Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:29 AM GMT

PDB ID	:	3ETG
Title	:	Glutamate dehydrogenase complexed with GW5074
Authors	:	Li, M.; Smith, T.J.
Deposited on	:	2008-10-07
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

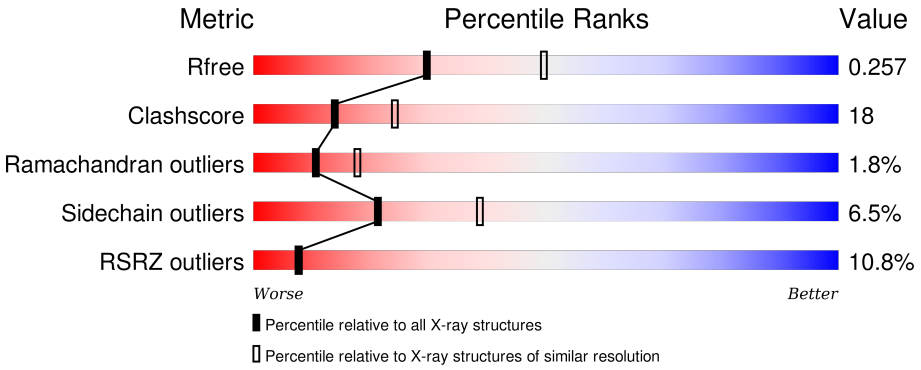
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	501	12% 64% 33% ·
1	B	501	13% 64% 33% ·
1	C	501	5% 64% 32% ·
1	D	501	12% 65% 31% ·
1	E	501	13% 62% 35% ·

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Mol	Chain	Length	Quality of chain
1	F	501	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLU	B	550	-	-	-	X
2	GLU	D	550	-	-	-	X
2	GLU	E	550	-	-	-	X
3	NDP	A	551	-	-	-	X
3	NDP	C	551	-	-	-	X
4	GTP	B	553	-	-	-	X
4	GTP	C	553	X	-	-	-
4	GTP	D	553	-	-	-	X
4	GTP	E	553	X	-	-	-
4	GTP	F	553	-	-	-	X
5	GWD	A	552	-	-	-	X
5	GWD	B	552	-	-	-	X
5	GWD	C	552	-	-	-	X
5	GWD	D	552	-	-	X	X
5	GWD	E	552	-	-	-	X
5	GWD	F	552	-	-	-	X

2 Entry composition

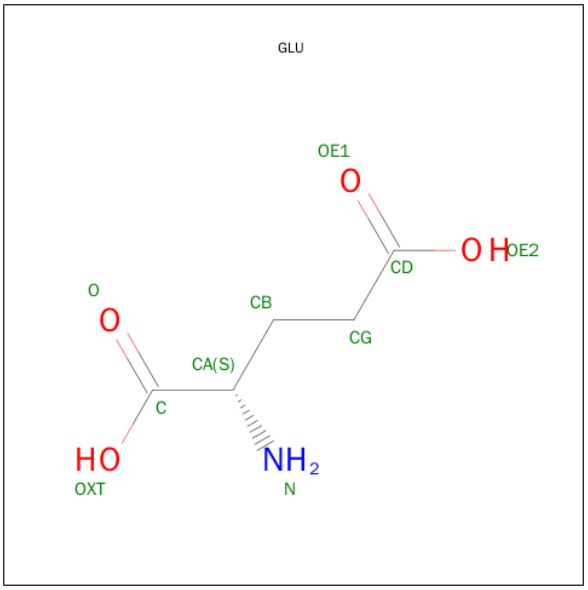
There are 6 unique types of molecules in this entry. The entry contains 24305 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glutamate dehydrogenase.

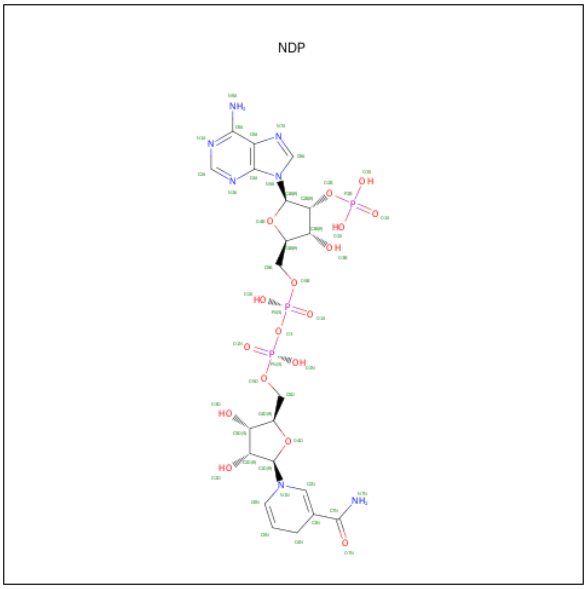
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			3915	2473	687	736	19			
1	B	501	Total	C	N	O	S	0	0	0
			3915	2473	687	736	19			
1	C	501	Total	C	N	O	S	0	0	0
			3915	2473	687	736	19			
1	D	501	Total	C	N	O	S	0	0	0
			3915	2473	687	736	19			
1	E	501	Total	C	N	O	S	0	0	0
			3915	2473	687	736	19			
1	F	501	Total	C	N	O	S	0	0	0
			3915	2473	687	736	19			

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	5	1	3		
2	B	1	Total	C	N	O	0	0
			9	5	1	3		
2	C	1	Total	C	N	O	0	0
			9	5	1	3		
2	D	1	Total	C	N	O	0	0
			9	5	1	3		
2	E	1	Total	C	N	O	0	0
			9	5	1	3		
2	F	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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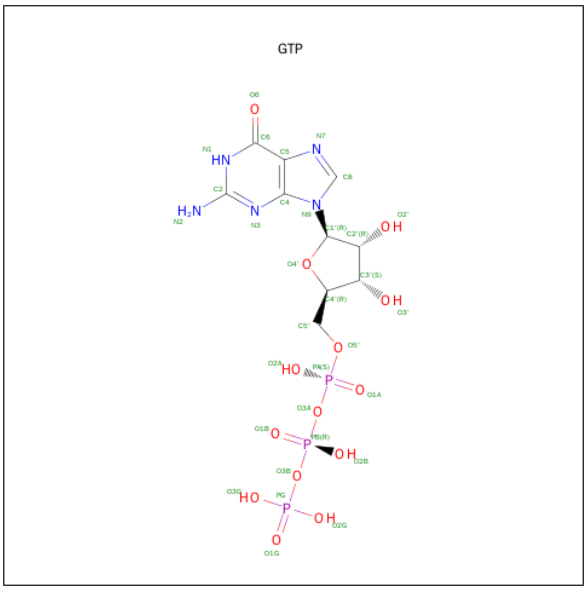
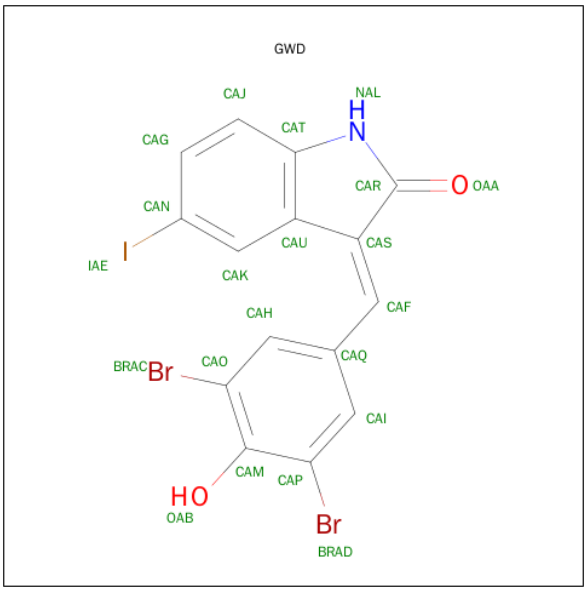
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	F	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is (3E)-3-[(3,5-DIBROMO-4-HYDROXYPHENYL)METHYLIDENE]-5-IODO-1,3-DIHYDRO-2H-INDOL-2-ONE (three-letter code: GWD) (formula: $C_{15}H_8Br_2INO_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	Br	C	I	N	O	0	0
			21	2	15	1	1	2		
5	B	1	Total	Br	C	I	N	O	0	0
			21	2	15	1	1	2		
5	C	1	Total	Br	C	I	N	O	0	0
			21	2	15	1	1	2		
5	D	1	Total	Br	C	I	N	O	0	0
			21	2	15	1	1	2		
5	E	1	Total	Br	C	I	N	O	0	0
			21	2	15	1	1	2		
5	F	1	Total	Br	C	I	N	O	0	0
			21	2	15	1	1	2		

- Molecule 6 is water.

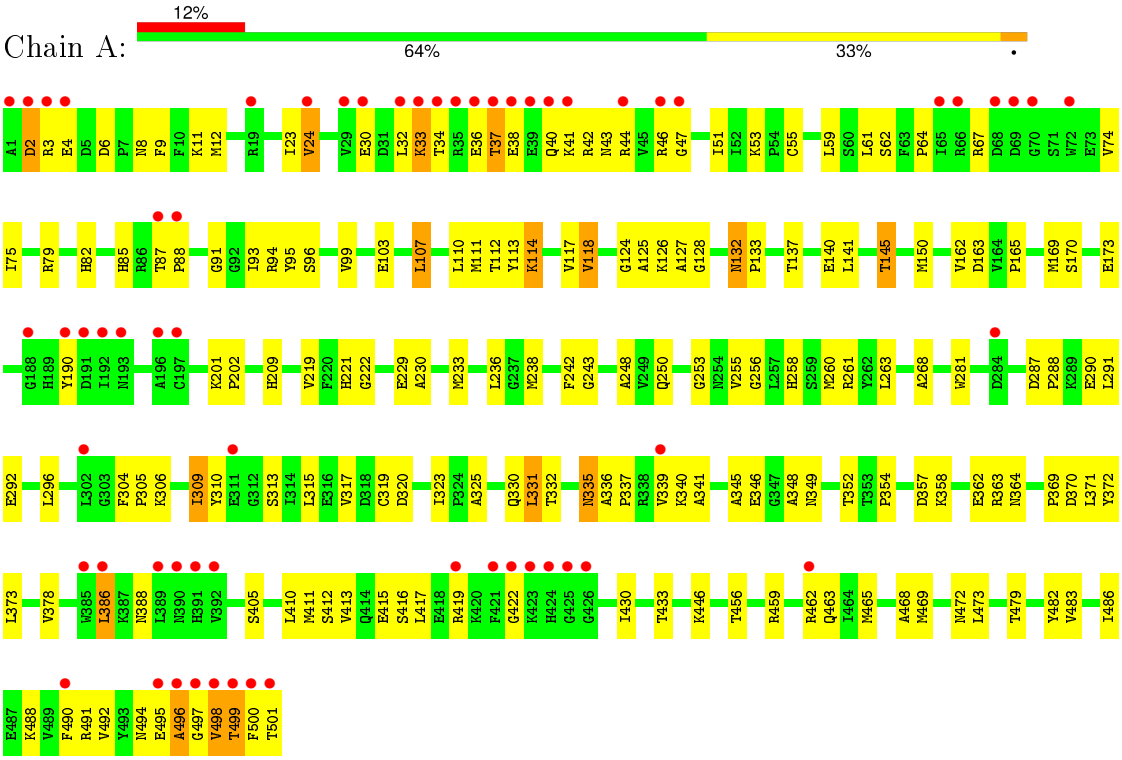
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	30	Total	O	0	0
			30	30		
6	B	29	Total	O	0	0
			29	29		
6	C	29	Total	O	0	0
			29	29		
6	D	30	Total	O	0	0
			30	30		
6	E	15	Total	O	0	0
			15	15		
6	F	22	Total	O	0	0
			22	22		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

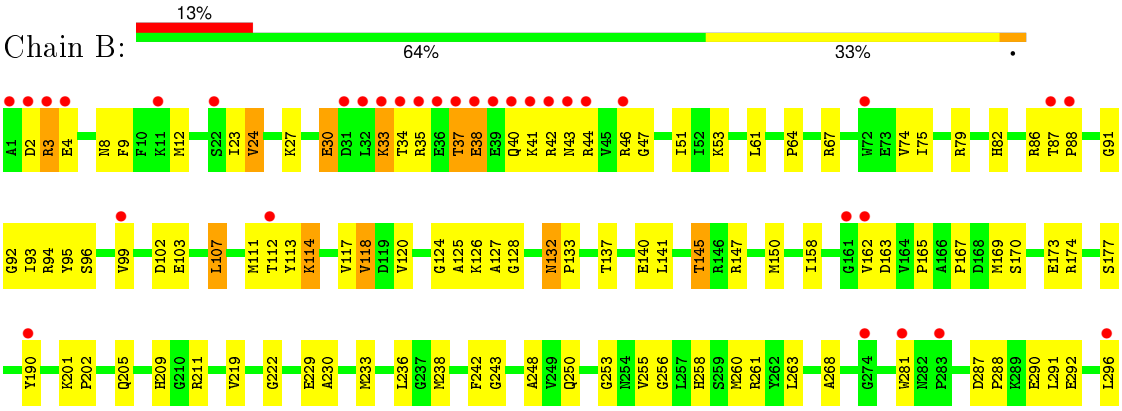
- Molecule 1: Glutamate dehydrogenase

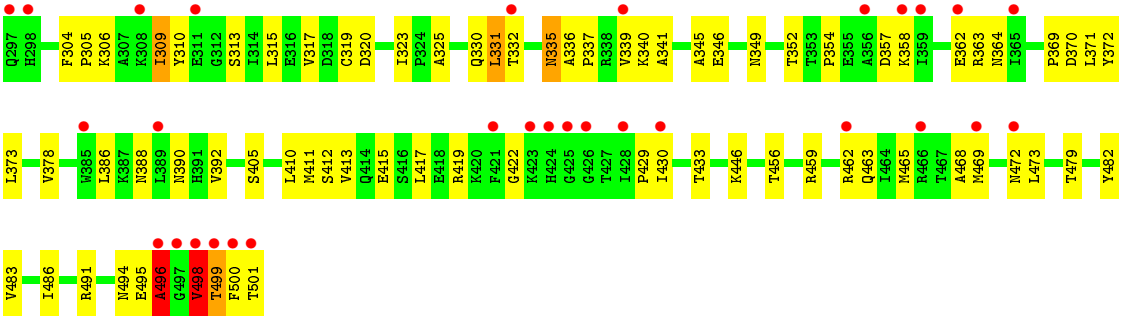
Chain A:



- Molecule 1: Glutamate dehydrogenase

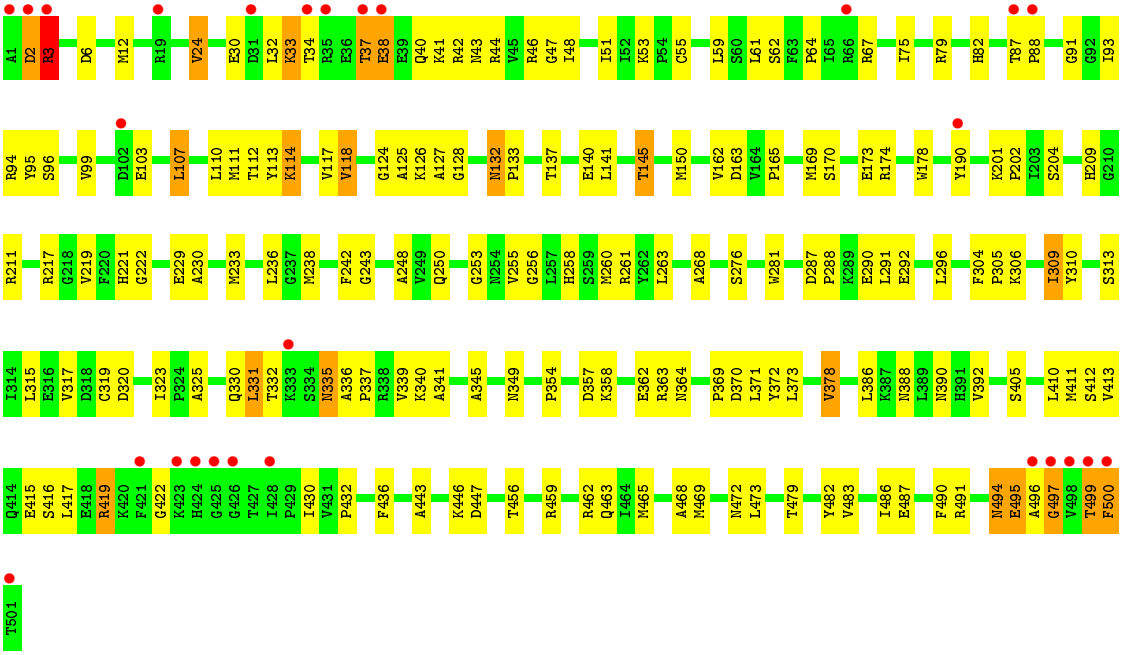
Chain B:





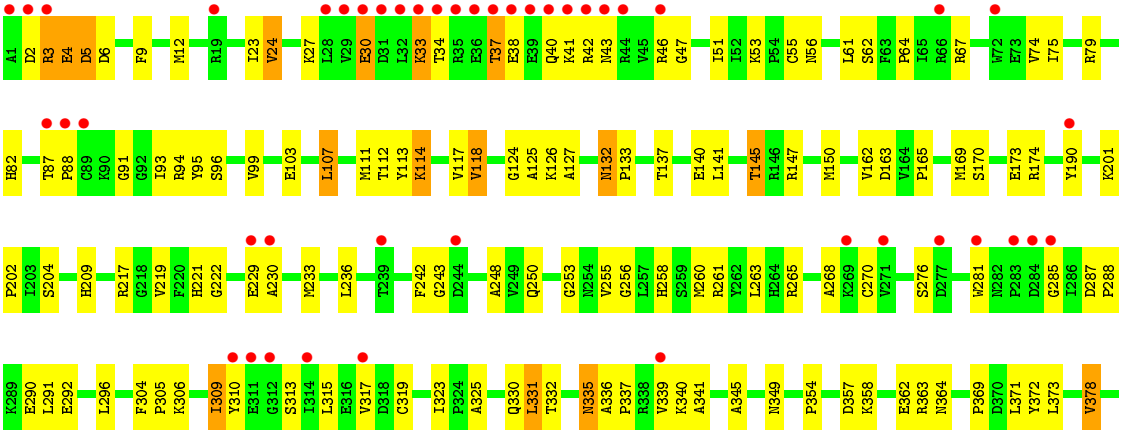
• Molecule 1: Glutamate dehydrogenase

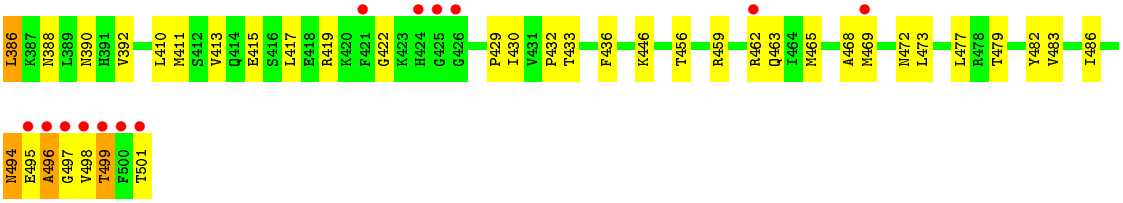
Chain C:



• Molecule 1: Glutamate dehydrogenase

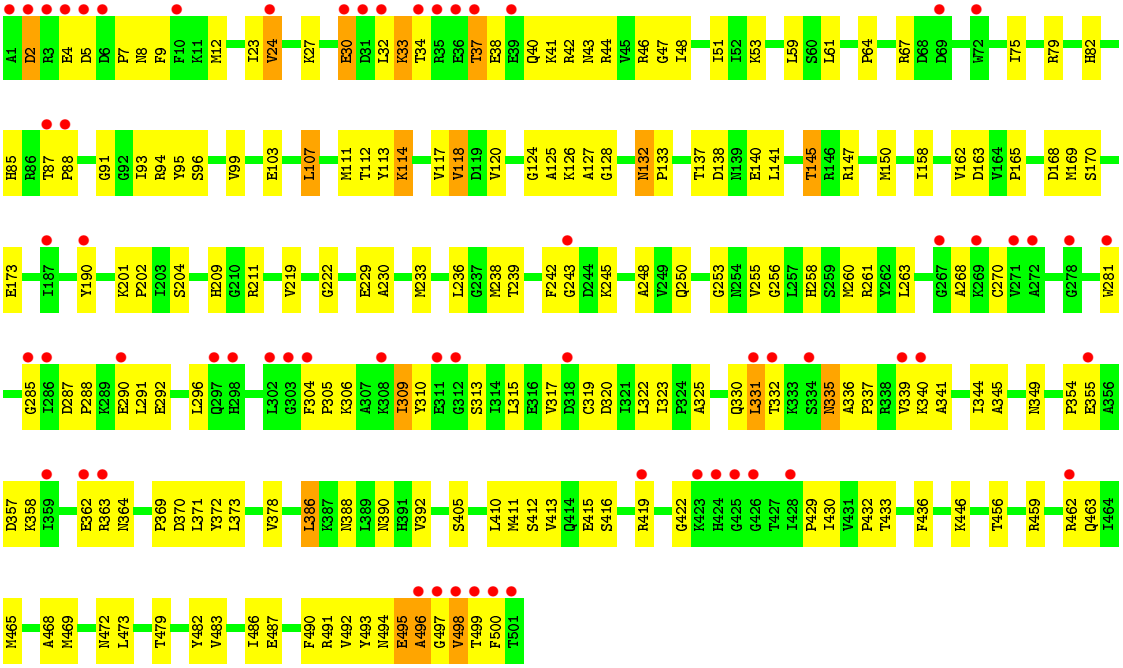
Chain D:





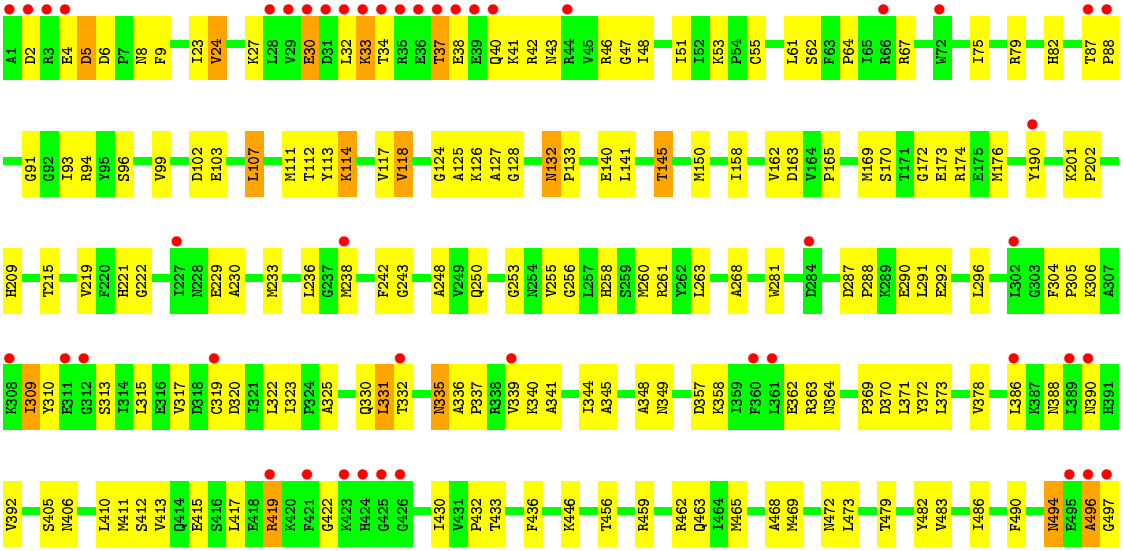
• Molecule 1: Glutamate dehydrogenase

Chain E:



• Molecule 1: Glutamate dehydrogenase

Chain F:




