Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:30 AM GMT

PDB ID	:	3ETD
Title	:	Structure of glutamate dehydrogenase complexed with bithionol
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:

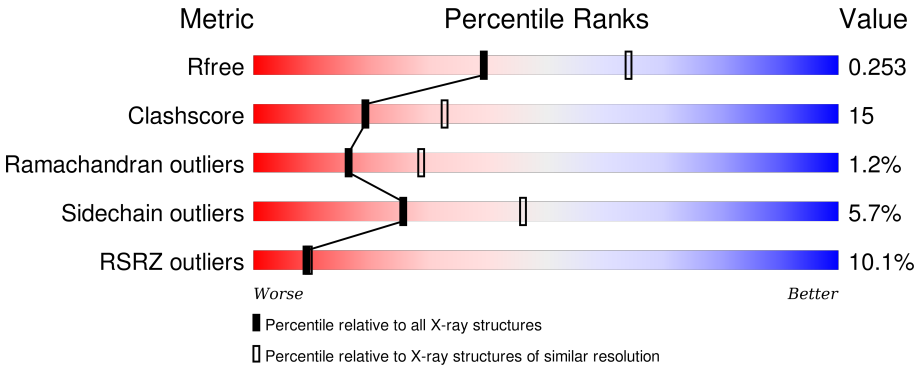
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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% 70% 26% ·
1	B	501	8% 70% 26% ·
1	C	501	7% 69% 27% ·
1	D	501	9% 71% 26% ·
1	E	501	10% 70% 26% ·

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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	A	550	-	-	-	X
2	GLU	D	550	-	-	X	-
2	GLU	E	550	-	-	X	X
3	NDP	D	551	-	-	-	X
4	GTP	A	553	-	-	-	X
4	GTP	B	553	-	-	-	X
4	GTP	C	553	-	-	-	X
4	GTP	D	553	-	-	-	X
4	GTP	E	553	X	-	-	X
4	GTP	F	553	-	-	-	X
5	B1T	A	552	-	-	-	X
5	B1T	B	552	-	-	-	X
5	B1T	C	552	-	-	-	X
5	B1T	F	552	-	-	-	X

2 Entry composition

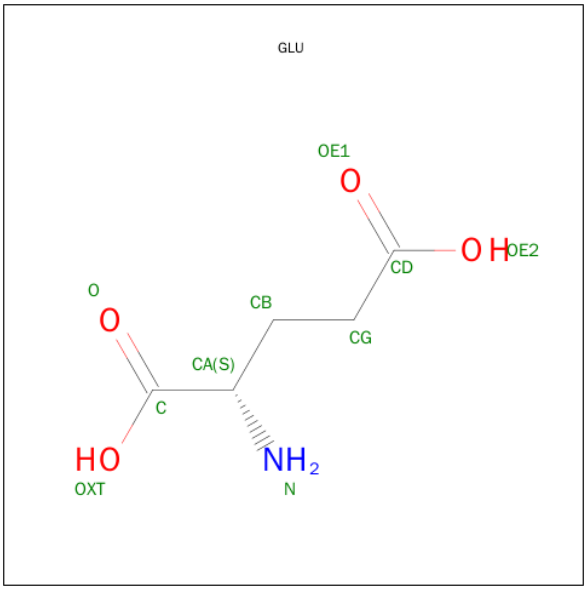
There are 6 unique types of molecules in this entry. The entry contains 24226 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUD1 protein.