V498
T499
P500
T501

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	122.30Å 102.20Å 167.70Å 90.00° 102.50° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 48.78 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.50) 95.9 (48.78-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	5.49 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.244 , 0.258 0.242 , 0.257	Depositor DCC
R_{free} test set	7054 reflections (5.54%)	DCC
Wilson B-factor (Å^2)	41.4	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 45.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 138957 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	24305	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, GWD, NDP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.43	0/3998	0.71	0/5396
1	B	0.43	0/3998	0.86	5/5396 (0.1%)
1	C	0.45	0/3998	0.71	0/5396
1	D	0.44	0/3998	0.71	1/5396 (0.0%)
1	E	0.44	0/3998	0.71	0/5396
1	F	0.45	0/3998	0.85	4/5396 (0.1%)
All	All	0.44	0/23988	0.76	10/32376 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	419	ARG	NE-CZ-NH2	23.80	132.20	120.30
1	B	35	ARG	NE-CZ-NH1	-23.28	108.66	120.30
1	B	35	ARG	NE-CZ-NH2	22.96	131.78	120.30
1	F	419	ARG	NE-CZ-NH1	-22.75	108.93	120.30
1	B	35	ARG	CD-NE-CZ	11.71	140.00	123.60
1	F	419	ARG	CD-NE-CZ	11.66	139.92	123.60
1	B	496	ALA	N-CA-C	-7.68	90.27	111.00
1	D	497	GLY	N-CA-C	-6.57	96.69	113.10
1	F	497	GLY	N-CA-C	-5.64	98.99	113.10
1	B	498	VAL	N-CA-C	-5.36	96.53	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3915	0	3880	145	0
1	B	3915	0	3880	155	0
1	C	3915	0	3880	153	0
1	D	3915	0	3880	149	0
1	E	3915	0	3880	160	0
1	F	3915	0	3880	144	0
2	A	9	0	5	1	0
2	B	9	0	5	2	0
2	C	9	0	5	2	0
2	D	9	0	5	1	0
2	E	9	0	5	3	0
2	F	9	0	5	0	0
3	A	48	0	26	6	0
3	B	48	0	26	8	0
3	C	48	0	26	9	0
3	D	48	0	26	5	0
3	E	48	0	26	6	0
3	F	48	0	26	7	0
4	A	32	0	11	1	0
4	B	32	0	10	2	0
4	C	32	0	12	0	0
4	D	32	0	10	2	0
4	E	32	0	12	3	0
4	F	32	0	10	1	0
5	A	21	0	7	3	0
5	B	21	0	8	5	0
5	C	21	0	7	3	0
5	D	21	0	7	7	0
5	E	21	0	7	5	0
5	F	21	0	7	3	0
6	A	30	0	0	1	0
6	B	29	0	0	3	0
6	C	29	0	0	3	0
6	D	30	0	0	5	0
6	E	15	0	0	0	0
6	F	22	0	0	1	0
All	All	24305	0	23574	879	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (879) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:VAL:HG21	1:F:174:ARG:HG3	1.33	1.10
5:C:552:GWD:HAK	5:C:552:GWD:HAI	1.09	1.08
1:E:112:THR:HG22	1:E:124:GLY:H	1.18	1.08
5:F:552:GWD:HAK	5:F:552:GWD:HAI	1.09	1.07
5:D:552:GWD:HAK	5:D:552:GWD:HAI	1.09	1.07
1:B:174:ARG:HG3	1:F:498:VAL:HG21	1.34	1.06
1:B:112:THR:HG22	1:B:124:GLY:H	1.19	1.06
5:E:552:GWD:HAI	5:E:552:GWD:HAK	1.08	1.06
5:A:552:GWD:HAI	5:A:552:GWD:HAK	1.07	1.06
1:D:112:THR:HG22	1:D:124:GLY:H	1.16	1.05
5:B:552:GWD:HAI	5:B:552:GWD:HAK	1.08	1.05
1:F:112:THR:HG22	1:F:124:GLY:H	1.18	1.03
1:A:112:THR:HG22	1:A:124:GLY:H	1.22	1.02
1:C:112:THR:HG22	1:C:124:GLY:H	1.24	1.00
5:A:552:GWD:CAK	5:A:552:GWD:HAI	1.92	1.00
5:B:552:GWD:CAK	5:B:552:GWD:HAI	1.93	0.98
5:F:552:GWD:CAK	5:F:552:GWD:HAI	1.94	0.98
5:C:552:GWD:CAK	5:C:552:GWD:HAI	1.94	0.98
5:D:552:GWD:CAK	5:D:552:GWD:HAI	1.94	0.97
5:E:552:GWD:HAI	5:E:552:GWD:CAK	1.93	0.97
1:D:112:THR:HG22	1:D:124:GLY:N	1.84	0.92
1:D:332:THR:H	1:D:335:ASN:HD21	1.19	0.91
1:E:112:THR:HG22	1:E:124:GLY:N	1.84	0.91
1:F:112:THR:HG22	1:F:124:GLY:N	1.85	0.90
1:B:112:THR:HG22	1:B:124:GLY:N	1.85	0.89
1:A:112:THR:HG22	1:A:124:GLY:N	1.87	0.89
1:A:51:ILE:HD12	1:D:64:PRO:HB3	1.52	0.89
1:B:332:THR:H	1:B:335:ASN:HD21	1.21	0.89
1:E:332:THR:H	1:E:335:ASN:HD21	1.21	0.88
1:C:51:ILE:HD12	1:F:64:PRO:HB3	1.54	0.87
1:B:64:PRO:HB3	1:E:51:ILE:HD12	1.57	0.86
1:C:112:THR:HG22	1:C:124:GLY:N	1.89	0.86
1:C:332:THR:H	1:C:335:ASN:HD21	1.22	0.86
1:D:3:ARG:HE	1:D:4:GLU:H	1.21	0.85
1:F:332:THR:H	1:F:335:ASN:HD21	1.20	0.85
1:C:64:PRO:HB3	1:F:51:ILE:HD12	1.57	0.84
1:A:498:VAL:HG21	1:F:174:ARG:CG	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:PRO:HB3	1:D:51:ILE:HD12	1.60	0.84
1:B:174:ARG:HG3	1:F:498:VAL:CG2	2.07	0.84
1:C:34:THR:HG21	1:C:40:GLN:HE22	1.42	0.83
1:A:202:PRO:HG2	1:B:496:ALA:HA	1.61	0.82
1:A:34:THR:HG21	1:A:40:GLN:HE22	1.45	0.82
1:D:258:HIS:HD2	1:D:261:ARG:HH11	1.27	0.82
1:C:44:ARG:NH2	1:C:500:PHE:HB3	1.93	0.82
1:E:5:ASP:OD1	1:E:355:GLU:HB2	1.79	0.81
1:C:221:HIS:HE1	6:C:559:HOH:O	1.62	0.81
1:A:332:THR:H	1:A:335:ASN:HD21	1.25	0.81
1:B:51:ILE:HD12	1:E:64:PRO:HB3	1.60	0.81
1:E:258:HIS:HD2	1:E:261:ARG:HH11	1.27	0.81
1:E:34:THR:HG21	1:E:40:GLN:HE22	1.45	0.80
1:F:258:HIS:HD2	1:F:261:ARG:HH11	1.28	0.80
1:C:258:HIS:HD2	1:C:261:ARG:HH11	1.29	0.80
1:F:34:THR:HG21	1:F:40:GLN:HE22	1.45	0.79
1:B:34:THR:HG21	1:B:40:GLN:HE22	1.48	0.79
1:D:34:THR:HG21	1:D:40:GLN:HE22	1.45	0.79
1:B:258:HIS:HD2	1:B:261:ARG:HH11	1.29	0.79
3:D:551:NDP:H52N	3:D:551:NDP:H2N	1.65	0.78
1:B:174:ARG:CG	1:F:498:VAL:HG21	2.13	0.78
1:A:258:HIS:HD2	1:A:261:ARG:HH11	1.27	0.78
1:C:497:GLY:H	1:D:174:ARG:HG3	1.49	0.77
1:A:287:ASP:HB3	1:A:290:GLU:HG2	1.67	0.76
1:B:287:ASP:HB3	1:B:290:GLU:HG2	1.67	0.76
1:F:287:ASP:HB3	1:F:290:GLU:HG2	1.68	0.75
1:C:287:ASP:HB3	1:C:290:GLU:HG2	1.69	0.75
1:C:44:ARG:CZ	1:C:500:PHE:HB3	2.16	0.74
1:B:141:LEU:O	1:B:145:THR:HG23	1.87	0.74
1:D:250:GLN:HE22	1:D:330:GLN:HE21	1.36	0.74
1:F:141:LEU:O	1:F:145:THR:HG23	1.87	0.74
1:C:141:LEU:O	1:C:145:THR:HG23	1.88	0.74
1:C:250:GLN:HE22	1:C:330:GLN:HE21	1.35	0.74
1:E:287:ASP:HB3	1:E:290:GLU:HG2	1.70	0.73
1:E:141:LEU:O	1:E:145:THR:HG23	1.88	0.73
1:D:255:VAL:HG22	6:D:578:HOH:O	1.87	0.73
1:D:287:ASP:HB3	1:D:290:GLU:HG2	1.69	0.73
1:C:82:HIS:HD2	1:C:112:THR:HG21	1.54	0.73
1:D:141:LEU:O	1:D:145:THR:HG23	1.88	0.72
1:E:250:GLN:HE22	1:E:330:GLN:HE21	1.37	0.72
1:D:495:GLU:HG3	1:E:204:SER:OG	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:ARG:HD3	5:E:552:GWD:BRAC	2.44	0.72
1:A:82:HIS:HD2	1:A:112:THR:HG21	1.53	0.72
1:B:82:HIS:HD2	1:B:112:THR:HG21	1.55	0.71
1:A:141:LEU:O	1:A:145:THR:HG23	1.90	0.71
1:F:233:MET:HE1	1:F:236:LEU:HD12	1.72	0.71
1:C:487:GLU:HG3	1:C:491:ARG:NH2	2.06	0.71
1:A:107:LEU:HB3	1:A:126:LYS:HG2	1.73	0.70
1:D:349:ASN:ND2	3:D:551:NDP:O2D	2.24	0.70
1:F:250:GLN:HE22	1:F:330:GLN:HE21	1.38	0.70
1:D:107:LEU:HB3	1:D:126:LYS:HG2	1.71	0.70
1:A:250:GLN:HE22	1:A:330:GLN:HE21	1.35	0.70
1:D:82:HIS:HD2	1:D:112:THR:HG21	1.55	0.70
1:F:82:HIS:HD2	1:F:112:THR:HG21	1.55	0.70
1:D:255:VAL:HG23	1:D:325:ALA:HB1	1.73	0.69
1:B:133:PRO:HG2	1:B:170:SER:HB3	1.75	0.69
1:E:498:VAL:HB	1:E:500:PHE:CE2	2.26	0.69
1:E:82:HIS:HD2	1:E:112:THR:HG21	1.56	0.69
1:E:118:VAL:HG22	1:E:456:THR:CG2	2.23	0.69
1:A:133:PRO:HG2	1:A:170:SER:HB3	1.74	0.69
1:A:498:VAL:CG2	1:F:174:ARG:HG3	2.20	0.69
1:C:255:VAL:HG23	1:C:325:ALA:HB1	1.74	0.69
1:F:107:LEU:HB3	1:F:126:LYS:HG2	1.73	0.69
1:F:496:ALA:C	1:F:498:VAL:H	1.95	0.68
1:E:233:MET:HE1	1:E:236:LEU:HD12	1.75	0.68
1:A:497:GLY:O	1:A:498:VAL:HG22	1.94	0.68
1:B:250:GLN:HE22	1:B:330:GLN:HE21	1.41	0.68
1:F:8:ASN:HD21	1:F:102:ASP:HB3	1.58	0.68
1:D:118:VAL:HG22	1:D:456:THR:CG2	2.24	0.68
1:B:255:VAL:HG23	1:B:325:ALA:HB1	1.77	0.67
1:C:150:MET:HE2	1:C:150:MET:HA	1.76	0.67
1:E:38:GLU:HG3	1:E:40:GLN:HG3	1.76	0.67
1:E:44:ARG:NH2	1:E:500:PHE:HD1	1.92	0.67
1:C:107:LEU:HB3	1:C:126:LYS:HG2	1.75	0.67
1:C:133:PRO:HG2	1:C:170:SER:HB3	1.77	0.67
1:B:3:ARG:CG	1:B:3:ARG:HH11	2.05	0.67
1:D:5:ASP:HB3	1:D:332:THR:HB	1.76	0.67
1:F:38:GLU:HG3	1:F:40:GLN:HG3	1.76	0.67
1:F:112:THR:HG22	1:F:124:GLY:CA	2.24	0.67
1:F:133:PRO:HG2	1:F:170:SER:HB3	1.75	0.67
1:E:133:PRO:HG2	1:E:170:SER:HB3	1.76	0.67
1:A:233:MET:HE1	1:A:236:LEU:HD12	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:GLU:HG3	1:B:40:GLN:HG3	1.75	0.67
1:D:38:GLU:HG3	1:D:40:GLN:HG3	1.76	0.67
1:A:38:GLU:HG3	1:A:40:GLN:HG3	1.76	0.66
1:A:255:VAL:HG23	1:A:325:ALA:HB1	1.76	0.66
1:B:349:ASN:ND2	3:B:551:NDP:O2D	2.28	0.66
1:A:150:MET:HA	1:A:150:MET:HE2	1.75	0.66
1:E:150:MET:HG3	5:E:552:GWD:HAH	1.76	0.66
1:E:112:THR:HG22	1:E:124:GLY:CA	2.25	0.66
1:C:38:GLU:HG3	1:C:40:GLN:HG3	1.77	0.66
1:D:118:VAL:HG22	1:D:456:THR:HG22	1.78	0.66
1:E:107:LEU:HB3	1:E:126:LYS:HG2	1.77	0.66
1:D:498:VAL:HG21	1:E:138:ASP:HB2	1.77	0.66
1:A:112:THR:HG22	1:A:124:GLY:CA	2.26	0.66
1:B:3:ARG:HG2	1:B:3:ARG:HH11	1.60	0.66
1:A:221:HIS:HE1	6:A:557:HOH:O	1.78	0.66
1:E:498:VAL:HG12	1:E:499:THR:H	1.61	0.66
2:B:550:GLU:HA	3:B:551:NDP:H41N	1.77	0.66
1:E:487:GLU:HG3	1:E:491:ARG:NH2	2.11	0.65
1:E:487:GLU:HG3	1:E:491:ARG:HH22	1.62	0.65
1:D:233:MET:HE1	1:D:236:LEU:HD12	1.79	0.65
1:B:112:THR:HG22	1:B:124:GLY:CA	2.25	0.65
1:F:209:HIS:HE1	4:F:553:GTP:O2A	1.79	0.65
1:B:233:MET:HE1	1:B:236:LEU:HD12	1.78	0.65
1:B:219:VAL:HG22	1:B:373:LEU:HD13	1.77	0.65
1:D:133:PRO:HG2	1:D:170:SER:HB3	1.79	0.65
1:D:219:VAL:HG22	1:D:373:LEU:HD13	1.78	0.65
1:F:255:VAL:HG23	1:F:325:ALA:HB1	1.77	0.65
1:B:150:MET:HE2	1:B:150:MET:HA	1.78	0.65
1:A:85:HIS:HD2	1:A:492:VAL:HG21	1.61	0.65
1:B:44:ARG:HE	1:B:500:PHE:HD2	1.46	0.64
1:D:79:ARG:HD3	1:D:127:ALA:HB2	1.79	0.64
1:C:233:MET:HE1	1:C:236:LEU:HD12	1.78	0.64
1:A:219:VAL:HG22	1:A:373:LEU:HD13	1.80	0.64
1:B:99:VAL:HA	1:B:103:GLU:OE1	1.97	0.64
1:E:99:VAL:HA	1:E:103:GLU:OE1	1.98	0.64
1:E:255:VAL:HG23	1:E:325:ALA:HB1	1.78	0.64
1:D:112:THR:HG22	1:D:124:GLY:CA	2.28	0.64
1:E:150:MET:HA	1:E:150:MET:HE2	1.78	0.64
1:E:219:VAL:HG22	1:E:373:LEU:HD13	1.80	0.64
1:D:335:ASN:H	1:D:335:ASN:HD22	1.45	0.64
1:D:150:MET:HA	1:D:150:MET:HE2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:150:MET:HE2	1:F:150:MET:HA	1.79	0.63
1:C:112:THR:HG22	1:C:124:GLY:CA	2.26	0.63
1:A:118:VAL:HG22	1:A:456:THR:CG2	2.27	0.63
1:C:219:VAL:HG22	1:C:373:LEU:HD13	1.79	0.63
1:D:150:MET:HG3	5:D:552:GWD:HAH	1.80	0.63
1:B:107:LEU:HB3	1:B:126:LYS:HG2	1.80	0.63
1:F:118:VAL:HG22	1:F:456:THR:CG2	2.29	0.63
1:C:91:GLY:HA3	1:C:125:ALA:O	1.99	0.63
1:F:335:ASN:H	1:F:335:ASN:HD22	1.46	0.63
1:C:67:ARG:HD2	1:C:140:GLU:OE2	1.99	0.63
1:B:91:GLY:HA3	1:B:125:ALA:O	1.99	0.63
1:C:118:VAL:HG22	1:C:456:THR:CG2	2.28	0.63
3:B:551:NDP:H2N	3:B:551:NDP:H52N	1.81	0.63
1:A:219:VAL:HG13	1:A:373:LEU:HD11	1.81	0.63
1:E:79:ARG:HD3	1:E:127:ALA:HB2	1.80	0.63
1:E:335:ASN:H	1:E:335:ASN:HD22	1.46	0.62
1:B:335:ASN:H	1:B:335:ASN:HD22	1.47	0.62
1:E:118:VAL:HG22	1:E:456:THR:HG22	1.80	0.62
1:A:44:ARG:HH21	1:A:500:PHE:HD2	1.47	0.62
1:A:496:ALA:C	1:A:498:VAL:H	2.00	0.62
1:D:53:LYS:O	1:D:82:HIS:HE1	1.83	0.62
1:B:211:ARG:HH22	3:B:551:NDP:H71N	1.45	0.62
1:B:67:ARG:HD2	1:B:140:GLU:OE2	1.99	0.62
1:E:53:LYS:O	1:E:82:HIS:HE1	1.83	0.62
1:F:91:GLY:HA3	1:F:125:ALA:O	1.99	0.62
1:D:147:ARG:HD3	5:D:552:GWD:BRAC	2.55	0.61
1:C:79:ARG:HD3	1:C:127:ALA:HB2	1.81	0.61
1:C:204:SER:OG	1:E:495:GLU:HG3	2.00	0.61
1:A:79:ARG:HD3	1:A:127:ALA:HB2	1.82	0.61
1:C:53:LYS:O	1:C:82:HIS:HE1	1.83	0.61
1:D:91:GLY:HA3	1:D:125:ALA:O	2.01	0.61
1:F:332:THR:H	1:F:335:ASN:ND2	1.96	0.61
1:C:335:ASN:H	1:C:335:ASN:HD22	1.48	0.61
1:D:219:VAL:HG13	1:D:373:LEU:HD11	1.82	0.61
1:E:219:VAL:HG13	1:E:373:LEU:HD11	1.81	0.61
1:C:44:ARG:HH22	1:C:494:ASN:ND2	1.99	0.61
1:D:67:ARG:HD2	1:D:140:GLU:OE2	2.00	0.61
1:D:99:VAL:HA	1:D:103:GLU:OE1	2.01	0.61
1:E:91:GLY:HA3	1:E:125:ALA:O	2.01	0.61
1:D:173:GLU:HB3	1:D:202:PRO:HG3	1.83	0.61
1:A:91:GLY:HA3	1:A:125:ALA:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:173:GLU:HB3	1:F:202:PRO:HG3	1.83	0.60
1:B:118:VAL:HG22	1:B:456:THR:CG2	2.31	0.60
1:C:118:VAL:HG22	1:C:456:THR:HG22	1.82	0.60
1:C:99:VAL:HA	1:C:103:GLU:OE1	2.01	0.60
1:F:219:VAL:HG13	1:F:373:LEU:HD11	1.82	0.60
1:B:173:GLU:HB3	1:B:202:PRO:HG3	1.83	0.60
1:D:3:ARG:NE	1:D:4:GLU:H	1.96	0.60
1:F:219:VAL:HG22	1:F:373:LEU:HD13	1.81	0.60
1:D:332:THR:N	1:D:335:ASN:HD21	1.96	0.60
1:A:332:THR:H	1:A:335:ASN:ND2	1.99	0.60
1:E:498:VAL:HB	1:E:500:PHE:HE2	1.63	0.60
1:E:67:ARG:HD2	1:E:140:GLU:OE2	2.01	0.60
1:F:118:VAL:HG22	1:F:456:THR:HG22	1.83	0.60
1:F:53:LYS:O	1:F:82:HIS:HE1	1.84	0.60
1:E:44:ARG:NH2	1:E:500:PHE:CD1	2.69	0.60
1:B:332:THR:H	1:B:335:ASN:ND2	1.96	0.60
1:B:413:VAL:HG23	1:B:430:ILE:HG13	1.84	0.59
1:F:99:VAL:HA	1:F:103:GLU:OE1	2.01	0.59
1:B:500:PHE:O	1:B:501:THR:HG22	2.02	0.59
1:A:335:ASN:HD22	1:A:335:ASN:H	1.49	0.59
1:A:118:VAL:HG22	1:A:456:THR:HG22	1.83	0.59
1:E:465:MET:O	1:E:469:MET:HG2	2.02	0.59
1:B:253:GLY:HA3	3:B:551:NDP:O1A	2.03	0.59
1:F:79:ARG:HD3	1:F:127:ALA:HB2	1.84	0.59
1:B:53:LYS:O	1:B:82:HIS:HE1	1.85	0.59
1:D:332:THR:H	1:D:335:ASN:ND2	1.95	0.59
1:C:332:THR:N	1:C:335:ASN:HD21	1.98	0.59
1:B:3:ARG:HG2	1:B:3:ARG:NH1	2.15	0.59
1:F:253:GLY:HA3	3:F:551:NDP:O1A	2.02	0.59
1:B:79:ARG:HD3	1:B:127:ALA:HB2	1.83	0.59
1:E:349:ASN:ND2	3:E:551:NDP:O2D	2.36	0.59
1:F:67:ARG:HD2	1:F:140:GLU:OE2	2.02	0.59
1:D:465:MET:O	1:D:469:MET:HG2	2.03	0.59
1:C:217:ARG:NH1	6:C:559:HOH:O	2.24	0.59
1:A:99:VAL:HA	1:A:103:GLU:OE1	2.02	0.59
1:D:495:GLU:O	1:D:496:ALA:HB3	2.03	0.59
1:B:219:VAL:HG13	1:B:373:LEU:HD11	1.84	0.59
1:C:219:VAL:HG13	1:C:373:LEU:HD11	1.84	0.59
1:A:67:ARG:HD2	1:A:140:GLU:OE2	2.03	0.58
1:E:332:THR:H	1:E:335:ASN:ND2	1.97	0.58
1:E:281:TRP:HB2	1:E:310:TYR:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:HIS:HE1	4:B:553:GTP:O1A	1.86	0.58
1:B:40:GLN:HA	1:B:43:ASN:HD22	1.68	0.58
1:C:173:GLU:HB3	1:C:202:PRO:HG3	1.85	0.58
1:C:495:GLU:HG3	1:D:204:SER:OG	2.03	0.58
3:C:551:NDP:H52N	3:C:551:NDP:H2N	1.84	0.58
1:A:53:LYS:O	1:A:82:HIS:HE1	1.86	0.58
1:A:332:THR:N	1:A:335:ASN:HD21	2.01	0.58
1:A:173:GLU:HB3	1:A:202:PRO:HG3	1.86	0.58
1:B:499:THR:HG23	1:B:500:PHE:H	1.67	0.57
1:A:40:GLN:HA	1:A:43:ASN:HD22	1.69	0.57
1:B:118:VAL:HG22	1:B:456:THR:HG22	1.85	0.57
1:B:465:MET:O	1:B:469:MET:HG2	2.04	0.57
1:D:40:GLN:HA	1:D:43:ASN:HD22	1.68	0.57
1:A:488:LYS:HG2	1:A:491:ARG:HH21	1.68	0.57
1:F:91:GLY:O	1:F:165:PRO:HA	2.05	0.57
1:E:34:THR:HB	1:E:41:LYS:HD3	1.87	0.57
1:D:56:ASN:ND2	6:D:570:HOH:O	2.38	0.57
4:E:553:GTP:H8	4:E:553:GTP:H5'	1.70	0.57
1:A:82:HIS:CD2	1:A:112:THR:HG21	2.38	0.57
1:D:258:HIS:HD2	1:D:261:ARG:NH1	2.01	0.57
1:B:287:ASP:HB3	1:B:290:GLU:CG	2.35	0.57
2:D:550:GLU:HA	3:D:551:NDP:H41N	1.86	0.57
1:F:169:MET:HG2	3:F:551:NDP:O1N	2.04	0.57
1:C:201:LYS:HZ2	1:C:388:ASN:HD21	1.53	0.57
1:D:413:VAL:HG23	1:D:430:ILE:HG13	1.87	0.56
1:D:433:THR:HG23	1:E:412:SER:HA	1.87	0.56
1:C:211:ARG:HH22	3:C:551:NDP:H71N	1.52	0.56
1:B:205:GLN:NE2	1:F:496:ALA:HA	2.20	0.56
1:E:40:GLN:HA	1:E:43:ASN:HD22	1.70	0.56
1:F:40:GLN:HA	1:F:43:ASN:HD22	1.70	0.56
1:C:174:ARG:HD2	1:E:499:THR:HG21	1.86	0.56
3:A:551:NDP:H2N	3:A:551:NDP:H52N	1.87	0.56
1:A:190:TYR:HD2	1:B:162:VAL:HG11	1.70	0.56
1:F:281:TRP:HB2	1:F:310:TYR:HB2	1.86	0.56
1:E:173:GLU:HB3	1:E:202:PRO:HG3	1.87	0.56
1:D:281:TRP:HB2	1:D:310:TYR:HB2	1.87	0.56
1:C:40:GLN:HA	1:C:43:ASN:HD22	1.70	0.56
1:C:468:ALA:HA	1:C:473:LEU:HD12	1.88	0.56
1:A:413:VAL:HG23	1:A:430:ILE:HG13	1.86	0.56
1:D:34:THR:HG21	1:D:40:GLN:NE2	2.19	0.56
1:A:287:ASP:HB3	1:A:290:GLU:CG	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:TRP:HB2	1:C:310:TYR:HB2	1.88	0.56
1:C:150:MET:HG3	5:C:552:GWD:BRAC	2.60	0.56
1:F:465:MET:O	1:F:469:MET:HG2	2.06	0.56
1:B:44:ARG:NH2	1:B:494:ASN:HD22	2.04	0.56
1:F:34:THR:HB	1:F:41:LYS:HD3	1.88	0.56
1:A:465:MET:O	1:A:469:MET:HG2	2.04	0.56
1:D:79:ARG:CD	1:D:127:ALA:HB2	2.36	0.56
1:E:255:VAL:HG23	1:E:256:GLY:N	2.21	0.56
1:B:281:TRP:HB2	1:B:310:TYR:HB2	1.88	0.56
1:A:2:ASP:O	1:A:6:ASP:HB2	2.06	0.56
1:A:281:TRP:HB2	1:A:310:TYR:HB2	1.87	0.56
1:A:169:MET:HG2	3:A:551:NDP:O1N	2.05	0.55
1:B:468:ALA:HA	1:B:473:LEU:HD12	1.88	0.55
1:C:292:GLU:O	1:C:296:LEU:HD23	2.06	0.55
1:C:174:ARG:HG3	1:E:499:THR:OG1	2.07	0.55
1:B:150:MET:HG3	5:B:552:GWD:HAH	1.87	0.55
1:E:79:ARG:CD	1:E:127:ALA:HB2	2.37	0.55
3:F:551:NDP:H52N	3:F:551:NDP:H2N	1.88	0.55
1:A:498:VAL:O	1:A:500:PHE:N	2.40	0.55
1:E:258:HIS:HD2	1:E:261:ARG:NH1	2.01	0.55
1:B:94:ARG:HG3	1:B:169:MET:HB2	1.88	0.55
1:B:336:ALA:HB3	1:B:337:PRO:HD3	1.89	0.55
1:C:12:MET:HG3	1:C:354:PRO:HD3	1.88	0.55
1:F:332:THR:N	1:F:335:ASN:HD21	1.98	0.55
1:C:255:VAL:HG23	1:C:256:GLY:N	2.22	0.55
1:D:386:LEU:HD11	1:E:392:VAL:HG22	1.89	0.55
1:E:332:THR:N	1:E:335:ASN:HD21	1.99	0.55
1:A:150:MET:HG3	5:A:552:GWD:BRAC	2.62	0.54
1:E:91:GLY:O	1:E:165:PRO:HA	2.07	0.54
1:B:255:VAL:HG23	1:B:256:GLY:N	2.22	0.54
1:E:336:ALA:HB3	1:E:337:PRO:HD3	1.88	0.54
1:C:332:THR:H	1:C:335:ASN:ND2	1.97	0.54
1:E:34:THR:HB	1:E:41:LYS:CD	2.38	0.54
1:C:91:GLY:O	1:C:165:PRO:HA	2.07	0.54
1:C:465:MET:O	1:C:469:MET:HG2	2.07	0.54
1:C:413:VAL:HG23	1:C:430:ILE:HG13	1.90	0.54
1:E:413:VAL:HG23	1:E:430:ILE:HG13	1.89	0.54
1:B:34:THR:HB	1:B:41:LYS:HD3	1.90	0.54
1:F:348:ALA:HA	3:F:551:NDP:H1D	1.89	0.54
2:C:550:GLU:HA	3:C:551:NDP:H41N	1.89	0.54
1:A:468:ALA:HA	1:A:473:LEU:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:HIS:CD2	1:D:112:THR:HG21	2.40	0.54
1:B:42:ARG:O	1:B:46:ARG:HG3	2.07	0.54
1:B:112:THR:HG22	1:B:124:GLY:HA3	1.89	0.54
1:F:112:THR:HG22	1:F:124:GLY:HA3	1.88	0.54
1:C:287:ASP:HB3	1:C:290:GLU:CG	2.36	0.54
1:C:349:ASN:N	3:C:551:NDP:O2D	2.41	0.54
1:A:42:ARG:O	1:A:46:ARG:HG3	2.07	0.54
4:D:553:GTP:O1G	4:D:553:GTP:O1B	2.26	0.54
1:A:412:SER:HA	1:B:433:THR:HG23	1.90	0.54
1:D:42:ARG:O	1:D:46:ARG:HG3	2.07	0.54
1:B:82:HIS:CD2	1:B:112:THR:HG21	2.40	0.54
1:A:348:ALA:HA	3:A:551:NDP:H1D	1.90	0.54
1:E:468:ALA:HA	1:E:473:LEU:HD12	1.90	0.54
1:B:91:GLY:O	1:B:165:PRO:HA	2.07	0.53
1:C:494:ASN:C	1:C:494:ASN:HD22	2.10	0.53
1:F:42:ARG:O	1:F:46:ARG:HG3	2.08	0.53
1:F:468:ALA:HA	1:F:473:LEU:HD12	1.90	0.53
1:E:48:ILE:HD12	1:E:490:PHE:HE1	1.73	0.53
1:E:44:ARG:CZ	1:E:500:PHE:HD1	2.20	0.53
1:A:255:VAL:HG23	1:A:256:GLY:N	2.22	0.53
1:A:91:GLY:O	1:A:165:PRO:HA	2.08	0.53
1:D:468:ALA:HA	1:D:473:LEU:HD12	1.90	0.53
1:D:255:VAL:HG23	1:D:256:GLY:N	2.22	0.53
1:D:91:GLY:O	1:D:165:PRO:HA	2.09	0.53
1:E:42:ARG:O	1:E:46:ARG:HG3	2.08	0.53
1:E:209:HIS:CD2	1:E:446:LYS:HG3	2.43	0.53
1:F:292:GLU:O	1:F:296:LEU:HD23	2.08	0.53
1:F:94:ARG:HG3	1:F:169:MET:HB2	1.90	0.53
1:C:169:MET:HG2	3:C:551:NDP:O1N	2.08	0.53
1:D:287:ASP:HB3	1:D:290:GLU:CG	2.36	0.53
1:B:332:THR:N	1:B:335:ASN:HD21	1.98	0.53
1:C:34:THR:HB	1:C:41:LYS:HD3	1.89	0.53
1:F:287:ASP:HB3	1:F:290:GLU:CG	2.36	0.53
1:C:112:THR:HG22	1:C:124:GLY:HA3	1.90	0.53
1:B:79:ARG:CD	1:B:127:ALA:HB2	2.39	0.53
1:A:349:ASN:ND2	3:A:551:NDP:O2D	2.42	0.53
1:B:190:TYR:HD2	1:F:162:VAL:HG11	1.74	0.53
1:E:112:THR:HG22	1:E:124:GLY:HA3	1.90	0.52
1:F:82:HIS:CD2	1:F:112:THR:HG21	2.40	0.52
1:B:34:THR:HG21	1:B:40:GLN:NE2	2.22	0.52
1:E:5:ASP:OD2	1:E:7:PRO:HD3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:THR:HG21	1:F:40:GLN:NE2	2.20	0.52
1:D:34:THR:HB	1:D:41:LYS:HD3	1.90	0.52
1:C:201:LYS:NZ	1:C:388:ASN:HD21	2.07	0.52
1:C:82:HIS:CD2	1:C:112:THR:HG21	2.38	0.52
1:F:255:VAL:HG23	1:F:256:GLY:N	2.24	0.52
1:A:386:LEU:HD11	1:F:392:VAL:HG22	1.91	0.52
1:A:32:LEU:HD13	1:A:490:PHE:HZ	1.74	0.52
1:A:112:THR:HG22	1:A:124:GLY:HA3	1.90	0.52
1:F:258:HIS:HD2	1:F:261:ARG:NH1	2.03	0.52
1:D:253:GLY:HA3	3:D:551:NDP:O1A	2.09	0.52
1:E:287:ASP:HB3	1:E:290:GLU:CG	2.38	0.52
1:D:162:VAL:HG11	1:E:190:TYR:HD2	1.74	0.52
1:A:258:HIS:HD2	1:A:261:ARG:NH1	2.03	0.52
1:E:209:HIS:NE2	1:E:446:LYS:HG3	2.24	0.52
1:A:433:THR:HG23	1:F:412:SER:HA	1.91	0.52
1:A:260:MET:HG2	1:A:288:PRO:HG3	1.91	0.52
1:C:42:ARG:O	1:C:46:ARG:HG3	2.09	0.52
1:A:133:PRO:HG2	1:A:170:SER:CB	2.40	0.52
1:B:3:ARG:O	1:B:4:GLU:HB3	2.09	0.52
1:D:94:ARG:HG3	1:D:169:MET:HB2	1.91	0.52
1:C:79:ARG:CD	1:C:127:ALA:HB2	2.40	0.52
1:C:309:ILE:N	1:C:309:ILE:HD12	2.25	0.52
1:C:2:ASP:HB3	1:C:6:ASP:HB2	1.91	0.52
1:C:162:VAL:HG11	1:D:190:TYR:HD2	1.75	0.52
1:E:44:ARG:NE	1:E:500:PHE:HD1	2.07	0.52
1:A:34:THR:HB	1:A:41:LYS:HD3	1.92	0.52
1:E:44:ARG:NE	1:E:500:PHE:CD1	2.78	0.52
1:B:9:PHE:CE1	1:B:107:LEU:HD13	2.44	0.52
1:A:93:ILE:HG12	1:A:127:ALA:HB3	1.91	0.52
1:F:79:ARG:CD	1:F:127:ALA:HB2	2.39	0.52
1:E:335:ASN:HD22	1:E:335:ASN:N	2.07	0.52
1:F:34:THR:HB	1:F:41:LYS:CD	2.40	0.52
1:B:93:ILE:HG12	1:B:127:ALA:HB3	1.92	0.52
1:E:85:HIS:HD2	1:E:492:VAL:HG21	1.75	0.52
1:B:34:THR:HB	1:B:41:LYS:CD	2.40	0.51
1:E:292:GLU:O	1:E:296:LEU:HD23	2.10	0.51
1:B:3:ARG:CB	1:B:3:ARG:HH11	2.23	0.51
1:B:201:LYS:NZ	1:B:388:ASN:HD21	2.08	0.51
1:E:94:ARG:HG3	1:E:169:MET:HB2	1.91	0.51
1:D:255:VAL:CG2	1:D:325:ALA:HB1	2.40	0.51
1:C:34:THR:HB	1:C:41:LYS:CD	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:THR:HG21	1:C:40:GLN:NE2	2.19	0.51
1:A:34:THR:HG21	1:A:40:GLN:NE2	2.19	0.51
1:D:260:MET:HG2	1:D:288:PRO:HG3	1.92	0.51
1:E:253:GLY:HA3	3:E:551:NDP:O1A	2.11	0.51
1:E:493:TYR:O	1:E:496:ALA:HB2	2.11	0.51
1:D:3:ARG:C	1:D:5:ASP:H	2.14	0.51
1:E:2:ASP:HB2	1:E:332:THR:OG1	2.10	0.51
1:D:34:THR:HB	1:D:41:LYS:CD	2.41	0.51
1:B:133:PRO:HG2	1:B:170:SER:CB	2.40	0.51
1:F:113:TYR:O	1:F:117:VAL:HG23	2.11	0.51
1:A:255:VAL:HG23	1:A:256:GLY:H	1.76	0.51
1:A:79:ARG:CD	1:A:127:ALA:HB2	2.40	0.50
1:C:24:VAL:HG22	1:C:483:VAL:HG22	1.93	0.50
1:F:335:ASN:HD22	1:F:335:ASN:N	2.07	0.50
1:F:133:PRO:HG2	1:F:170:SER:CB	2.42	0.50
1:D:292:GLU:O	1:D:296:LEU:HD23	2.11	0.50
1:A:336:ALA:HB3	1:A:337:PRO:HD3	1.92	0.50
4:A:553:GTP:O1B	4:A:553:GTP:O1G	2.28	0.50
1:D:265:ARG:NH1	4:D:553:GTP:O2G	2.38	0.50
1:A:162:VAL:HG11	1:F:190:TYR:HD2	1.76	0.50
1:A:113:TYR:O	1:A:117:VAL:HG23	2.11	0.50
1:C:94:ARG:HG3	1:C:169:MET:HB2	1.93	0.50
1:F:87:THR:HB	1:F:88:PRO:HD3	1.94	0.50
1:D:132:ASN:C	1:D:132:ASN:HD22	2.15	0.50
1:F:336:ALA:HB3	1:F:337:PRO:HD3	1.92	0.50
1:D:255:VAL:HG23	1:D:256:GLY:H	1.77	0.50
1:A:292:GLU:O	1:A:296:LEU:HD23	2.10	0.50
1:D:2:ASP:HB3	1:D:332:THR:HG21	1.94	0.50
1:F:255:VAL:CG2	1:F:325:ALA:HB1	2.42	0.50
1:E:260:MET:HG2	1:E:288:PRO:HG3	1.92	0.50
1:F:413:VAL:HG23	1:F:430:ILE:HG13	1.92	0.50
1:C:44:ARG:HH21	1:C:499:THR:HG22	1.76	0.50
1:C:93:ILE:HG12	1:C:127:ALA:HB3	1.93	0.50
1:C:61:LEU:HD12	1:C:61:LEU:N	2.27	0.50
1:A:309:ILE:HD12	1:A:309:ILE:N	2.26	0.50
1:F:309:ILE:HD12	1:F:309:ILE:N	2.27	0.50
1:D:4:GLU:O	1:D:5:ASP:HB2	2.11	0.50
1:E:255:VAL:HG23	1:E:256:GLY:H	1.76	0.50
1:B:255:VAL:HG23	1:B:256:GLY:H	1.77	0.49
1:D:498:VAL:HG11	1:E:138:ASP:HB3	1.94	0.49
1:C:260:MET:HG2	1:C:288:PRO:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:TRP:HD1	1:E:497:GLY:O	1.94	0.49
1:F:111:MET:SD	1:F:114:LYS:HE3	2.52	0.49
1:D:47:GLY:O	1:D:51:ILE:HG12	2.12	0.49
1:E:34:THR:HG21	1:E:40:GLN:NE2	2.20	0.49
1:C:255:VAL:HG23	1:C:256:GLY:H	1.77	0.49
1:F:260:MET:HG2	1:F:288:PRO:HG3	1.94	0.49
1:D:217:ARG:NH1	6:D:579:HOH:O	2.31	0.49
1:B:309:ILE:HD12	1:B:309:ILE:N	2.27	0.49
1:A:94:ARG:HG3	1:A:169:MET:HB2	1.94	0.49
1:E:201:LYS:NZ	1:E:388:ASN:HD21	2.11	0.49
1:D:336:ALA:HB3	1:D:337:PRO:HD3	1.93	0.49
1:C:250:GLN:NE2	1:C:330:GLN:HE21	2.07	0.49
1:F:93:ILE:HG12	1:F:127:ALA:HB3	1.94	0.49
4:E:553:GTP:C8	4:E:553:GTP:H5'	2.47	0.49
1:A:34:THR:HB	1:A:41:LYS:CD	2.42	0.49
1:C:32:LEU:HD13	1:C:490:PHE:HZ	1.78	0.49
1:B:260:MET:HG2	1:B:288:PRO:HG3	1.93	0.49
1:D:93:ILE:HG12	1:D:127:ALA:HB3	1.93	0.49
1:B:201:LYS:HZ1	1:B:388:ASN:HD21	1.60	0.49
1:D:221:HIS:HE1	6:D:579:HOH:O	1.96	0.49
1:C:87:THR:HB	1:C:88:PRO:HD3	1.94	0.49
1:E:48:ILE:HD12	1:E:490:PHE:CE1	2.47	0.49
1:E:47:GLY:O	1:E:51:ILE:HG12	2.13	0.49
1:B:47:GLY:O	1:B:51:ILE:HG12	2.12	0.49
1:E:37:THR:HA	1:E:41:LYS:HG3	1.95	0.49
1:F:250:GLN:NE2	1:F:330:GLN:HE21	2.09	0.49
1:B:258:HIS:HD2	1:B:261:ARG:NH1	2.03	0.49
1:B:242:PHE:HB3	1:B:268:ALA:HB2	1.95	0.49
1:A:3:ARG:O	1:A:4:GLU:HB2	2.13	0.49
1:F:349:ASN:ND2	3:F:551:NDP:O2D	2.46	0.49
1:B:132:ASN:C	1:B:132:ASN:HD22	2.16	0.49
1:A:44:ARG:NH2	1:A:500:PHE:HD2	2.09	0.48
1:E:82:HIS:CD2	1:E:112:THR:HG21	2.40	0.48
1:E:93:ILE:HG12	1:E:127:ALA:HB3	1.93	0.48
1:C:494:ASN:ND2	1:C:494:ASN:C	2.67	0.48
1:E:255:VAL:CG2	1:E:325:ALA:HB1	2.44	0.48
1:B:87:THR:HB	1:B:88:PRO:HD3	1.95	0.48
1:F:479:THR:O	1:F:483:VAL:HG23	2.13	0.48
1:E:132:ASN:HD22	1:E:132:ASN:C	2.16	0.48
1:D:112:THR:HG22	1:D:124:GLY:HA3	1.94	0.48
1:D:276:SER:HB2	3:D:551:NDP:O2X	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:GLN:NE2	1:E:330:GLN:HE21	2.07	0.48
1:E:222:GLY:HA2	1:E:372:TYR:OH	2.13	0.48
1:E:229:GLU:O	1:E:230:ALA:HB3	2.14	0.48
1:E:479:THR:O	1:E:483:VAL:HG23	2.13	0.48
1:C:47:GLY:O	1:C:51:ILE:HG12	2.14	0.48
1:E:24:VAL:CG2	1:E:483:VAL:HG13	2.44	0.48
1:B:61:LEU:HD12	1:B:61:LEU:N	2.28	0.48
1:D:250:GLN:NE2	1:D:330:GLN:HE21	2.07	0.48
1:D:133:PRO:HG2	1:D:170:SER:CB	2.43	0.48
1:C:190:TYR:HD2	1:E:162:VAL:HG11	1.77	0.48
1:B:222:GLY:HA2	1:B:372:TYR:OH	2.14	0.48
1:F:229:GLU:O	1:F:230:ALA:HB3	2.14	0.48
1:B:44:ARG:HH22	1:B:494:ASN:HD22	1.60	0.48
1:C:133:PRO:HG2	1:C:170:SER:CB	2.42	0.48
1:E:133:PRO:HG2	1:E:170:SER:CB	2.42	0.48
1:F:255:VAL:HG23	1:F:256:GLY:H	1.78	0.48
1:C:111:MET:SD	1:C:114:LYS:HE3	2.53	0.48
1:C:336:ALA:HB3	1:C:337:PRO:HD3	1.95	0.48
1:B:292:GLU:O	1:B:296:LEU:HD23	2.13	0.48
1:C:48:ILE:HD11	1:C:499:THR:HG21	1.96	0.48
1:B:167:PRO:O	2:B:550:GLU:N	2.46	0.48
1:E:369:PRO:HB2	1:E:371:LEU:HD23	1.95	0.48
1:A:47:GLY:O	1:A:51:ILE:HG12	2.14	0.48
1:E:118:VAL:O	1:E:118:VAL:HG13	2.14	0.48
1:D:309:ILE:HD12	1:D:309:ILE:N	2.28	0.48
1:C:229:GLU:O	1:C:230:ALA:HB3	2.12	0.48
1:A:255:VAL:CG2	1:A:325:ALA:HB1	2.42	0.48
1:F:47:GLY:O	1:F:51:ILE:HG12	2.13	0.47
1:D:12:MET:HG3	1:D:354:PRO:HD3	1.95	0.47
1:B:147:ARG:HD3	5:B:552:GWD:OAB	2.14	0.47
1:B:255:VAL:CG2	1:B:325:ALA:HB1	2.43	0.47
1:A:132:ASN:C	1:A:132:ASN:HD22	2.18	0.47
1:E:309:ILE:HD12	1:E:309:ILE:N	2.30	0.47
1:E:95:TYR:OH	1:E:145:THR:HG22	2.15	0.47
1:C:174:ARG:CD	1:E:499:THR:HG21	2.44	0.47
1:C:201:LYS:HZ2	1:C:388:ASN:ND2	2.11	0.47
1:E:339:VAL:HG22	1:E:363:ARG:HH21	1.79	0.47
1:F:339:VAL:HG22	1:F:363:ARG:HH21	1.80	0.47
1:E:113:TYR:O	1:E:117:VAL:HG23	2.15	0.47
1:F:48:ILE:HD12	1:F:490:PHE:CE1	2.49	0.47
1:F:150:MET:HG3	5:F:552:GWD:HAH	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:495:GLU:O	1:D:496:ALA:CB	2.63	0.47
1:D:219:VAL:HG22	1:D:373:LEU:CD1	2.45	0.47
1:D:242:PHE:HB3	1:D:268:ALA:HB2	1.96	0.47
1:F:242:PHE:HB3	1:F:268:ALA:HB2	1.96	0.47
1:D:147:ARG:HD3	5:D:552:GWD:OAB	2.15	0.47
1:B:37:THR:HA	1:B:41:LYS:HG3	1.97	0.47
1:F:369:PRO:HB2	1:F:371:LEU:HD23	1.97	0.47
1:B:412:SER:HA	1:F:433:THR:HG23	1.97	0.47
1:A:201:LYS:NZ	1:A:388:ASN:HD21	2.11	0.47
1:D:339:VAL:HG22	1:D:363:ARG:HH21	1.80	0.47
1:A:482:TYR:O	1:A:486:ILE:HG13	2.14	0.47
1:C:412:SER:HA	1:E:433:THR:HG23	1.96	0.47
1:A:263:LEU:HD11	1:A:323:ILE:HD11	1.97	0.47
1:A:209:HIS:CD2	1:A:446:LYS:HG3	2.49	0.47
1:C:255:VAL:CG2	1:C:325:ALA:HB1	2.42	0.47
1:D:229:GLU:O	1:D:230:ALA:HB3	2.15	0.47
1:D:61:LEU:HD12	1:D:61:LEU:N	2.30	0.47
1:F:61:LEU:HD12	1:F:61:LEU:N	2.29	0.47
1:D:222:GLY:HA2	1:D:372:TYR:OH	2.15	0.47
1:A:107:LEU:CB	1:A:126:LYS:HG2	2.44	0.47
1:D:107:LEU:CB	1:D:126:LYS:HG2	2.44	0.47
1:B:162:VAL:HG23	1:B:163:ASP:N	2.30	0.47
1:E:87:THR:HB	1:E:88:PRO:HD3	1.97	0.47
1:A:253:GLY:HA3	3:A:551:NDP:O1A	2.14	0.46
1:B:263:LEU:HD11	1:B:323:ILE:HD11	1.96	0.46
1:D:87:THR:HB	1:D:88:PRO:HD3	1.95	0.46
1:A:369:PRO:HB2	1:A:371:LEU:HD23	1.97	0.46
1:A:55:CYS:O	1:D:62:SER:HB3	2.16	0.46
1:B:369:PRO:HB2	1:B:371:LEU:HD23	1.98	0.46
1:C:459:ARG:O	1:C:463:GLN:HG3	2.15	0.46
1:F:162:VAL:HG23	1:F:163:ASP:N	2.31	0.46
1:E:459:ARG:O	1:E:463:GLN:HG3	2.15	0.46
1:C:242:PHE:HB3	1:C:268:ALA:HB2	1.96	0.46
1:E:315:LEU:HD13	1:E:331:LEU:CD1	2.45	0.46
1:B:250:GLN:NE2	1:B:330:GLN:HE21	2.11	0.46
1:D:118:VAL:O	1:D:118:VAL:HG13	2.15	0.46
1:E:32:LEU:HD13	1:E:490:PHE:HZ	1.80	0.46
1:C:369:PRO:HB2	1:C:371:LEU:HD23	1.97	0.46
1:A:459:ARG:HA	1:A:462:ARG:HE	1.81	0.46
1:F:201:LYS:HZ1	1:F:388:ASN:HD21	1.63	0.46
1:E:242:PHE:HB3	1:E:268:ALA:HB2	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:369:PRO:HB2	1:D:371:LEU:HD23	1.97	0.46
1:A:250:GLN:NE2	1:A:330:GLN:HE21	2.08	0.46
1:C:479:THR:O	1:C:483:VAL:HG23	2.16	0.46
1:B:24:VAL:CG2	1:B:483:VAL:HG13	2.45	0.46