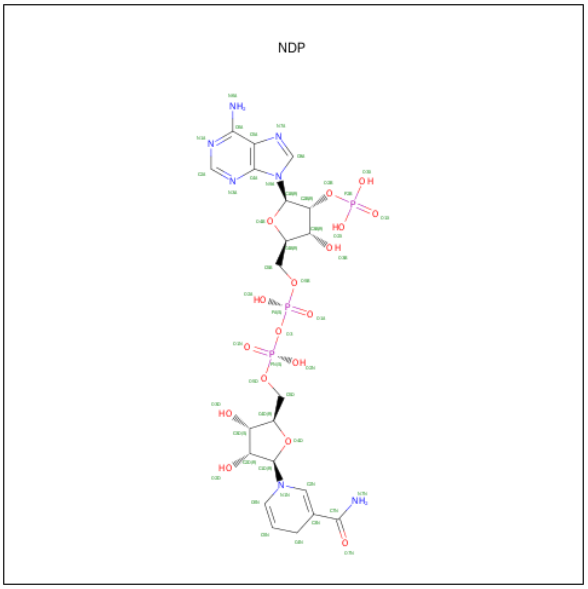
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			3915	2473	687	736	19			
1	B	501	Total	C	N	O	S	0	0	0
			3915	2473	687	736	19			
1	C	501	Total	C	N	O	S	0	0	0
			3915	2473	687	736	19			
1	D	501	Total	C	N	O	S	0	0	0
			3915	2473	687	736	19			
1	E	501	Total	C	N	O	S	0	0	0
			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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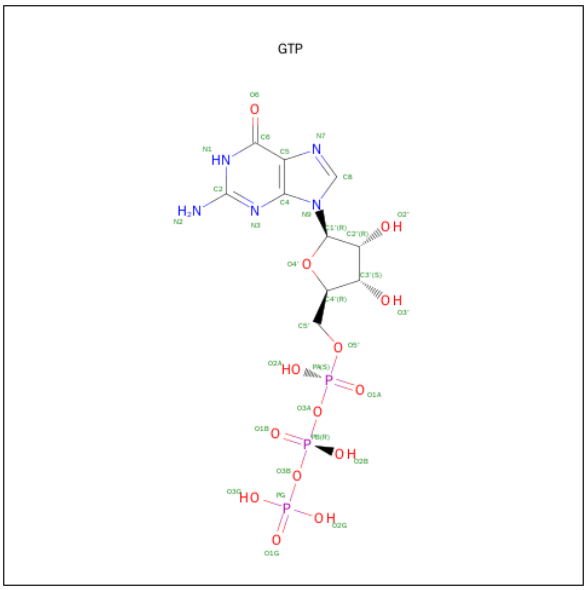
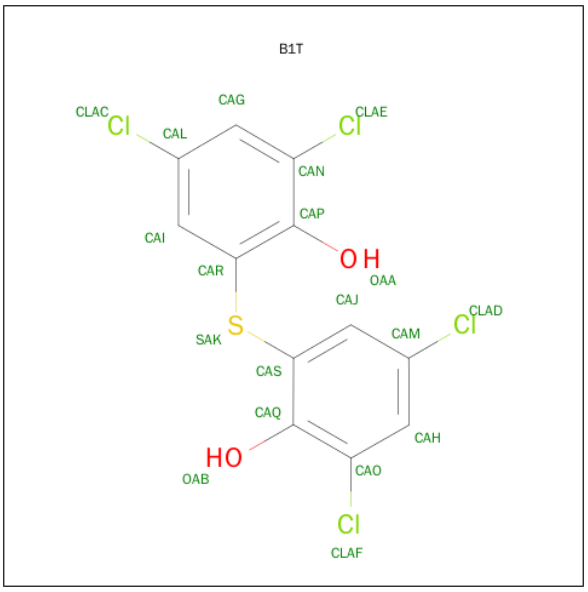
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- 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 2,2'-SULFANEDIYLBIS(4,6-DICHLOROPHENOL) (three-letter code: B1T) (formula: $C_{12}H_6Cl_4O_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Cl	O	S	0	0
			19	12	4	2	1		
5	B	1	Total	C	Cl	O	S	0	0
			19	12	4	2	1		
5	C	1	Total	C	Cl	O	S	0	0
			19	12	4	2	1		
5	D	1	Total	C	Cl	O	S	0	0
			19	12	4	2	1		
5	E	1	Total	C	Cl	O	S	0	0
			19	12	4	2	1		
5	F	1	Total	C	Cl	O	S	0	0
			19	12	4	2	1		

- Molecule 6 is water.