1:B:24:VAL:HG22	1:B:483:VAL:HG22	1.96	0.46
1:B:339:VAL:HG22	1:B:363:ARG:HH21	1.80	0.46
1:B:459:ARG:O	1:B:463:GLN:HG3	2.16	0.46
1:B:495:GLU:O	1:B:496:ALA:HB2	2.16	0.46
1:B:253:GLY:HA3	3:B:551:NDP:H51A	1.98	0.46
1:F:209:HIS:CD2	1:F:446:LYS:HG3	2.51	0.46
1:E:219:VAL:HG22	1:E:373:LEU:CD1	2.45	0.46
1:A:162:VAL:HG23	1:A:163:ASP:N	2.31	0.46
1:B:323:ILE:HG12	1:B:345:ALA:HB3	1.97	0.46
1:D:369:PRO:HD3	1:D:477:LEU:HB2	1.97	0.46
1:E:162:VAL:HG23	1:E:163:ASP:N	2.31	0.46
1:C:113:TYR:O	1:C:117:VAL:HG23	2.15	0.46
1:E:61:LEU:N	1:E:61:LEU:HD12	2.31	0.46
1:C:459:ARG:HA	1:C:462:ARG:HE	1.81	0.46
1:A:61:LEU:HD12	1:A:61:LEU:N	2.31	0.46
1:E:211:ARG:HH22	3:E:551:NDP:H72N	1.64	0.46
1:A:24:VAL:CG2	1:A:483:VAL:HG13	2.46	0.46
1:D:459:ARG:O	1:D:463:GLN:HG3	2.16	0.46
1:A:496:ALA:C	1:A:498:VAL:N	2.64	0.46
1:C:219:VAL:HG22	1:C:373:LEU:CD1	2.45	0.46
1:B:12:MET:HG3	1:B:354:PRO:HD3	1.98	0.46
1:C:132:ASN:C	1:C:132:ASN:HD22	2.18	0.46
1:A:498:VAL:O	1:A:499:THR:C	2.53	0.46
1:B:118:VAL:O	1:B:118:VAL:HG13	2.15	0.46
1:E:137:THR:OG1	1:E:140:GLU:HG3	2.17	0.46
2:C:550:GLU:HA	3:C:551:NDP:C4N	2.45	0.46
1:E:111:MET:SD	1:E:114:LYS:HE3	2.56	0.46
1:C:358:LYS:O	1:C:362:GLU:HG3	2.15	0.46
1:A:111:MET:SD	1:A:114:LYS:HE3	2.56	0.46
1:E:319:CYS:O	1:E:341:ALA:HA	2.16	0.46
1:A:51:ILE:HD13	1:D:74:VAL:HG22	1.98	0.45
1:F:2:ASP:OD2	1:F:5:ASP:N	2.49	0.45
1:A:242:PHE:HB3	1:A:268:ALA:HB2	1.97	0.45
1:A:229:GLU:O	1:A:230:ALA:HB3	2.16	0.45
1:D:3:ARG:O	1:D:5:ASP:N	2.50	0.45
1:E:335:ASN:ND2	1:E:335:ASN:H	2.13	0.45
1:D:37:THR:HA	1:D:41:LYS:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:THR:O	1:B:483:VAL:HG23	2.16	0.45
1:B:417:LEU:HD21	1:F:417:LEU:HD13	1.97	0.45
1:A:37:THR:HA	1:A:41:LYS:HG3	1.98	0.45
1:D:258:HIS:CD2	1:D:261:ARG:HH11	2.19	0.45
1:B:413:VAL:CG2	1:B:430:ILE:HG13	2.45	0.45
1:B:459:ARG:HA	1:B:462:ARG:HE	1.80	0.45
1:D:113:TYR:O	1:D:117:VAL:HG23	2.17	0.45
1:E:482:TYR:O	1:E:486:ILE:HG13	2.17	0.45
1:F:37:THR:HA	1:F:41:LYS:HG3	1.98	0.45
1:D:137:THR:OG1	1:D:140:GLU:HG3	2.17	0.45
1:A:319:CYS:O	1:A:341:ALA:HA	2.16	0.45
1:C:263:LEU:HD11	1:C:323:ILE:HD11	1.97	0.45
1:F:24:VAL:CG2	1:F:483:VAL:HG13	2.46	0.45
1:D:479:THR:O	1:D:483:VAL:HG23	2.15	0.45
1:C:417:LEU:HD13	1:D:417:LEU:HD21	1.99	0.45
1:A:87:THR:HB	1:A:88:PRO:HD3	1.98	0.45
1:C:95:TYR:OH	1:C:145:THR:HG22	2.16	0.45
1:F:132:ASN:C	1:F:132:ASN:HD22	2.19	0.45
1:B:3:ARG:CA	1:B:3:ARG:HH11	2.29	0.45
1:C:162:VAL:HG23	1:C:163:ASP:N	2.32	0.45
1:B:229:GLU:O	1:B:230:ALA:HB3	2.16	0.45
1:F:172:GLY:O	1:F:176:MET:HG2	2.17	0.45
1:F:319:CYS:O	1:F:341:ALA:HA	2.16	0.45
1:E:147:ARG:CD	5:E:552:GWD:BRAC	3.19	0.45
1:A:3:ARG:O	1:A:4:GLU:CB	2.65	0.45
1:A:479:THR:O	1:A:483:VAL:HG23	2.16	0.45
1:D:201:LYS:NZ	1:D:388:ASN:HD21	2.15	0.45
1:D:319:CYS:O	1:D:341:ALA:HA	2.17	0.45
1:B:44:ARG:HH22	1:B:494:ASN:ND2	2.15	0.45
1:E:168:ASP:OD1	2:E:550:GLU:N	2.50	0.45
1:D:162:VAL:HG23	1:D:163:ASP:N	2.32	0.45
1:E:459:ARG:HA	1:E:462:ARG:HE	1.81	0.45
1:D:111:MET:SD	1:D:114:LYS:HE3	2.57	0.45
1:C:432:PRO:HB3	1:C:436:PHE:HD2	1.82	0.45
1:F:496:ALA:C	1:F:498:VAL:N	2.65	0.45
1:C:487:GLU:HG3	1:C:491:ARG:HH22	1.80	0.45
1:C:349:ASN:ND2	3:C:551:NDP:O2D	2.50	0.45
1:D:263:LEU:HD11	1:D:323:ILE:HD11	1.99	0.45
1:D:482:TYR:O	1:D:486:ILE:HG13	2.17	0.45
1:A:304:PHE:CD1	1:A:305:PRO:HD2	2.52	0.45
1:E:263:LEU:HD11	1:E:323:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:TYR:O	1:B:117:VAL:HG23	2.17	0.45
1:E:411:MET:CE	1:E:415:GLU:HG3	2.47	0.44
1:F:221:HIS:HE1	6:F:563:HOH:O	1.99	0.44
1:D:3:ARG:C	1:D:5:ASP:N	2.70	0.44
1:C:37:THR:HA	1:C:41:LYS:HG3	1.98	0.44
1:C:44:ARG:HH21	1:C:499:THR:CG2	2.30	0.44
1:C:107:LEU:CB	1:C:126:LYS:HG2	2.46	0.44
1:D:459:ARG:HA	1:D:462:ARG:HE	1.81	0.44
1:F:482:TYR:O	1:F:486:ILE:HG13	2.17	0.44
1:E:358:LYS:O	1:E:362:GLU:HG3	2.16	0.44
1:B:8:ASN:HD21	1:B:102:ASP:HB3	1.82	0.44
1:C:482:TYR:O	1:C:486:ILE:HG13	2.17	0.44
1:E:487:GLU:CG	1:E:491:ARG:HH22	2.29	0.44
1:A:219:VAL:HG22	1:A:373:LEU:CD1	2.46	0.44
1:B:482:TYR:O	1:B:486:ILE:HG13	2.17	0.44
1:D:24:VAL:CG2	1:D:483:VAL:HG13	2.48	0.44
1:B:95:TYR:OH	1:B:145:THR:HG22	2.17	0.44
1:C:137:THR:OG1	1:C:140:GLU:HG3	2.18	0.44
1:D:248:ALA:CB	1:D:317:VAL:HG11	2.48	0.44
1:A:12:MET:HG3	1:A:354:PRO:HD3	1.99	0.44
1:A:358:LYS:O	1:A:362:GLU:HG3	2.18	0.44
1:D:315:LEU:HD13	1:D:331:LEU:CD1	2.47	0.44
1:F:304:PHE:CD1	1:F:305:PRO:HD2	2.53	0.44
1:B:150:MET:HG3	5:B:552:GWD:CAH	2.48	0.44
1:C:82:HIS:HD2	1:C:112:THR:CG2	2.28	0.44
1:F:118:VAL:O	1:F:118:VAL:HG13	2.18	0.44
1:C:209:HIS:CD2	1:C:446:LYS:HG3	2.52	0.44
1:F:459:ARG:HA	1:F:462:ARG:HE	1.82	0.44
1:C:499:THR:HG23	1:C:499:THR:O	2.16	0.44
1:A:335:ASN:N	1:A:335:ASN:HD22	2.09	0.44
1:E:258:HIS:CD2	1:E:261:ARG:HH11	2.19	0.44
1:B:469:MET:HE2	6:B:582:HOH:O	2.17	0.44
1:F:459:ARG:O	1:F:463:GLN:HG3	2.18	0.44
1:B:319:CYS:O	1:B:341:ALA:HA	2.18	0.44
1:B:238:MET:CE	1:B:320:ASP:HB3	2.48	0.44
1:C:319:CYS:O	1:C:341:ALA:HA	2.18	0.44
1:B:358:LYS:O	1:B:362:GLU:HG3	2.18	0.44
1:D:33:LYS:N	1:D:33:LYS:HD2	2.33	0.44
1:B:290:GLU:OE2	1:B:306:LYS:HD2	2.18	0.44
1:D:95:TYR:OH	1:D:145:THR:HG22	2.16	0.44
2:E:550:GLU:HA	3:E:551:NDP:H41N	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:201:LYS:NZ	1:F:388:ASN:HD21	2.16	0.44
1:D:323:ILE:HG12	1:D:345:ALA:HB3	2.00	0.44
1:A:95:TYR:OH	1:A:145:THR:HG22	2.18	0.43
1:B:9:PHE:HE1	1:B:107:LEU:HD13	1.80	0.43
1:E:94:ARG:O	1:E:128:GLY:HA2	2.18	0.43
1:E:292:GLU:HG2	1:E:296:LEU:HD23	2.00	0.43
1:A:8:ASN:OD1	1:A:11:LYS:HG2	2.18	0.43
1:C:497:GLY:N	1:D:174:ARG:HG3	2.24	0.43
1:B:469:MET:CE	6:B:582:HOH:O	2.64	0.43
2:A:550:GLU:HA	3:A:551:NDP:H41N	2.00	0.43
1:E:24:VAL:HG22	1:E:483:VAL:HG13	1.99	0.43
1:A:459:ARG:O	1:A:463:GLN:HG3	2.18	0.43
1:E:323:ILE:HG12	1:E:345:ALA:HB3	2.00	0.43
1:D:411:MET:CE	1:D:415:GLU:HG3	2.47	0.43
1:C:339:VAL:HG22	1:C:363:ARG:HH21	1.83	0.43
1:E:12:MET:HG3	1:E:354:PRO:HD3	2.00	0.43
1:B:111:MET:SD	1:B:114:LYS:HE3	2.58	0.43
1:F:107:LEU:CB	1:F:126:LYS:HG2	2.47	0.43
1:C:118:VAL:HG13	1:C:118:VAL:O	2.18	0.43
1:A:137:THR:OG1	1:A:140:GLU:HG3	2.17	0.43
1:F:292:GLU:HG2	1:F:296:LEU:HD23	2.00	0.43
1:A:339:VAL:HG22	1:A:363:ARG:HH21	1.82	0.43
1:C:55:CYS:O	1:F:62:SER:HB3	2.19	0.43
1:D:201:LYS:HZ2	1:D:388:ASN:HD21	1.66	0.43
1:B:169:MET:HA	3:B:551:NDP:O1N	2.19	0.43
1:C:276:SER:HB2	3:C:551:NDP:O2X	2.18	0.43
1:C:24:VAL:CG2	1:C:483:VAL:HG13	2.48	0.43
1:D:432:PRO:HB3	1:D:436:PHE:HD2	1.83	0.43
1:C:416:SER:HB3	1:E:429:PRO:O	2.18	0.43
1:C:258:HIS:HD2	1:C:261:ARG:NH1	2.04	0.43
1:A:118:VAL:O	1:A:118:VAL:HG13	2.19	0.43
1:C:392:VAL:HG22	1:E:386:LEU:HD21	2.01	0.43
1:B:335:ASN:H	1:B:335:ASN:ND2	2.15	0.43
1:F:169:MET:HG2	3:F:551:NDP:H51N	1.99	0.43
1:A:201:LYS:HZ2	1:A:388:ASN:HD21	1.65	0.43
1:D:358:LYS:O	1:D:362:GLU:HG3	2.19	0.43
1:E:248:ALA:CB	1:E:317:VAL:HG11	2.49	0.43
1:B:304:PHE:CD1	1:B:305:PRO:HD2	2.54	0.43
1:F:432:PRO:HB3	1:F:436:PHE:HD2	1.83	0.43
1:B:209:HIS:CE1	4:B:553:GTP:O1A	2.71	0.43
1:A:315:LEU:HD13	1:A:331:LEU:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:222:GLY:HA2	1:F:372:TYR:OH	2.19	0.43
1:A:82:HIS:HD2	1:A:112:THR:CG2	2.27	0.43
1:B:137:THR:OG1	1:B:140:GLU:HG3	2.18	0.43
1:E:446:LYS:HD2	4:E:553:GTP:O2B	2.19	0.43
1:C:411:MET:CE	1:C:415:GLU:HG3	2.49	0.43
1:E:304:PHE:CD1	1:E:305:PRO:HD2	2.54	0.43
1:E:33:LYS:N	1:E:33:LYS:HD2	2.34	0.43
1:E:2:ASP:OD2	1:E:5:ASP:HB3	2.18	0.43
1:B:491:ARG:O	1:B:495:GLU:HB2	2.19	0.43
1:A:238:MET:CE	1:A:320:ASP:HB3	2.49	0.43
1:B:211:ARG:HB3	6:B:562:HOH:O	2.18	0.42
1:B:94:ARG:O	1:B:128:GLY:HA2	2.18	0.42
1:A:209:HIS:NE2	1:A:446:LYS:HG3	2.34	0.42
1:A:416:SER:HB3	1:B:429:PRO:O	2.19	0.42
1:D:498:VAL:HG23	1:D:499:THR:N	2.34	0.42
1:A:413:VAL:CG2	1:A:430:ILE:HG13	2.49	0.42
1:C:323:ILE:HG12	1:C:345:ALA:HB3	2.01	0.42
1:D:378:VAL:HG22	6:D:560:HOH:O	2.17	0.42
1:E:2:ASP:HB3	1:E:5:ASP:O	2.19	0.42
1:B:248:ALA:CB	1:B:317:VAL:HG11	2.49	0.42
1:E:432:PRO:HB3	1:E:436:PHE:HD2	1.84	0.42
1:B:86:ARG:HD3	1:B:86:ARG:HA	1.90	0.42
1:F:315:LEU:HD13	1:F:331:LEU:CD1	2.49	0.42
1:B:219:VAL:HG22	1:B:373:LEU:CD1	2.46	0.42
1:A:292:GLU:HG2	1:A:296:LEU:HD23	2.01	0.42
1:A:3:ARG:H	1:A:3:ARG:HG2	1.66	0.42
1:D:304:PHE:CD1	1:D:305:PRO:HD2	2.54	0.42
1:E:27:LYS:HA	1:E:30:GLU:HB2	2.01	0.42
1:F:82:HIS:HD2	1:F:112:THR:CG2	2.29	0.42
1:E:290:GLU:OE2	1:E:306:LYS:HD2	2.19	0.42
1:B:158:ILE:HA	1:B:163:ASP:O	2.19	0.42
1:E:390:ASN:O	1:E:392:VAL:HG23	2.19	0.42
1:D:27:LYS:HA	1:D:30:GLU:HB2	2.01	0.42
1:A:24:VAL:HG22	1:A:483:VAL:HG13	2.00	0.42
1:C:248:ALA:CB	1:C:317:VAL:HG11	2.50	0.42
1:D:2:ASP:O	1:D:6:ASP:HB2	2.19	0.42
1:F:290:GLU:OE2	1:F:306:LYS:HD2	2.19	0.42
1:C:292:GLU:HG2	1:C:296:LEU:HD23	2.01	0.42
1:C:419:ARG:NH2	1:E:429:PRO:HD2	2.35	0.42
1:F:411:MET:CE	1:F:415:GLU:HG3	2.49	0.42
1:F:323:ILE:HG12	1:F:345:ALA:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:443:ALA:HA	1:C:447:ASP:OD1	2.20	0.42
1:F:33:LYS:HD2	1:F:33:LYS:N	2.34	0.42
1:F:112:THR:CG2	1:F:124:GLY:HA3	2.49	0.42
1:B:74:VAL:HG22	1:E:51:ILE:HD13	2.01	0.42
1:F:94:ARG:O	1:F:128:GLY:HA2	2.20	0.42
1:A:323:ILE:HG12	1:A:345:ALA:HB3	2.02	0.42
1:F:358:LYS:O	1:F:362:GLU:HG3	2.20	0.42
1:F:27:LYS:HA	1:F:30:GLU:HB2	2.00	0.42
1:D:209:HIS:CD2	1:D:446:LYS:HG3	2.55	0.42
1:D:24:VAL:HG22	1:D:483:VAL:HG22	2.02	0.42
1:F:263:LEU:HD11	1:F:323:ILE:HD11	2.01	0.42
1:C:335:ASN:N	1:C:335:ASN:HD22	2.09	0.42
1:B:33:LYS:N	1:B:33:LYS:HD2	2.35	0.42
1:F:219:VAL:HG22	1:F:373:LEU:CD1	2.49	0.42
1:B:411:MET:CE	1:B:415:GLU:HG3	2.49	0.42
1:C:315:LEU:HD13	1:C:331:LEU:CD1	2.50	0.42
1:C:335:ASN:ND2	1:C:335:ASN:H	2.16	0.41
1:C:94:ARG:O	1:C:128:GLY:HA2	2.20	0.41
1:A:370:ASP:OD1	1:A:371:LEU:N	2.52	0.41
1:C:370:ASP:OD1	1:C:371:LEU:N	2.53	0.41
1:B:315:LEU:HD13	1:B:331:LEU:CD1	2.50	0.41
1:F:406:ASN:HD22	1:F:406:ASN:HA	1.72	0.41
1:A:290:GLU:OE2	1:A:306:LYS:HD2	2.19	0.41
1:B:253:GLY:HA3	3:B:551:NDP:C5B	2.50	0.41
1:C:304:PHE:CD1	1:C:305:PRO:HD2	2.55	0.41
1:E:238:MET:CE	1:E:320:ASP:HB3	2.50	0.41
1:D:270:CYS:O	1:D:285:GLY:HA2	2.20	0.41
1:B:112:THR:CG2	1:B:124:GLY:HA3	2.50	0.41
1:F:158:ILE:HA	1:F:163:ASP:O	2.21	0.41
1:F:2:ASP:HB2	1:F:332:THR:HG21	2.02	0.41
1:C:2:ASP:HB3	1:C:3:ARG:H	1.65	0.41
1:A:59:LEU:HG	1:A:61:LEU:HD11	2.02	0.41
1:C:378:VAL:HG22	6:C:555:HOH:O	2.19	0.41
1:F:32:LEU:HD12	1:F:494:ASN:HD21	1.84	0.41
1:C:222:GLY:HA2	1:C:372:TYR:OH	2.20	0.41
1:B:346:GLU:OE1	1:B:352:THR:HG23	2.21	0.41
1:C:62:SER:HB3	1:F:55:CYS:O	2.21	0.41
1:E:239:THR:O	1:E:245:LYS:NZ	2.46	0.41
1:A:33:LYS:N	1:A:33:LYS:HD2	2.35	0.41
1:B:177:SER:OG	1:F:496:ALA:O	2.24	0.41
1:B:496:ALA:CB	1:B:499:THR:HB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:491:ARG:O	1:C:495:GLU:HG2	2.21	0.41
1:A:59:LEU:HG	1:A:61:LEU:CD1	2.51	0.41
1:A:346:GLU:OE1	1:A:352:THR:HG23	2.19	0.41
1:C:33:LYS:N	1:C:33:LYS:HD2	2.35	0.41
1:A:411:MET:CE	1:A:415:GLU:HG3	2.50	0.41
1:B:370:ASP:OD1	1:B:371:LEU:N	2.54	0.41
1:E:322:LEU:HB3	1:E:344:ILE:HD13	2.03	0.41
1:F:248:ALA:CB	1:F:317:VAL:HG11	2.50	0.41
1:A:94:ARG:O	1:A:128:GLY:HA2	2.21	0.41
1:D:292:GLU:HG2	1:D:296:LEU:HD23	2.01	0.41
1:C:390:ASN:O	1:C:392:VAL:HG23	2.21	0.41
1:D:498:VAL:HG11	1:E:138:ASP:CB	2.51	0.41
1:F:209:HIS:NE2	1:F:446:LYS:HG3	2.36	0.41
1:A:417:LEU:HD13	1:F:417:LEU:HD21	2.02	0.41
1:A:222:GLY:HA2	1:A:372:TYR:OH	2.21	0.41
1:B:33:LYS:HG2	1:B:495:GLU:OE2	2.21	0.41
1:A:34:THR:HG22	1:A:36:GLU:N	2.36	0.41
1:C:258:HIS:CD2	1:C:261:ARG:HD3	2.56	0.41
1:B:118:VAL:CG1	1:B:120:VAL:HG23	2.51	0.41
1:E:169:MET:HA	3:E:551:NDP:O1N	2.20	0.41
1:C:59:LEU:HG	1:C:61:LEU:HD11	2.03	0.41
1:F:370:ASP:OD1	1:F:371:LEU:N	2.54	0.41
1:E:59:LEU:HG	1:E:61:LEU:HD11	2.03	0.41
1:F:322:LEU:HB3	1:F:344:ILE:HD13	2.02	0.41
1:B:27:LYS:HA	1:B:30:GLU:HB2	2.03	0.41
1:A:62:SER:HB3	1:D:55:CYS:O	2.21	0.41
1:D:494:ASN:C	1:D:494:ASN:HD22	2.25	0.41
1:F:335:ASN:ND2	1:F:335:ASN:H	2.14	0.41
1:E:118:VAL:CG1	1:E:120:VAL:HG23	2.51	0.41
1:B:92:GLY:O	1:B:126:LYS:HD3	2.20	0.41
1:F:24:VAL:HG22	1:F:483:VAL:HG13	2.03	0.41
1:E:59:LEU:HG	1:E:61:LEU:CD1	2.51	0.41
1:E:270:CYS:O	1:E:285:GLY:HA2	2.21	0.41
1:A:248:ALA:CB	1:A:317:VAL:HG11	2.50	0.41
1:D:147:ARG:CD	5:D:552:GWD:BRAC	3.24	0.40
1:F:258:HIS:CD2	1:F:261:ARG:HD3	2.56	0.40
1:C:253:GLY:HA3	3:C:551:NDP:O1A	2.21	0.40
1:F:390:ASN:O	1:F:392:VAL:HG23	2.20	0.40
1:D:24:VAL:HG22	1:D:483:VAL:HG13	2.03	0.40
1:D:150:MET:HG3	5:D:552:GWD:CAH	2.51	0.40
1:C:290:GLU:OE2	1:C:306:LYS:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:215:THR:O	1:F:219:VAL:HG23	2.20	0.40
2:E:550:GLU:HA	3:E:551:NDP:C4N	2.51	0.40
1:F:281:TRP:CB	1:F:310:TYR:HB2	2.51	0.40
1:D:390:ASN:O	1:D:392:VAL:HG23	2.22	0.40
1:B:390:ASN:O	1:B:392:VAL:HG23	2.21	0.40
1:A:74:VAL:HG22	1:D:51:ILE:HD13	2.04	0.40
1:A:258:HIS:CD2	1:A:261:ARG:HD3	2.56	0.40
1:F:169:MET:HA	3:F:551:NDP:O1N	2.22	0.40
1:B:209:HIS:CD2	1:B:446:LYS:HG3	2.56	0.40
1:B:201:LYS:HZ1	1:B:388:ASN:ND2	2.18	0.40
1:E:158:ILE:HA	1:E:163:ASP:O	2.21	0.40
1:E:370:ASP:OD1	1:E:371:LEU:N	2.55	0.40
1:C:238:MET:CE	1:C:320:ASP:HB3	2.51	0.40
1:F:238:MET:CE	1:F:320:ASP:HB3	2.52	0.40
1:D:258:HIS:CD2	1:D:261:ARG:HD3	2.56	0.40
1:C:494:ASN:O	1:C:495:GLU:C	2.60	0.40
1:D:287:ASP:HA	1:D:288:PRO:HD3	1.97	0.40
1:D:290:GLU:OE2	1:D:306:LYS:HD2	2.21	0.40
1:C:3:ARG:HA	1:C:3:ARG:HE	1.86	0.40
1:C:110:LEU:O	1:C:114:LYS:HB3	2.22	0.40
1:A:110:LEU:O	1:A:114:LYS:HB3	2.21	0.40
1:D:429:PRO:O	1:E:416:SER:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	499/501 (100%)	462 (93%)	27 (5%)	10 (2%)	9 15
1	B	499/501 (100%)	466 (93%)	25 (5%)	8 (2%)	12 21
1	C	499/501 (100%)	460 (92%)	28 (6%)	11 (2%)	8 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	499/501 (100%)	460 (92%)	30 (6%)	9 (2%)	11	18
1	E	499/501 (100%)	464 (93%)	27 (5%)	8 (2%)	12	21
1	F	499/501 (100%)	462 (93%)	29 (6%)	8 (2%)	12	21
All	All	2994/3006 (100%)	2774 (93%)	166 (6%)	54 (2%)	11	18

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	498	VAL
1	B	496	ALA
1	B	498	VAL
1	C	3	ARG
1	C	495	GLU
1	D	5	ASP
1	D	499	THR
1	E	496	ALA
1	F	496	ALA
1	F	498	VAL
1	A	499	THR
1	E	2	ASP
1	F	5	ASP
1	A	243	GLY
1	C	496	ALA
1	D	4	GLU
1	E	30	GLU
1	E	243	GLY
1	F	243	GLY
1	A	30	GLU
1	A	313	SER
1	A	495	GLU
1	A	496	ALA
1	B	30	GLU
1	B	243	GLY
1	B	313	SER
1	C	2	ASP
1	C	30	GLU
1	C	243	GLY
1	C	313	SER
1	D	30	GLU
1	D	243	GLY

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Mol	Chain	Res	Type
1	D	313	SER
1	D	496	ALA
1	E	313	SER
1	E	498	VAL
1	F	30	GLU
1	F	313	SER
1	C	38	GLU
1	E	422	GLY
1	B	38	GLU
1	D	422	GLY
1	A	422	GLY
1	B	422	GLY
1	C	422	GLY
1	E	309	ILE
1	A	309	ILE
1	C	309	ILE
1	C	497	GLY
1	F	309	ILE
1	B	309	ILE
1	D	309	ILE
1	F	422	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	417/417 (100%)	391 (94%)	26 (6%)	23	41
1	B	417/417 (100%)	390 (94%)	27 (6%)	21	39
1	C	417/417 (100%)	391 (94%)	26 (6%)	23	41
1	D	417/417 (100%)	391 (94%)	26 (6%)	23	41
1	E	417/417 (100%)	389 (93%)	28 (7%)	20	37
1	F	417/417 (100%)	389 (93%)	28 (7%)	20	37
All	All	2502/2502 (100%)	2341 (94%)	161 (6%)	21	39

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	PHE
1	A	23	ILE
1	A	24	VAL
1	A	33	LYS
1	A	37	THR
1	A	75	ILE
1	A	96	SER
1	A	107	LEU
1	A	114	LYS
1	A	118	VAL
1	A	132	ASN
1	A	145	THR
1	A	291	LEU
1	A	331	LEU
1	A	335	ASN
1	A	340	LYS
1	A	357	ASP
1	A	364	ASN
1	A	378	VAL
1	A	386	LEU
1	A	405	SER
1	A	410	LEU
1	A	419	ARG
1	A	472	ASN
1	A	494	ASN
1	A	501	THR
1	B	2	ASP
1	B	3	ARG
1	B	23	ILE
1	B	24	VAL
1	B	33	LYS
1	B	37	THR
1	B	75	ILE
1	B	96	SER
1	B	107	LEU
1	B	114	LYS
1	B	118	VAL
1	B	132	ASN
1	B	145	THR
1	B	291	LEU
1	B	331	LEU
1	B	335	ASN

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Mol	Chain	Res	Type
1	B	340	LYS
1	B	357	ASP
1	B	364	ASN
1	B	378	VAL
1	B	386	LEU
1	B	405	SER
1	B	410	LEU
1	B	419	ARG
1	B	472	ASN
1	B	498	VAL
1	B	499	THR
1	C	3	ARG
1	C	24	VAL
1	C	33	LYS
1	C	37	THR
1	C	75	ILE
1	C	96	SER
1	C	107	LEU
1	C	114	LYS
1	C	118	VAL
1	C	132	ASN
1	C	145	THR
1	C	291	LEU
1	C	331	LEU
1	C	335	ASN
1	C	340	LYS
1	C	357	ASP
1	C	364	ASN
1	C	378	VAL
1	C	386	LEU
1	C	405	SER
1	C	410	LEU
1	C	419	ARG
1	C	472	ASN
1	C	494	ASN
1	C	499	THR
1	C	500	PHE
1	D	3	ARG
1	D	9	PHE
1	D	23	ILE
1	D	24	VAL
1	D	33	LYS

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Mol	Chain	Res	Type
1	D	37	THR
1	D	75	ILE
1	D	96	SER
1	D	107	LEU
1	D	114	LYS
1	D	118	VAL
1	D	132	ASN
1	D	145	THR
1	D	291	LEU
1	D	331	LEU
1	D	335	ASN
1	D	340	LYS
1	D	357	ASP
1	D	364	ASN
1	D	378	VAL
1	D	386	LEU
1	D	410	LEU
1	D	419	ARG
1	D	472	ASN
1	D	494	ASN
1	D	501	THR
1	E	4	GLU
1	E	8	ASN
1	E	9	PHE
1	E	23	ILE
1	E	24	VAL
1	E	33	LYS
1	E	37	THR
1	E	75	ILE
1	E	96	SER
1	E	107	LEU
1	E	114	LYS
1	E	118	VAL
1	E	132	ASN
1	E	145	THR
1	E	291	LEU
1	E	331	LEU
1	E	335	ASN
1	E	340	LYS
1	E	357	ASP
1	E	364	ASN
1	E	378	VAL

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Mol	Chain	Res	Type
1	E	386	LEU
1	E	405	SER
1	E	410	LEU
1	E	419	ARG
1	E	472	ASN
1	E	494	ASN
1	E	495	GLU
1	F	4	GLU
1	F	6	ASP
1	F	9	PHE
1	F	23	ILE
1	F	24	VAL
1	F	33	LYS
1	F	37	THR
1	F	75	ILE
1	F	96	SER
1	F	107	LEU
1	F	114	LYS
1	F	118	VAL
1	F	132	ASN
1	F	145	THR
1	F	291	LEU
1	F	331	LEU
1	F	335	ASN
1	F	340	LYS
1	F	357	ASP
1	F	364	ASN
1	F	378	VAL
1	F	386	LEU
1	F	405	SER
1	F	410	LEU
1	F	419	ARG
1	F	472	ASN
1	F	494	ASN
1	F	498	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	43	ASN
1	A	56	ASN

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Mol	Chain	Res	Type
1	A	82	HIS
1	A	132	ASN
1	A	221	HIS
1	A	254	ASN
1	A	258	HIS
1	A	330	GLN
1	A	335	ASN
1	A	388	ASN
1	A	390	ASN
1	A	406	ASN
1	A	424	HIS
1	A	494	ASN
1	B	40	GLN
1	B	43	ASN
1	B	56	ASN
1	B	82	HIS
1	B	132	ASN
1	B	205	GLN
1	B	209	HIS
1	B	254	ASN
1	B	258	HIS
1	B	330	GLN
1	B	335	ASN
1	B	388	ASN
1	B	406	ASN
1	B	424	HIS
1	B	494	ASN
1	C	40	GLN
1	C	43	ASN
1	C	56	ASN
1	C	82	HIS
1	C	132	ASN
1	C	221	HIS
1	C	254	ASN
1	C	258	HIS
1	C	330	GLN
1	C	335	ASN
1	C	388	ASN
1	C	406	ASN
1	C	424	HIS
1	C	494	ASN
1	D	40	GLN

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Mol	Chain	Res	Type
1	D	43	ASN
1	D	56	ASN
1	D	82	HIS
1	D	132	ASN
1	D	205	GLN
1	D	221	HIS
1	D	254	ASN
1	D	258	HIS
1	D	330	GLN
1	D	335	ASN
1	D	388	ASN
1	D	406	ASN
1	D	424	HIS
1	D	494	ASN
1	E	8	ASN
1	E	40	GLN
1	E	43	ASN
1	E	56	ASN
1	E	82	HIS
1	E	132	ASN
1	E	205	GLN
1	E	254	ASN
1	E	258	HIS
1	E	330	GLN
1	E	335	ASN
1	E	388	ASN
1	E	390	ASN
1	E	406	ASN
1	E	424	HIS
1	E	494	ASN
1	F	8	ASN
1	F	40	GLN
1	F	43	ASN
1	F	56	ASN
1	F	82	HIS
1	F	132	ASN
1	F	205	GLN
1	F	209	HIS
1	F	254	ASN
1	F	258	HIS
1	F	330	GLN
1	F	335	ASN

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Mol	Chain	Res	Type
1	F	388	ASN
1	F	406	ASN
1	F	424	HIS
1	F	494	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GLU	A	550	-	4,8,9	1.50	1 (25%)	3,9,11	1.18	0
3	NDP	A	551	-	42,52,52	1.45	5 (11%)	55,80,80	3.71	23 (41%)
5	GWD	A	552	-	23,23,23	2.40	6 (26%)	33,34,34	1.69	6 (18%)
4	GTP	A	553	-	25,34,34	2.04	5 (20%)	34,54,54	5.15	18 (52%)
2	GLU	B	550	-	4,8,9	0.81	0	3,9,11	1.26	0
3	NDP	B	551	-	42,52,52	1.61	6 (14%)	55,80,80	3.63	19 (34%)
5	GWD	B	552	-	23,23,23	2.57	6 (26%)	33,34,34	1.61	5 (15%)
4	GTP	B	553	-	25,34,34	1.48	3 (12%)	34,54,54	5.49	18 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GLU	C	550	-	4,8,9	1.60	1 (25%)	3,9,11	1.18	1 (33%)
3	NDP	C	551	-	42,52,52	1.43	4 (9%)	55,80,80	3.75	22 (40%)
5	GWD	C	552	-	23,23,23	2.48	6 (26%)	33,34,34	1.73	5 (15%)
4	GTP	C	553	-	25,34,34	2.47	5 (20%)	34,54,54	5.45	24 (70%)
2	GLU	D	550	-	4,8,9	0.50	0	3,9,11	1.18	1 (33%)
3	NDP	D	551	-	42,52,52	1.39	3 (7%)	55,80,80	3.59	19 (34%)
5	GWD	D	552	-	23,23,23	2.23	6 (26%)	33,34,34	1.63	5 (15%)
4	GTP	D	553	-	25,34,34	1.86	4 (16%)	34,54,54	5.06	16 (47%)
2	GLU	E	550	-	4,8,9	0.52	0	3,9,11	1.02	0
3	NDP	E	551	-	42,52,52	1.74	7 (16%)	55,80,80	3.55	22 (40%)
5	GWD	E	552	-	23,23,23	2.33	6 (26%)	33,34,34	1.61	5 (15%)
4	GTP	E	553	-	25,34,34	2.48	4 (16%)	34,54,54	4.47	18 (52%)
2	GLU	F	550	-	4,8,9	1.08	0	3,9,11	1.01	0
3	NDP	F	551	-	42,52,52	1.38	5 (11%)	55,80,80	3.63	21 (38%)
5	GWD	F	552	-	23,23,23	2.38	6 (26%)	33,34,34	1.57	4 (12%)
4	GTP	F	553	-	25,34,34	1.59	5 (20%)	34,54,54	5.85	18 (52%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLU	A	550	-	-	0/3/7/9	0/0/0/0
3	NDP	A	551	-	-	0/30/77/77	0/5/5/5
5	GWD	A	552	-	-	0/4/16/16	0/3/3/3
4	GTP	A	553	-	-	0/18/38/38	0/3/3/3
2	GLU	B	550	-	-	0/3/7/9	0/0/0/0
3	NDP	B	551	-	-	0/30/77/77	0/5/5/5
5	GWD	B	552	-	-	0/4/16/16	0/3/3/3
4	GTP	B	553	-	-	0/18/38/38	0/3/3/3
2	GLU	C	550	-	-	0/3/7/9	0/0/0/0
3	NDP	C	551	-	-	0/30/77/77	0/5/5/5
5	GWD	C	552	-	-	0/4/16/16	0/3/3/3
4	GTP	C	553	-	1/1/7/7	0/18/38/38	0/3/3/3
2	GLU	D	550	-	-	0/3/7/9	0/0/0/0
3	NDP	D	551	-	-	0/30/77/77	0/5/5/5
5	GWD	D	552	-	-	0/4/16/16	0/3/3/3
4	GTP	D	553	-	-	0/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLU	E	550	-	-	0/3/7/9	0/0/0/0
3	NDP	E	551	-	-	0/30/77/77	0/5/5/5
5	GWD	E	552	-	-	0/4/16/16	0/3/3/3
4	GTP	E	553	-	1/1/7/7	0/18/38/38	0/3/3/3
2	GLU	F	550	-	-	0/3/7/9	0/0/0/0
3	NDP	F	551	-	-	0/30/77/77	0/5/5/5
5	GWD	F	552	-	-	0/4/16/16	0/3/3/3
4	GTP	F	553	-	-	0/18/38/38	0/3/3/3

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	552	GWD	CAS-CAR	-9.41	1.38	1.50
5	C	552	GWD	CAS-CAR	-9.20	1.38	1.50
5	A	552	GWD	CAS-CAR	-8.77	1.39	1.50
5	F	552	GWD	CAS-CAR	-8.65	1.39	1.50
5	E	552	GWD	CAS-CAR	-8.48	1.39	1.50
5	D	552	GWD	CAS-CAR	-8.27	1.39	1.50
5	B	552	GWD	CAU-CAS	-4.03	1.38	1.45
5	A	552	GWD	CAQ-CAF	-3.88	1.39	1.46
5	C	552	GWD	CAQ-CAF	-3.70	1.39	1.46
5	C	552	GWD	CAU-CAS	-3.67	1.39	1.45
5	E	552	GWD	CAQ-CAF	-3.61	1.39	1.46
5	B	552	GWD	CAQ-CAF	-3.60	1.39	1.46
5	F	552	GWD	CAQ-CAF	-3.55	1.39	1.46
4	B	553	GTP	C8-N7	-3.48	1.27	1.34
5	F	552	GWD	CAU-CAS	-3.46	1.39	1.45
5	D	552	GWD	CAQ-CAF	-3.33	1.40	1.46
5	E	552	GWD	CAU-CAS	-3.27	1.39	1.45
5	A	552	GWD	CAU-CAS	-3.22	1.40	1.45
5	F	552	GWD	CAR-NAL	-3.12	1.32	1.36
5	B	552	GWD	CAT-NAL	-3.04	1.33	1.38
5	A	552	GWD	CAT-NAL	-2.97	1.33	1.38
5	D	552	GWD	CAU-CAS	-2.97	1.40	1.45
5	E	552	GWD	CAR-NAL	-2.95	1.33	1.36
5	D	552	GWD	CAR-NAL	-2.91	1.33	1.36
4	F	553	GTP	C8-N7	-2.89	1.29	1.34
5	E	552	GWD	CAT-NAL	-2.84	1.33	1.38
5	D	552	GWD	CAT-NAL	-2.78	1.33	1.38
5	C	552	GWD	CAT-NAL	-2.75	1.33	1.38
4	A	553	GTP	PA-O1A	-2.72	1.41	1.51
5	B	552	GWD	CAR-NAL	-2.55	1.33	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	552	GWD	CAR-NAL	-2.54	1.33	1.36
5	F	552	GWD	CAT-NAL	-2.50	1.34	1.38
3	B	551	NDP	C8A-N7A	-2.45	1.29	1.34
3	E	551	NDP	C8A-N7A	-2.39	1.30	1.34
5	C	552	GWD	CAR-NAL	-2.39	1.33	1.36
3	F	551	NDP	C8A-N7A	-2.36	1.30	1.34
3	A	551	NDP	C2D-C3D	-2.23	1.47	1.53
4	E	553	GTP	O5'-C5'	-2.04	1.36	1.44
4	D	553	GTP	C2-N1	2.02	1.39	1.35
3	B	551	NDP	C2N-C3N	2.05	1.39	1.34
4	F	553	GTP	C3'-C4'	2.05	1.58	1.53
3	A	551	NDP	P2B-O3X	2.06	1.62	1.54
3	C	551	NDP	P2B-O2X	2.10	1.62	1.54
3	E	551	NDP	PN-O2N	2.10	1.63	1.54
3	B	551	NDP	PN-O2N	2.11	1.64	1.54
3	A	551	NDP	P2B-O2X	2.15	1.62	1.54
3	E	551	NDP	P2B-O2X	2.21	1.62	1.54
4	A	553	GTP	O4'-C4'	2.22	1.50	1.45
4	D	553	GTP	C6-C5	2.23	1.45	1.41
4	A	553	GTP	PG-O2G	2.25	1.62	1.54
3	D	551	NDP	C2N-C3N	2.28	1.40	1.34
4	F	553	GTP	C2-N1	2.32	1.39	1.35
3	E	551	NDP	P2B-O3X	2.33	1.63	1.54
3	F	551	NDP	P2B-O2X	2.38	1.63	1.54
3	C	551	NDP	O4B-C4B	2.42	1.50	1.45
4	C	553	GTP	C6-C5	2.43	1.46	1.41
3	B	551	NDP	PA-O5B	2.46	1.70	1.59
3	F	551	NDP	P2B-O3X	2.46	1.63	1.54
3	E	551	NDP	PA-O5B	2.53	1.70	1.59
4	B	553	GTP	C2'-C3'	2.55	1.60	1.53
4	B	553	GTP	C3'-C4'	2.62	1.60	1.53
4	C	553	GTP	C5'-C4'	2.66	1.60	1.51
5	D	552	GWD	CAF-CAS	2.70	1.38	1.34
3	E	551	NDP	O4D-C1D	2.71	1.48	1.42
4	F	553	GTP	C6-N1	2.74	1.38	1.33
2	A	550	GLU	CB-CA	2.84	1.56	1.53
4	D	553	GTP	C6-N1	2.88	1.38	1.33
4	E	553	GTP	C6-N1	2.91	1.38	1.33
4	C	553	GTP	C6-N1	3.03	1.38	1.33
5	E	552	GWD	CAF-CAS	3.08	1.39	1.34
2	C	550	GLU	CB-CA	3.08	1.56	1.53
4	A	553	GTP	C6-N1	3.14	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	553	GTP	O4'-C1'	3.15	1.45	1.41
3	A	551	NDP	O4D-C1D	3.16	1.49	1.42
5	F	552	GWD	CAF-CAS	3.23	1.39	1.34
3	D	551	NDP	O4D-C1D	3.26	1.50	1.42
5	A	552	GWD	CAF-CAS	3.57	1.39	1.34
3	F	551	NDP	O4D-C1D	3.59	1.51	1.42
5	C	552	GWD	CAF-CAS	3.68	1.40	1.34
3	B	551	NDP	O4D-C1D	3.69	1.51	1.42
3	F	551	NDP	O4B-C1B	3.74	1.45	1.41
5	B	552	GWD	CAF-CAS	3.85	1.40	1.34
3	C	551	NDP	O4D-C1D	3.98	1.51	1.42
3	C	551	NDP	O4B-C1B	4.24	1.46	1.41
4	E	553	GTP	C3'-C4'	4.30	1.64	1.53
3	D	551	NDP	O4B-C1B	4.62	1.47	1.41
4	C	553	GTP	C3'-C4'	4.79	1.65	1.53
3	A	551	NDP	O4B-C1B	4.93	1.47	1.41
3	B	551	NDP	O4B-C1B	5.99	1.48	1.41
4	D	553	GTP	O4'-C1'	6.91	1.49	1.41
3	E	551	NDP	O4B-C1B	7.05	1.50	1.41
4	A	553	GTP	O4'-C1'	7.07	1.50	1.41
4	C	553	GTP	O4'-C1'	8.92	1.52	1.41
4	E	553	GTP	O4'-C1'	9.46	1.53	1.41