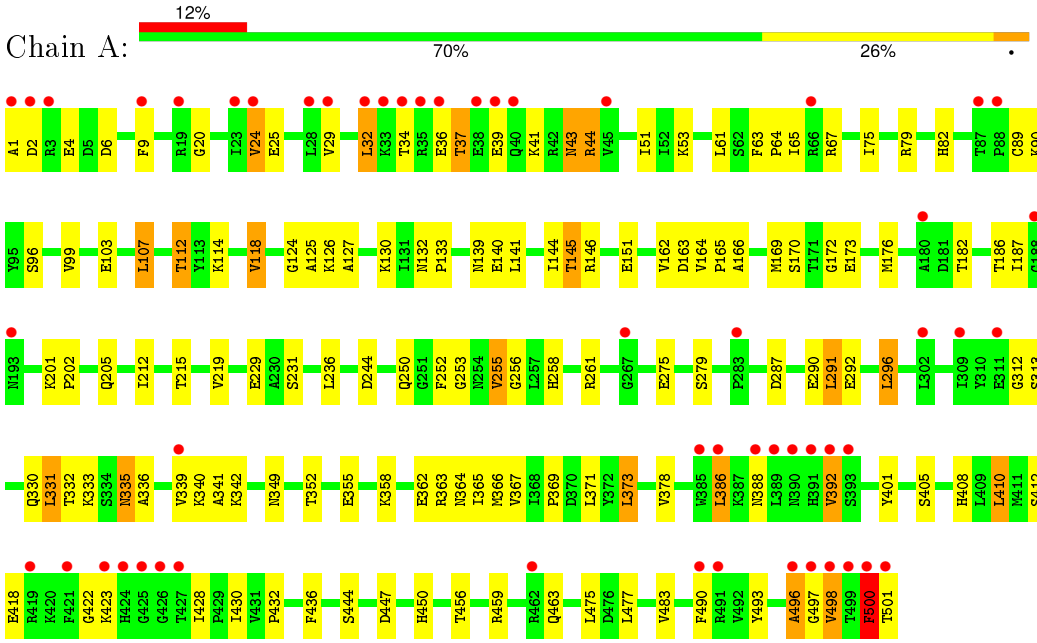
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	13	Total	O	0	0
			13	13		
6	B	17	Total	O	0	0
			17	17		
6	C	19	Total	O	0	0
			19	19		
6	D	20	Total	O	0	0
			20	20		
6	E	13	Total	O	0	0
			13	13		
6	F	6	Total	O	0	0
			6	6		

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.

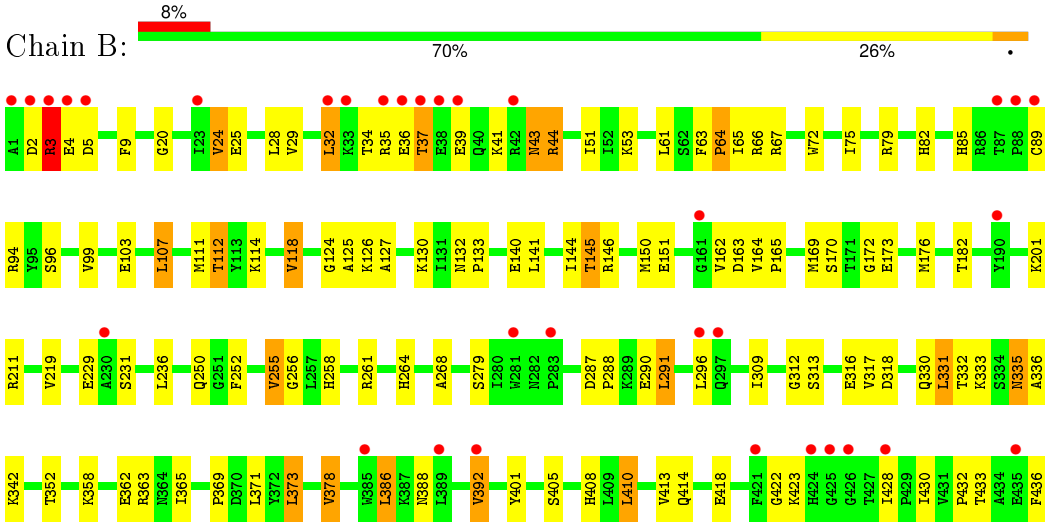
- Molecule 1: GLUD1 protein

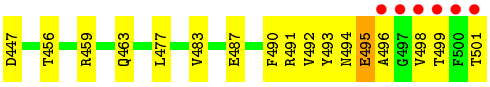
Chain A:



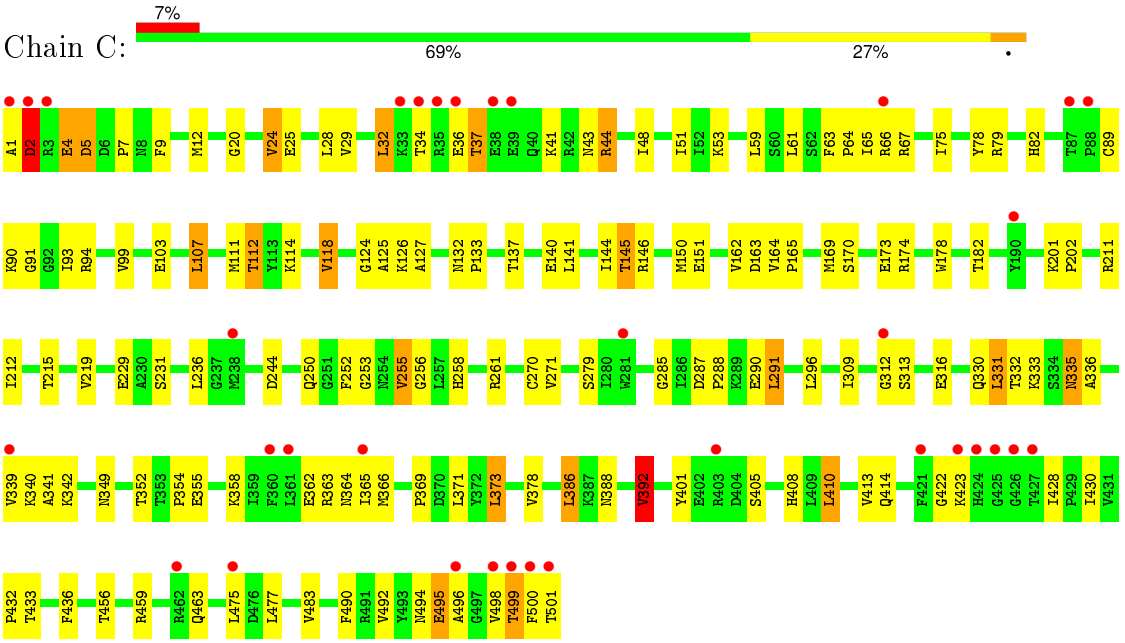
- Molecule 1: GLUD1 protein

Chain B:

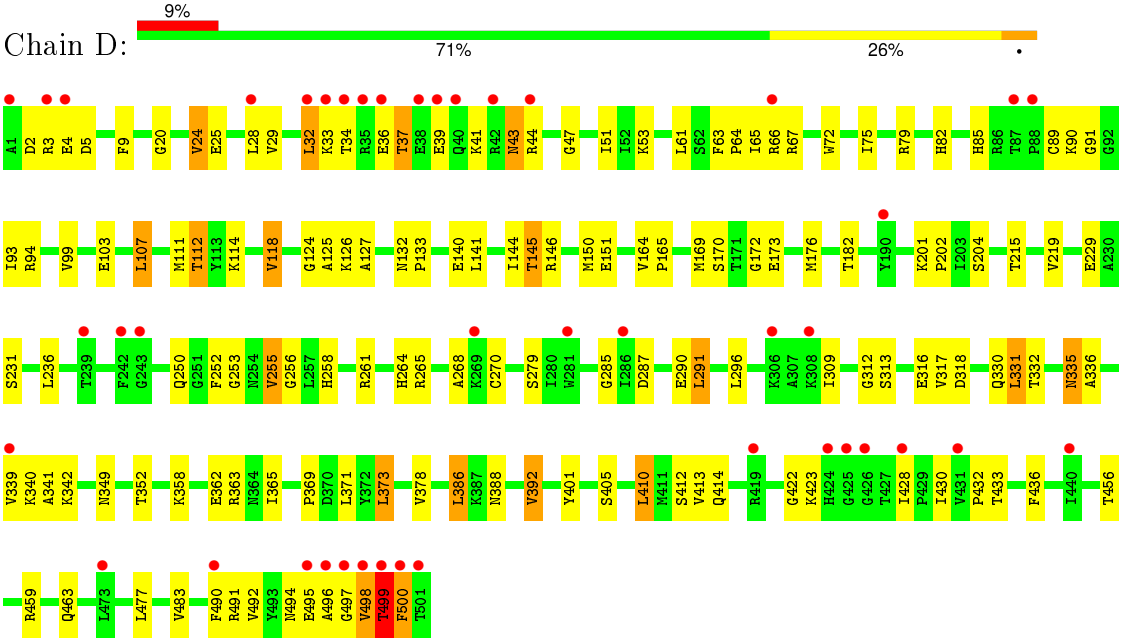




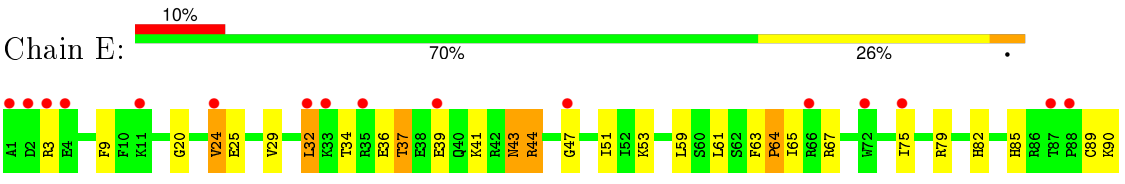
• Molecule 1: GLUD1 protein

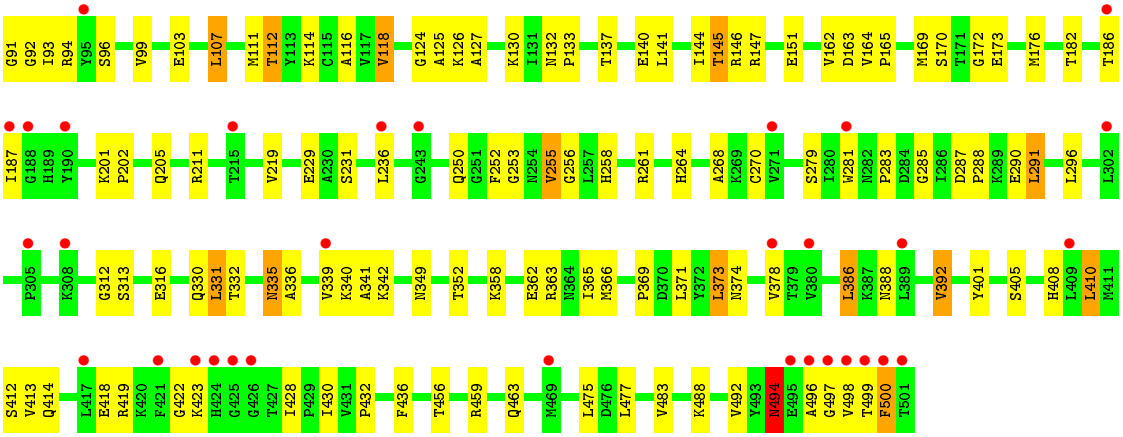


• Molecule 1: GLUD1 protein



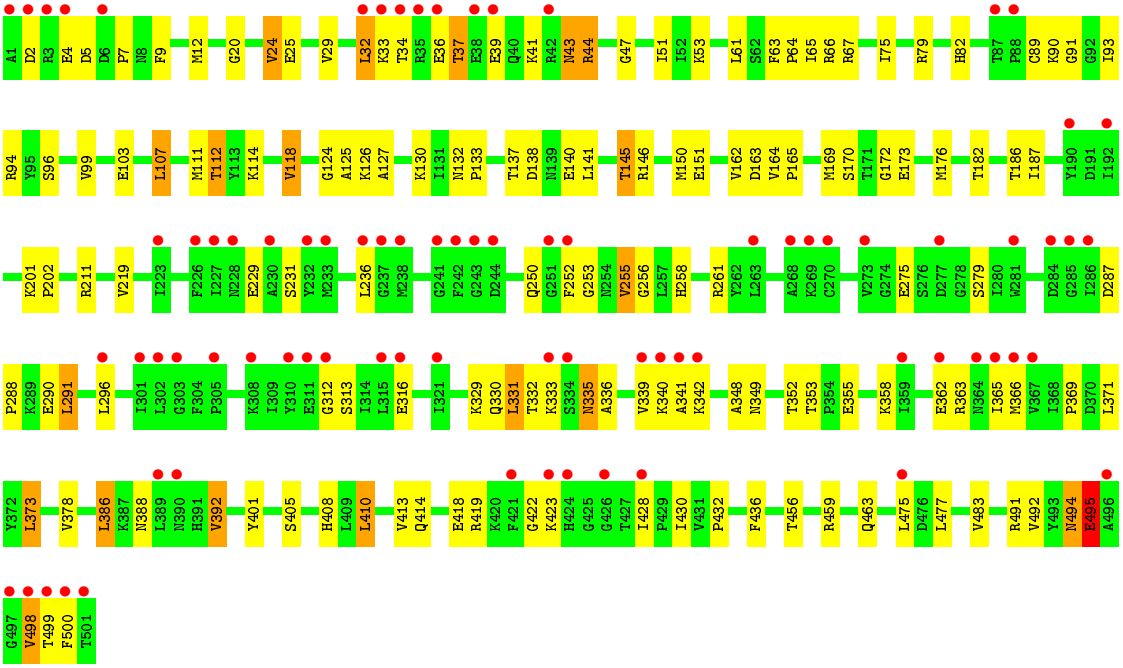
• Molecule 1: GLUD1 protein





- Molecule 1: GLUD1 protein

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	122.38Å 101.30Å 166.59Å 90.00° 102.46° 90.00°	Depositor
Resolution (Å)	48.34 – 2.50 48.36 – 2.49	Depositor EDS
% Data completeness (in resolution range)	94.7 (48.34-2.50) 94.1 (48.36-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.239 , 0.257 0.234 , 0.253	Depositor DCC
R_{free} test set	6941 reflections (5.61%)	DCC
Wilson B-factor (Å^2)	51.1	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 36.9	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 137717 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	24226	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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, NDP, B1T

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	0.74	3/5396 (0.1%)
1	B	0.44	0/3998	0.91	6/5396 (0.1%)
1	C	0.44	0/3998	0.73	4/5396 (0.1%)
1	D	0.43	0/3998	0.79	3/5396 (0.1%)
1	E	0.43	0/3998	0.73	4/5396 (0.1%)
1	F	0.43	0/3998	0.86	6/5396 (0.1%)