All (270) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	553	GTP	C4'-O4'-C1'	-26.67	80.41	109.72
4	F	553	GTP	C4'-O4'-C1'	-24.56	82.74	109.72
4	F	553	GTP	O3A-PA-O5'	-16.31	59.66	102.94
4	D	553	GTP	PA-O3A-PB	-14.87	90.98	132.73
3	A	551	NDP	O3-PA-O5B	-13.26	67.75	102.94
3	C	551	NDP	O3-PA-O5B	-13.01	68.41	102.94
3	F	551	NDP	O3-PA-O5B	-12.72	69.19	102.94
3	B	551	NDP	O3-PA-O5B	-12.40	70.04	102.94
4	A	553	GTP	PA-O3A-PB	-12.40	97.92	132.73
3	D	551	NDP	O3-PA-O5B	-12.31	70.27	102.94
4	C	553	GTP	O4'-C4'-C3'	-12.20	80.57	105.15
4	E	553	GTP	O4'-C4'-C3'	-11.59	81.79	105.15
3	E	551	NDP	O3-PA-O5B	-11.47	72.51	102.94
4	C	553	GTP	O3A-PA-O5'	-11.20	73.23	102.94
4	C	553	GTP	O2G-PG-O1G	-9.97	78.48	110.58
3	D	551	NDP	PN-O3-PA	-9.91	104.89	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	551	NDP	PN-O3-PA	-9.91	104.91	132.73
4	A	553	GTP	PB-O3B-PG	-9.89	99.51	132.67
3	F	551	NDP	N3A-C2A-N1A	-9.85	121.35	128.89
3	B	551	NDP	PN-O3-PA	-9.84	105.09	132.73
3	E	551	NDP	O3-PN-O5D	-9.77	77.02	102.94
3	B	551	NDP	N3A-C2A-N1A	-9.74	121.44	128.89
3	B	551	NDP	O3-PN-O5D	-9.66	77.30	102.94
3	E	551	NDP	PN-O3-PA	-9.65	105.64	132.73
3	F	551	NDP	PN-O3-PA	-9.59	105.78	132.73
4	E	553	GTP	O4'-C4'-C5'	-9.48	75.43	109.32
3	C	551	NDP	N3A-C2A-N1A	-9.42	121.68	128.89
4	C	553	GTP	O4'-C4'-C5'	-9.36	75.83	109.32
3	A	551	NDP	O3-PN-O5D	-9.25	78.39	102.94
3	D	551	NDP	O3-PN-O5D	-9.23	78.46	102.94
3	E	551	NDP	N3A-C2A-N1A	-9.20	121.85	128.89
3	C	551	NDP	PN-O3-PA	-9.18	106.95	132.73
3	A	551	NDP	N3A-C2A-N1A	-9.10	121.93	128.89
4	D	553	GTP	PB-O3B-PG	-8.83	103.08	132.67
3	C	551	NDP	O3-PN-O5D	-8.71	79.82	102.94
3	D	551	NDP	N3A-C2A-N1A	-8.57	122.33	128.89
4	E	553	GTP	O3A-PA-O5'	-8.52	80.33	102.94
3	F	551	NDP	O3-PN-O5D	-8.49	80.41	102.94
4	E	553	GTP	O5'-C5'-C4'	-8.18	78.95	109.12
4	C	553	GTP	O3G-PG-O2G	-7.61	78.39	107.38
4	D	553	GTP	O5'-PA-O1A	-7.42	80.82	109.62
4	C	553	GTP	O5'-C5'-C4'	-7.32	82.13	109.12
3	C	551	NDP	C4B-O4B-C1B	-7.20	101.81	109.72
3	B	551	NDP	P2B-O2B-C2B	-7.20	104.30	121.56
3	C	551	NDP	P2B-O2B-C2B	-6.89	105.04	121.56
4	A	553	GTP	O5'-PA-O1A	-6.80	83.22	109.62
3	E	551	NDP	P2B-O2B-C2B	-6.56	105.82	121.56
3	A	551	NDP	P2B-O2B-C2B	-6.51	105.96	121.56
3	D	551	NDP	C4B-O4B-C1B	-6.29	102.81	109.72
3	F	551	NDP	P2B-O2B-C2B	-6.24	106.61	121.56
3	F	551	NDP	C4B-O4B-C1B	-6.06	103.06	109.72
4	A	553	GTP	C5'-C4'-C3'	-5.85	91.98	115.21
3	D	551	NDP	P2B-O2B-C2B	-5.85	107.54	121.56
3	D	551	NDP	O5D-PN-O1N	-5.62	87.80	109.62
3	E	551	NDP	O5B-PA-O1A	-5.50	88.28	109.62
4	C	553	GTP	O3G-PG-O3B	-5.48	80.21	105.09
3	B	551	NDP	O5B-PA-O1A	-5.48	88.36	109.62
3	F	551	NDP	O5D-PN-O1N	-5.47	88.38	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	551	NDP	O5B-PA-O1A	-5.46	88.42	109.62
4	F	553	GTP	PB-O3B-PG	-5.35	114.74	132.67
3	C	551	NDP	O5D-PN-O1N	-5.30	89.06	109.62
3	C	551	NDP	O5B-PA-O1A	-5.29	89.07	109.62
5	C	552	GWD	CAT-NAL-CAR	-5.23	108.15	111.35
4	B	553	GTP	O3A-PA-O5'	-5.20	89.13	102.94
3	B	551	NDP	C4B-O4B-C1B	-5.16	104.05	109.72
3	A	551	NDP	C4B-O4B-C1B	-5.12	104.10	109.72
3	A	551	NDP	O5D-PN-O1N	-5.05	90.01	109.62
3	E	551	NDP	O5D-PN-O1N	-4.89	90.64	109.62
3	A	551	NDP	O5B-PA-O1A	-4.84	90.83	109.62
3	A	551	NDP	O2N-PN-O5D	-4.81	84.19	108.46
3	C	551	NDP	O4B-C1B-C2B	-4.80	97.92	106.60
3	B	551	NDP	O5D-PN-O1N	-4.80	90.99	109.62
3	B	551	NDP	O2N-PN-O5D	-4.77	84.39	108.46
3	E	551	NDP	O2N-PN-O5D	-4.75	84.49	108.46
3	D	551	NDP	O4B-C1B-C2B	-4.74	98.02	106.60
3	C	551	NDP	O2N-PN-O5D	-4.70	84.78	108.46
5	A	552	GWD	CAT-NAL-CAR	-4.70	108.47	111.35
4	B	553	GTP	PB-O3B-PG	-4.69	116.93	132.67
3	F	551	NDP	O2N-PN-O5D	-4.69	84.80	108.46
3	D	551	NDP	O5B-PA-O1A	-4.66	91.53	109.62
3	A	551	NDP	O4B-C1B-C2B	-4.57	98.34	106.60
5	F	552	GWD	CAT-NAL-CAR	-4.56	108.56	111.35
5	E	552	GWD	CAT-NAL-CAR	-4.51	108.58	111.35
5	B	552	GWD	CAT-NAL-CAR	-4.51	108.59	111.35
5	D	552	GWD	CAT-NAL-CAR	-4.44	108.63	111.35
3	B	551	NDP	O4B-C1B-C2B	-4.41	98.63	106.60
3	E	551	NDP	O4B-C1B-C2B	-4.40	98.63	106.60
4	D	553	GTP	O2A-PA-O5'	-4.39	86.31	108.46
4	F	553	GTP	C5-C6-N1	-4.31	117.70	123.59
3	D	551	NDP	O2N-PN-O5D	-4.28	86.88	108.46
4	A	553	GTP	O2A-PA-O3A	-4.26	85.77	105.09
3	F	551	NDP	O4B-C1B-C2B	-4.23	98.96	106.60
4	C	553	GTP	C5-C6-N1	-4.10	117.98	123.59
4	F	553	GTP	O5'-PA-O1A	-4.09	93.75	109.62
4	D	553	GTP	O2A-PA-O3A	-4.06	86.67	105.09
4	D	553	GTP	C5-C6-N1	-4.00	118.11	123.59
4	C	553	GTP	C1'-N9-C4	-4.00	120.90	126.94
4	E	553	GTP	PB-O3B-PG	-4.00	119.27	132.67
4	E	553	GTP	C2'-C1'-N9	-3.89	108.34	114.29
4	A	553	GTP	O2A-PA-O5'	-3.85	89.03	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	551	NDP	O2A-PA-O5B	-3.81	89.25	108.46
4	C	553	GTP	N3-C2-N1	-3.79	121.68	127.44
4	E	553	GTP	C5-C6-N1	-3.75	118.46	123.59
4	B	553	GTP	O5'-C5'-C4'	-3.75	95.31	109.12
4	E	553	GTP	N3-C2-N1	-3.71	121.80	127.44
4	F	553	GTP	N3-C2-N1	-3.70	121.81	127.44
3	E	551	NDP	O2A-PA-O5B	-3.68	89.90	108.46
4	A	553	GTP	N3-C2-N1	-3.64	121.90	127.44
4	F	553	GTP	O2A-PA-O5'	-3.62	90.19	108.46
4	D	553	GTP	C5'-C4'-C3'	-3.62	100.85	115.21
4	B	553	GTP	C5-C6-N1	-3.58	118.69	123.59
4	A	553	GTP	C5-C6-N1	-3.57	118.70	123.59
4	B	553	GTP	N3-C2-N1	-3.56	122.02	127.44
4	B	553	GTP	O2B-PB-O3A	-3.54	89.02	105.09
3	E	551	NDP	C4B-O4B-C1B	-3.46	105.91	109.72
4	D	553	GTP	N3-C2-N1	-3.43	122.23	127.44
3	A	551	NDP	O2A-PA-O5B	-3.40	91.31	108.46
4	F	553	GTP	PA-O3A-PB	-3.40	123.19	132.73
3	A	551	NDP	C5D-C4D-C3D	-3.36	101.88	115.21
4	E	553	GTP	O2B-PB-O3A	-3.34	89.94	105.09
4	B	553	GTP	C2'-C3'-C4'	-3.33	95.76	102.61
3	F	551	NDP	O2A-PA-O5B	-3.33	91.68	108.46
3	A	551	NDP	C2D-C1D-N1N	-3.27	104.49	113.34
3	C	551	NDP	C4A-C5A-N7A	-3.24	106.50	109.48
4	C	553	GTP	C4-C5-N7	-3.19	106.55	109.48
3	C	551	NDP	O2A-PA-O5B	-3.14	92.61	108.46
3	F	551	NDP	C5D-C4D-C3D	-3.06	103.07	115.21
4	A	553	GTP	C4-C5-N7	-2.99	106.73	109.48
3	B	551	NDP	O2A-PA-O5B	-2.98	93.44	108.46
4	E	553	GTP	C4-C5-N7	-2.92	106.80	109.48
3	D	551	NDP	C5D-C4D-C3D	-2.91	103.67	115.21
4	C	553	GTP	C6-C5-C4	-2.91	117.42	120.90
4	F	553	GTP	O5'-C5'-C4'	-2.86	98.57	109.12
5	A	552	GWD	OAA-CAR-CAS	-2.80	124.25	127.74
5	F	552	GWD	OAA-CAR-CAS	-2.75	124.32	127.74
3	D	551	NDP	C4A-C5A-N7A	-2.72	106.97	109.48
3	A	551	NDP	C4A-C5A-N7A	-2.72	106.98	109.48
5	C	552	GWD	OAA-CAR-CAS	-2.71	124.36	127.74
3	B	551	NDP	C5B-C4B-C3B	-2.71	104.47	115.21
5	D	552	GWD	OAA-CAR-CAS	-2.69	124.39	127.74
3	A	551	NDP	C3N-C2N-N1N	-2.65	119.34	123.14
3	E	551	NDP	C1D-N1N-C6N	-2.63	114.93	120.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	553	GTP	C4-C5-N7	-2.60	107.09	109.48
3	E	551	NDP	C5D-C4D-C3D	-2.58	104.98	115.21
5	E	552	GWD	OAA-CAR-CAS	-2.57	124.54	127.74
3	C	551	NDP	C5D-C4D-C3D	-2.54	105.12	115.21
3	C	551	NDP	C1B-N9A-C4A	-2.48	123.20	126.94
3	A	551	NDP	C1D-N1N-C6N	-2.47	115.28	120.81
4	D	553	GTP	C6-C5-C4	-2.46	117.95	120.90
3	B	551	NDP	C5D-C4D-C3D	-2.46	105.46	115.21
4	C	553	GTP	PB-O3B-PG	-2.42	124.54	132.67
3	C	551	NDP	C2D-C1D-N1N	-2.42	106.81	113.34
3	F	551	NDP	C2D-C1D-N1N	-2.41	106.84	113.34
3	E	551	NDP	C5B-C4B-C3B	-2.40	105.67	115.21
3	F	551	NDP	C4A-C5A-N7A	-2.36	107.31	109.48
4	F	553	GTP	C2'-C3'-C4'	-2.32	97.84	102.61
4	B	553	GTP	PA-O3A-PB	-2.32	126.21	132.73
3	A	551	NDP	C5B-C4B-C3B	-2.29	106.11	115.21
3	E	551	NDP	C2D-C1D-N1N	-2.29	107.15	113.34
3	E	551	NDP	C4A-C5A-N7A	-2.27	107.39	109.48
3	B	551	NDP	C4A-C5A-N7A	-2.26	107.40	109.48
4	A	553	GTP	C6-C5-C4	-2.26	118.20	120.90
5	B	552	GWD	OAA-CAR-CAS	-2.25	124.94	127.74
3	E	551	NDP	C3N-C2N-N1N	-2.23	119.95	123.14
5	A	552	GWD	CAJ-CAT-CAU	-2.23	119.78	122.19
4	C	553	GTP	C2'-C1'-N9	-2.21	110.92	114.29
5	D	552	GWD	CAJ-CAT-CAU	-2.16	119.85	122.19
3	F	551	NDP	C5B-C4B-C3B	-2.16	106.65	115.21
4	F	553	GTP	C4-C5-N7	-2.14	107.51	109.48
4	E	553	GTP	C1'-N9-C4	-2.12	123.74	126.94
3	C	551	NDP	O4D-C4D-C5D	-2.11	101.78	109.32
3	D	551	NDP	C1D-N1N-C6N	-2.06	116.19	120.81
4	B	553	GTP	C6-C5-C4	-2.05	118.44	120.90
4	E	553	GTP	C6-C5-C4	-2.05	118.45	120.90
4	D	553	GTP	C2'-C1'-N9	-2.05	111.17	114.29
3	E	551	NDP	O4D-C4D-C5D	-2.04	102.01	109.32
5	A	552	GWD	CAT-CAU-CAS	-2.04	105.31	106.67
2	C	550	GLU	O-C-CA	-2.03	120.21	125.49
2	D	550	GLU	O-C-CA	-2.01	120.27	125.49
5	E	552	GWD	CAJ-CAT-CAU	-2.00	120.03	122.19
4	C	553	GTP	N2-C2-N1	2.02	120.55	117.20
3	B	551	NDP	O5D-C5D-C4D	2.03	116.59	109.12
4	D	553	GTP	C2'-C3'-C4'	2.03	106.78	102.61
4	A	553	GTP	O4'-C4'-C3'	2.07	109.31	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	551	NDP	O2A-PA-O3	2.08	114.53	105.09
5	F	552	GWD	CAP-CAM-CAO	2.08	119.43	116.52
3	A	551	NDP	O4B-C1B-N9A	2.11	112.53	108.10
4	A	553	GTP	O3G-PG-O2G	2.14	115.54	107.38
4	B	553	GTP	O2B-PB-O3B	2.15	114.86	105.09
4	E	553	GTP	O2B-PB-O3B	2.22	115.18	105.09
5	D	552	GWD	CAP-CAM-CAO	2.24	119.65	116.52
4	F	553	GTP	O2B-PB-O3A	2.26	115.33	105.09
5	E	552	GWD	CAP-CAM-CAO	2.29	119.72	116.52
3	A	551	NDP	O2A-PA-O3	2.32	115.61	105.09
3	E	551	NDP	O5D-C5D-C4D	2.34	117.76	109.12
5	C	552	GWD	CAP-CAM-CAO	2.44	119.92	116.52
3	C	551	NDP	O2N-PN-O3	2.46	116.24	105.09
4	B	553	GTP	O5'-PA-O1A	2.47	119.20	109.62
3	B	551	NDP	O2B-C2B-C1B	2.49	119.74	110.02
3	F	551	NDP	O2A-PA-O3	2.50	116.42	105.09
4	B	553	GTP	C5'-C4'-C3'	2.52	125.19	115.21
4	C	553	GTP	O5'-PA-O1A	2.54	119.47	109.62
4	A	553	GTP	O2A-PA-O1A	2.56	126.43	112.53
5	C	552	GWD	CAU-CAS-CAR	2.57	106.83	105.32
3	D	551	NDP	O2A-PA-O3	2.58	116.78	105.09
3	F	551	NDP	O4B-C1B-N9A	2.59	113.53	108.10
3	F	551	NDP	O2N-PN-O3	2.60	116.87	105.09
5	A	552	GWD	CAP-CAM-CAO	2.61	120.16	116.52
5	B	552	GWD	CAU-CAS-CAR	2.72	106.92	105.32
3	C	551	NDP	O5D-C5D-C4D	2.74	119.22	109.12
5	B	552	GWD	CAP-CAM-CAO	2.74	120.35	116.52
3	E	551	NDP	O2N-PN-O3	2.75	117.56	105.09
3	D	551	NDP	O5D-C5D-C4D	2.76	119.28	109.12
4	D	553	GTP	O4'-C1'-N9	2.77	113.91	108.10
4	E	553	GTP	O5'-PA-O1A	2.78	120.39	109.62
4	A	553	GTP	C6-N1-C2	2.84	119.87	115.94
3	A	551	NDP	O5D-C5D-C4D	2.96	120.04	109.12
4	C	553	GTP	C6-N1-C2	2.97	120.06	115.94
4	A	553	GTP	C2'-C3'-C4'	2.97	108.72	102.61
4	F	553	GTP	C1'-N9-C4	2.98	131.43	126.94
3	F	551	NDP	O5D-C5D-C4D	2.98	120.12	109.12
4	A	553	GTP	O4'-C1'-N9	2.99	114.36	108.10
3	D	551	NDP	O4B-C1B-N9A	3.00	114.38	108.10
3	A	551	NDP	O2N-PN-O3	3.02	118.78	105.09
3	B	551	NDP	O2N-PN-O3	3.03	118.83	105.09
4	D	553	GTP	C6-N1-C2	3.06	120.19	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	551	NDP	O4D-C1D-N1N	3.12	114.65	108.07
4	F	553	GTP	C6-N1-C2	3.21	120.39	115.94
4	B	553	GTP	C6-N1-C2	3.25	120.44	115.94
4	C	553	GTP	O2B-PB-O3A	3.26	119.90	105.09
4	E	553	GTP	C6-N1-C2	3.28	120.49	115.94
3	B	551	NDP	O4D-C1D-N1N	3.42	115.29	108.07
3	D	551	NDP	O4D-C1D-N1N	3.58	115.63	108.07
4	F	553	GTP	O2A-PA-O3A	3.64	121.60	105.09
4	C	553	GTP	PA-O3A-PB	4.01	144.00	132.73
3	A	551	NDP	O4D-C1D-N1N	4.06	116.64	108.07
3	E	551	NDP	O4D-C1D-N1N	4.07	116.66	108.07
3	E	551	NDP	C2D-C3D-C4D	4.11	111.06	102.61
3	A	551	NDP	C2D-C3D-C4D	4.16	111.17	102.61
4	B	553	GTP	O4'-C4'-C5'	4.30	124.71	109.32
3	C	551	NDP	O4B-C1B-N9A	4.38	117.27	108.10
5	B	552	GWD	CAS-CAR-NAL	4.41	109.39	106.98
3	B	551	NDP	C2D-C3D-C4D	4.41	111.68	102.61
3	D	551	NDP	C2D-C3D-C4D	4.43	111.71	102.61
3	C	551	NDP	O4D-C1D-N1N	4.52	117.60	108.07
3	C	551	NDP	C2D-C3D-C4D	4.62	112.10	102.61
4	B	553	GTP	C1'-N9-C4	4.62	133.91	126.94
3	F	551	NDP	C2D-C3D-C4D	4.64	112.14	102.61
5	F	552	GWD	CAS-CAR-NAL	4.71	109.56	106.98
5	C	552	GWD	CAS-CAR-NAL	4.78	109.60	106.98
5	A	552	GWD	CAS-CAR-NAL	4.94	109.68	106.98
4	C	553	GTP	O2G-PG-O3B	5.14	128.43	105.09
4	F	553	GTP	O4'-C4'-C5'	5.15	127.75	109.32
5	D	552	GWD	CAS-CAR-NAL	5.16	109.81	106.98
5	E	552	GWD	CAS-CAR-NAL	5.34	109.91	106.98
4	D	553	GTP	O5'-C5'-C4'	5.72	130.20	109.12
4	C	553	GTP	O3G-PG-O1G	5.76	129.12	110.58
4	B	553	GTP	C2'-C1'-N9	5.79	123.14	114.29
4	F	553	GTP	C2'-C1'-N9	5.82	123.19	114.29
4	C	553	GTP	C2'-C3'-C4'	5.98	114.91	102.61
4	E	553	GTP	C2'-C3'-C4'	6.17	115.29	102.61
4	A	553	GTP	O5'-C5'-C4'	7.39	136.34	109.12
4	F	553	GTP	O4'-C1'-N9	7.41	123.62	108.10
4	E	553	GTP	O4'-C1'-N9	7.46	123.71	108.10
4	B	553	GTP	O4'-C1'-N9	8.68	126.27	108.10
4	C	553	GTP	O4'-C1'-N9	9.12	127.19	108.10
4	C	553	GTP	C5'-C4'-C3'	9.83	154.24	115.21
4	E	553	GTP	C5'-C4'-C3'	10.15	155.49	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	553	GTP	O3A-PA-O5'	18.69	152.52	102.94
4	A	553	GTP	O3A-PA-O5'	19.67	155.13	102.94