All	All	0.44	0/23988	0.80	26/32376 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	419	ARG	NE-CZ-NH1	-22.85	108.87	120.30
1	F	419	ARG	NE-CZ-NH2	21.56	131.08	120.30
1	B	35	ARG	NE-CZ-NH1	-21.50	109.55	120.30
1	B	35	ARG	NE-CZ-NH2	21.09	130.85	120.30
1	B	44	ARG	NE-CZ-NH1	-19.57	110.51	120.30
1	D	44	ARG	NE-CZ-NH1	-18.97	110.81	120.30
1	B	44	ARG	NE-CZ-NH2	18.92	129.76	120.30
1	D	44	ARG	NE-CZ-NH2	18.54	129.57	120.30
1	A	44	ARG	NE-CZ-NH2	-11.39	114.60	120.30
1	F	44	ARG	NE-CZ-NH2	-11.11	114.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	44	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	F	419	ARG	CD-NE-CZ	10.70	138.58	123.60
1	C	44	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	C	44	ARG	NE-CZ-NH1	10.47	125.53	120.30
1	F	44	ARG	NE-CZ-NH1	10.46	125.53	120.30
1	E	44	ARG	NE-CZ-NH2	-10.19	115.21	120.30
1	B	44	ARG	CD-NE-CZ	10.03	137.64	123.60
1	D	44	ARG	CD-NE-CZ	10.02	137.63	123.60
1	B	35	ARG	CD-NE-CZ	9.90	137.46	123.60
1	E	44	ARG	NE-CZ-NH1	9.59	125.10	120.30
1	F	44	ARG	CD-NE-CZ	5.79	131.70	123.60
1	A	44	ARG	CD-NE-CZ	5.68	131.55	123.60
1	C	44	ARG	CD-NE-CZ	5.57	131.40	123.60
1	E	44	ARG	CD-NE-CZ	5.37	131.12	123.60
1	C	392	VAL	CB-CA-C	-5.08	101.75	111.40
1	E	419	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	500	PHE	Sidechain

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	124	0
1	B	3915	0	3880	127	0
1	C	3915	0	3880	125	0
1	D	3915	0	3880	124	0
1	E	3915	0	3880	131	0
1	F	3915	0	3880	123	0
2	A	9	0	5	1	0
2	B	9	0	5	3	0
2	C	9	0	5	0	0
2	D	9	0	5	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	9	0	5	5	0
2	F	9	0	5	2	0
3	A	48	0	26	8	0
3	B	48	0	26	5	0
3	C	48	0	26	6	0
3	D	48	0	26	8	0
3	E	48	0	26	8	0
3	F	48	0	26	9	0
4	A	32	0	12	2	0
4	B	32	0	10	1	0
4	C	32	0	12	1	0
4	D	32	0	12	1	0
4	E	32	0	12	0	0
4	F	32	0	12	0	0
5	A	19	0	4	2	0
5	B	19	0	4	2	0
5	C	19	0	4	3	0
5	D	19	0	4	4	0
5	E	19	0	4	1	0
5	F	19	0	4	2	0
6	A	13	0	0	1	0
6	B	17	0	0	0	0
6	C	19	0	0	0	0
6	D	20	0	0	2	0
6	E	13	0	0	1	0
6	F	6	0	0	1	0
All	All	24226	0	23560	724	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 15.