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	553	GTP	C4'
4	E	553	GTP	C4'

There are no torsion outliers.

There are no ring outliers.

22 monomers are involved in 78 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	550	GLU	1	0
3	A	551	NDP	6	0
5	A	552	GWD	3	0
4	A	553	GTP	1	0
2	B	550	GLU	2	0
3	B	551	NDP	8	0
5	B	552	GWD	5	0
4	B	553	GTP	2	0
2	C	550	GLU	2	0
3	C	551	NDP	9	0
5	C	552	GWD	3	0
2	D	550	GLU	1	0
3	D	551	NDP	5	0
5	D	552	GWD	7	0
4	D	553	GTP	2	0
2	E	550	GLU	3	0
3	E	551	NDP	6	0
5	E	552	GWD	5	0
4	E	553	GTP	3	0
3	F	551	NDP	7	0
5	F	552	GWD	3	0
4	F	553	GTP	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	501/501 (100%)	0.88	62 (12%) 5 5	26, 46, 68, 78	0
1	B	501/501 (100%)	0.98	63 (12%) 5 5	26, 47, 69, 78	0
1	C	501/501 (100%)	0.58	27 (5%) 29 33	22, 45, 67, 78	0
1	D	501/501 (100%)	0.87	58 (11%) 6 6	24, 46, 69, 78	0
1	E	501/501 (100%)	0.98	63 (12%) 5 5	28, 48, 69, 78	0
1	F	501/501 (100%)	0.80	51 (10%) 9 9	24, 46, 68, 78	0
All	All	3006/3006 (100%)	0.85	324 (10%) 8 8	22, 47, 69, 78	0

All (324) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	498	VAL	12.1
1	F	500	PHE	12.0
1	D	499	THR	11.6
1	E	497	GLY	10.8
1	A	499	THR	10.7
1	E	499	THR	10.3
1	D	500	PHE	10.2
1	B	501	THR	9.5
1	E	37	THR	9.3
1	F	499	THR	9.2
1	F	1	ALA	9.0
1	A	426	GLY	8.8
1	F	501	THR	8.8
1	C	501	THR	8.6
1	C	1	ALA	8.4
1	C	426	GLY	8.4
1	D	501	THR	8.0
1	B	1	ALA	8.0
1	A	500	PHE	7.9

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Mol	Chain	Res	Type	RSRZ
1	B	496	ALA	7.7
1	D	498	VAL	7.6
1	E	496	ALA	7.5
1	C	424	HIS	7.5
1	B	3	ARG	7.4
1	E	501	THR	7.4
1	B	497	GLY	6.8
1	E	424	HIS	6.8
1	B	500	PHE	6.7
1	D	425	GLY	6.4
1	D	424	HIS	6.4
1	A	501	THR	6.3
1	E	1	ALA	6.3
1	C	500	PHE	6.0
1	A	35	ARG	5.9
1	B	35	ARG	5.8
1	B	425	GLY	5.8
1	F	34	THR	5.7
1	F	33	LYS	5.6
1	D	496	ALA	5.6
1	E	271	VAL	5.6
1	A	424	HIS	5.5
1	A	497	GLY	5.5
1	B	499	THR	5.5
1	A	3	ARG	5.4
1	A	425	GLY	5.4
1	B	424	HIS	5.3
1	A	32	LEU	5.3
1	A	34	THR	5.2
1	C	425	GLY	5.1
1	C	190	TYR	5.0
1	F	3	ARG	5.0
1	F	498	VAL	5.0
1	F	496	ALA	5.0
1	F	35	ARG	5.0
1	D	37	THR	4.9
1	C	3	ARG	4.9
1	A	496	ALA	4.9
1	F	424	HIS	4.9
1	B	37	THR	4.9
1	C	37	THR	4.8
1	A	70	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	E	426	GLY	4.7
1	A	419	ARG	4.7
1	B	2	ASP	4.7
1	A	423	LYS	4.7
1	D	41	LYS	4.6
1	E	35	ARG	4.6
1	F	425	GLY	4.6
1	D	35	ARG	4.5
1	F	339	VAL	4.5
1	B	33	LYS	4.5
1	B	426	GLY	4.5
1	E	303	GLY	4.5
1	D	497	GLY	4.5
1	F	426	GLY	4.5
1	F	32	LEU	4.4
1	B	32	LEU	4.4
1	E	500	PHE	4.3
1	A	190	TYR	4.3
1	E	272	ALA	4.2
1	C	34	THR	4.2
1	F	37	THR	4.2
1	D	40	GLN	4.2
1	A	37	THR	4.2
1	D	1	ALA	4.2
1	A	421	PHE	4.2
1	E	2	ASP	4.2
1	D	32	LEU	4.1
1	F	190	TYR	4.1
1	B	87	THR	4.1
1	C	2	ASP	4.1
1	E	4	GLU	4.0
1	F	4	GLU	4.0
1	A	1	ALA	3.9
1	D	34	THR	3.9
1	A	87	THR	3.9
1	B	31	ASP	3.9
1	E	281	TRP	3.8
1	B	88	PRO	3.8
1	A	498	VAL	3.8
1	F	39	GLU	3.8
1	D	426	GLY	3.8
1	E	30	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	498	VAL	3.7
1	C	87	THR	3.7
1	E	359	ILE	3.7
1	B	38	GLU	3.7
1	E	36	GLU	3.7
1	E	285	GLY	3.7
1	E	278	GLY	3.6
1	E	34	THR	3.6
1	F	87	THR	3.6
1	A	33	LYS	3.6
1	D	87	THR	3.6
1	B	469	MET	3.5
1	E	190	TYR	3.5
1	D	339	VAL	3.5
1	C	35	ARG	3.5
1	B	39	GLU	3.5
1	D	281	TRP	3.4
1	A	422	GLY	3.4
1	F	360	PHE	3.4
1	B	44	ARG	3.4
1	A	24	VAL	3.4
1	D	72	TRP	3.4
1	E	297	GLN	3.3
1	B	42	ARG	3.3
1	B	274	GLY	3.3
1	F	311	GLU	3.3
1	B	190	TYR	3.3
1	C	499	THR	3.3
1	A	39	GLU	3.3
1	A	196	ALA	3.3
1	D	46	ARG	3.3
1	B	72	TRP	3.2
1	B	339	VAL	3.2
1	D	462	ARG	3.2
1	B	11	LYS	3.2
1	A	44	ARG	3.2
1	E	423	LYS	3.2
1	E	425	GLY	3.2
1	D	283	PRO	3.2
1	D	284	ASP	3.2
1	D	39	GLU	3.1
1	E	355	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	497	GLY	3.1
1	F	2	ASP	3.1
1	E	312	GLY	3.1
1	E	318	ASP	3.1
1	B	358	LYS	3.1
1	D	314	ILE	3.1
1	A	40	GLN	3.0
1	E	311	GLU	3.0
1	F	29	VAL	3.0
1	D	31	ASP	3.0
1	E	339	VAL	3.0
1	B	462	ARG	3.0
1	A	41	LYS	3.0
1	D	66	ARG	3.0
1	E	304	PHE	3.0
1	B	430	ILE	3.0
1	D	38	GLU	3.0
1	B	40	GLN	2.9
1	C	66	ARG	2.9
1	E	72	TRP	2.9
1	F	88	PRO	2.9
1	A	19	ARG	2.9
1	C	423	LYS	2.9
1	A	88	PRO	2.9
1	B	46	ARG	2.9
1	D	29	VAL	2.9
1	B	421	PHE	2.9
1	E	87	THR	2.9
1	F	40	GLN	2.9
1	B	362	GLU	2.9
1	B	34	THR	2.9
1	D	3	ARG	2.9
1	B	389	LEU	2.9
1	E	39	GLU	2.9
1	D	230	ALA	2.9
1	A	462	ARG	2.8
1	D	42	ARG	2.8
1	E	3	ARG	2.8
1	B	4	GLU	2.8
1	D	285	GLY	2.8
1	D	311	GLU	2.8
1	D	421	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	385	TRP	2.8
1	A	389	LEU	2.8
1	D	190	TYR	2.8
1	D	88	PRO	2.8
1	F	66	ARG	2.8
1	D	244	ASP	2.8
1	A	192	ILE	2.7
1	A	66	ARG	2.7
1	A	490	PHE	2.7
1	A	284	ASP	2.7
1	E	31	ASP	2.7
1	F	38	GLU	2.7
1	A	390	ASN	2.7
1	D	30	GLU	2.7
1	A	386	LEU	2.7
1	B	281	TRP	2.7
1	D	271	VAL	2.7
1	F	423	LYS	2.7
1	E	32	LEU	2.6
1	E	334	SER	2.6
1	A	29	VAL	2.6
1	C	421	PHE	2.6
1	E	24	VAL	2.6
1	F	421	PHE	2.6
1	B	297	GLN	2.6
1	D	28	LEU	2.6
1	A	30	GLU	2.6
1	E	290	GLU	2.6
1	F	419	ARG	2.6
1	E	6	ASP	2.5
1	A	47	GLY	2.5
1	D	36	GLU	2.5
1	E	88	PRO	2.5
1	D	33	LYS	2.5
1	A	72	TRP	2.5
1	A	4	GLU	2.5
1	A	495	GLU	2.5
1	D	43	ASN	2.5
1	F	390	ASN	2.5
1	D	317	VAL	2.5
1	D	312	GLY	2.5
1	B	296	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	19	ARG	2.5
1	B	311	GLU	2.5
1	F	312	GLY	2.5
1	E	340	LYS	2.4
1	E	428	ILE	2.4
1	F	30	GLU	2.4
1	E	308	LYS	2.4
1	D	2	ASP	2.4
1	E	269	LYS	2.4
1	A	311	GLU	2.4
1	E	298	HIS	2.4
1	E	267	GLY	2.4
1	F	495	GLU	2.4
1	A	339	VAL	2.4
1	F	332	THR	2.4
1	F	319	CYS	2.4
1	D	277	ASP	2.4
1	C	88	PRO	2.3
1	B	423	LYS	2.3
1	C	497	GLY	2.3
1	E	419	ARG	2.3
1	F	36	GLU	2.3
1	A	193	ASN	2.3
1	B	472	ASN	2.3
1	C	19	ARG	2.3
1	E	462	ARG	2.3
1	C	496	ALA	2.3
1	E	187	ILE	2.3
1	F	284	ASP	2.3
1	B	41	LYS	2.3
1	F	302	LEU	2.3
1	A	188	GLY	2.3
1	C	38	GLU	2.3
1	E	332	THR	2.3
1	F	308	LYS	2.3
1	A	391	HIS	2.3
1	B	162	VAL	2.3
1	A	191	ASP	2.3
1	C	31	ASP	2.3
1	C	333	LYS	2.3
1	A	197	CYS	2.3
1	A	392	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	36	GLU	2.2
1	B	22	SER	2.2
1	B	298	HIS	2.2
1	A	68	ASP	2.2
1	F	28	LEU	2.2
1	F	361	LEU	2.2
1	A	46	ARG	2.2
1	C	498	VAL	2.2
1	D	44	ARG	2.2
1	D	310	TYR	2.2
1	F	31	ASP	2.2
1	F	386	LEU	2.2
1	A	65	ILE	2.2
1	E	69	ASP	2.2
1	A	69	ASP	2.2
1	E	286	ILE	2.2
1	B	308	LYS	2.2
1	E	10	PHE	2.2
1	B	466	ARG	2.2
1	B	359	ILE	2.2
1	D	229	GLU	2.2
1	D	495	GLU	2.2
1	B	283	PRO	2.2
1	B	99	VAL	2.2
1	F	238	MET	2.2
1	F	72	TRP	2.2
1	A	2	ASP	2.2
1	A	38	GLU	2.1
1	F	44	ARG	2.1
1	D	239	THR	2.1
1	B	36	GLU	2.1
1	F	227	ILE	2.1
1	E	362	GLU	2.1
1	A	302	LEU	2.1
1	E	302	LEU	2.1
1	D	89	CYS	2.1
1	C	102	ASP	2.1
1	D	469	MET	2.1
1	B	43	ASN	2.1
1	E	363	ARG	2.1
1	B	161	GLY	2.1
1	E	5	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	356	ALA	2.1
1	B	385	TRP	2.1
1	B	428	ILE	2.0
1	C	428	ILE	2.0
1	E	243	GLY	2.0
1	B	365	ILE	2.0
1	F	389	LEU	2.0
1	B	112	THR	2.0
1	B	332	THR	2.0
1	E	331	LEU	2.0
1	D	269	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	GWD	A	552	21/21	0.37	0.40	7.64	85,102,111,118	0
5	GWD	C	552	21/21	0.42	0.35	7.44	83,101,110,116	0
5	GWD	F	552	21/21	0.47	0.37	6.13	83,101,109,117	0
5	GWD	B	552	21/21	0.41	0.34	5.83	85,101,110,117	0
5	GWD	D	552	21/21	0.37	0.37	5.48	80,101,110,118	0
4	GTP	F	553	32/32	0.79	0.29	4.94	58,64,69,72	0
2	GLU	E	550	9/10	0.88	0.32	4.42	48,52,55,56	0
4	GTP	B	553	32/32	0.76	0.30	4.37	61,66,72,73	0
4	GTP	D	553	32/32	0.80	0.25	4.00	47,60,69,70	0
5	GWD	E	552	21/21	0.46	0.37	3.91	88,102,111,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	GLU	D	550	9/10	0.86	0.30	3.80	38,43,49,50	0
2	GLU	B	550	9/10	0.86	0.29	3.28	39,44,48,49	0
3	NDP	C	551	48/48	0.87	0.25	2.72	36,48,54,65	0
3	NDP	A	551	48/48	0.87	0.23	2.32	48,53,59,67	0
4	GTP	E	553	32/32	0.82	0.26	1.88	65,69,73,76	0
4	GTP	A	553	32/32	0.85	0.21	1.87	46,59,64,68	0
2	GLU	A	550	9/10	0.93	0.23	1.58	37,40,48,48	0
4	GTP	C	553	32/32	0.92	0.19	1.50	44,50,57,62	0
3	NDP	E	551	48/48	0.84	0.23	1.49	55,61,68,72	0
3	NDP	D	551	48/48	0.89	0.24	1.28	44,49,57,63	0
3	NDP	B	551	48/48	0.86	0.24	1.04	48,55,62,65	0
2	GLU	F	550	9/10	0.92	0.19	0.93	27,33,40,41	0
3	NDP	F	551	48/48	0.86	0.21	0.82	45,53,61,63	0
2	GLU	C	550	9/10	0.93	0.18	0.55	26,32,35,37	0

6.5 Other polymers

There are no such residues in this entry.