All (724) 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:F:5:ASP:OD2	1:F:332:THR:HB	1.59	1.00
1:B:3:ARG:HH11	1:B:3:ARG:HG3	1.26	1.00
1:D:332:THR:H	1:D:335:ASN:HD21	1.12	0.98
1:C:150:MET:HG3	5:C:552:B1T:CLAE	2.03	0.95
1:B:150:MET:HG3	5:B:552:B1T:CLAE	2.04	0.94
1:E:332:THR:H	1:E:335:ASN:HD21	1.16	0.93
1:B:332:THR:H	1:B:335:ASN:HD21	1.17	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:THR:H	1:A:335:ASN:HD21	1.16	0.91
1:D:112:THR:HG22	1:D:124:GLY:HA3	1.52	0.91
1:F:150:MET:HG3	5:F:552:B1T:CLAE	2.08	0.90
1:C:332:THR:H	1:C:335:ASN:HD21	1.15	0.90
1:F:332:THR:H	1:F:335:ASN:HD21	1.16	0.90
1:F:112:THR:HG22	1:F:124:GLY:HA3	1.53	0.90
1:B:34:THR:HG22	1:B:36:GLU:H	1.38	0.89
1:B:112:THR:HG22	1:B:124:GLY:CA	2.03	0.88
1:B:112:THR:HG22	1:B:124:GLY:HA3	1.53	0.88
1:E:34:THR:HG22	1:E:36:GLU:H	1.39	0.88
1:C:112:THR:HG22	1:C:124:GLY:HA3	1.54	0.88
1:A:34:THR:HG22	1:A:36:GLU:H	1.38	0.88
1:F:250:GLN:HE22	1:F:330:GLN:HE21	1.22	0.87
1:C:250:GLN:HE22	1:C:330:GLN:HE21	1.22	0.87
1:D:250:GLN:HE22	1:D:330:GLN:HE21	1.22	0.87
1:D:34:THR:HG22	1:D:36:GLU:H	1.39	0.87
1:D:32:LEU:HD23	1:D:494:ASN:HD21	1.40	0.86
1:C:34:THR:HG22	1:C:36:GLU:H	1.37	0.86
1:F:34:THR:HG22	1:F:36:GLU:H	1.37	0.86
1:B:211:ARG:HH22	3:B:551:NDP:H71N	1.24	0.86
1:E:112:THR:HG22	1:E:124:GLY:CA	2.06	0.86
1:F:112:THR:HG22	1:F:124:GLY:CA	2.06	0.86
1:A:112:THR:HG22	1:A:124:GLY:HA3	1.57	0.86
1:E:126:LYS:HZ3	2:E:550:GLU:N	1.73	0.85
1:D:112:THR:HG22	1:D:124:GLY:CA	2.05	0.85
1:E:112:THR:HG22	1:E:124:GLY:HA3	1.57	0.85
1:A:250:GLN:HE22	1:A:330:GLN:HE21	1.24	0.85
1:C:112:THR:HG22	1:C:124:GLY:CA	2.06	0.84
1:A:112:THR:HG22	1:A:124:GLY:CA	2.07	0.84
1:E:250:GLN:HE22	1:E:330:GLN:HE21	1.21	0.84
3:D:551:NDP:H2N	3:D:551:NDP:H52N	1.58	0.83
1:B:250:GLN:HE22	1:B:330:GLN:HE21	1.26	0.83
1:C:48:ILE:HD11	1:C:499:THR:HG21	1.61	0.82
1:B:126:LYS:HZ3	2:B:550:GLU:N	1.78	0.82
1:B:112:THR:HG22	1:B:124:GLY:N	1.97	0.79
1:E:112:THR:HG22	1:E:124:GLY:N	1.98	0.79
1:F:32:LEU:HD23	1:F:494:ASN:HD21	1.46	0.79
1:B:112:THR:HG22	1:B:124:GLY:H	1.48	0.79
1:B:51:ILE:HD12	1:E:64:PRO:HB3	1.65	0.79
1:E:112:THR:HG22	1:E:124:GLY:H	1.48	0.79
1:A:205:GLN:HE22	1:B:496:ALA:HB2	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:THR:HG22	1:A:124:GLY:H	1.49	0.78
1:A:112:THR:HG22	1:A:124:GLY:N	1.99	0.78
1:E:211:ARG:HH22	3:E:551:NDP:H71N	1.31	0.76
1:B:72:TRP:HE1	1:E:499:THR:HG21	1.51	0.76
1:C:112:THR:HG22	1:C:124:GLY:N	2.01	0.76
1:C:91:GLY:HA3	1:C:125:ALA:O	1.86	0.75
1:E:173:GLU:HB3	1:E:202:PRO:HG3	1.68	0.75
1:C:112:THR:HG22	1:C:124:GLY:H	1.52	0.74
1:D:112:THR:HG22	1:D:124:GLY:N	2.01	0.74
3:A:551:NDP:H52N	3:A:551:NDP:H2N	1.69	0.74
1:F:107:LEU:HB3	1:F:126:LYS:HE3	1.69	0.74
1:B:64:PRO:HB3	1:E:51:ILE:HD12	1.70	0.73
3:F:551:NDP:H2N	3:F:551:NDP:H52N	1.70	0.73
1:D:255:VAL:HG23	6:D:557:HOH:O	1.88	0.73
1:F:112:THR:HG22	1:F:124:GLY:N	2.03	0.73
1:D:107:LEU:HB3	1:D:126:LYS:HE3	1.70	0.73
1:A:91:GLY:HA3	1:A:125:ALA:O	1.89	0.73
1:D:112:THR:HG22	1:D:124:GLY:H	1.52	0.72
1:F:112:THR:HG22	1:F:124:GLY:H	1.54	0.72
1:B:91:GLY:HA3	1:B:125:ALA:O	1.89	0.72
1:C:250:GLN:HE22	1:C:330:GLN:NE2	1.87	0.72
1:E:94:ARG:HG3	1:E:169:MET:HB2	1.72	0.72
1:F:91:GLY:HA3	1:F:125:ALA:O	1.89	0.72
1:A:107:LEU:HB3	1:A:126:LYS:HE3	1.72	0.72
1:D:250:GLN:HE22	1:D:330:GLN:NE2	1.88	0.71
1:C:107:LEU:HB3	1:C:126:LYS:HE3	1.71	0.71
1:C:212:ILE:HB	4:C:553:GTP:O3'	1.90	0.71
1:B:94:ARG:HG3	1:B:169:MET:HB2	1.72	0.71
1:F:94:ARG:HG3	1:F:169:MET:HB2	1.72	0.71
1:F:250:GLN:HE22	1:F:330:GLN:NE2	1.89	0.71
1:D:386:LEU:HD21	1:E:392:VAL:HG13	1.73	0.71
1:E:107:LEU:HB3	1:E:126:LYS:HE3	1.72	0.71
1:F:173:GLU:HB3	1:F:202:PRO:HG3	1.73	0.71
1:B:173:GLU:HB3	1:B:202:PRO:HG3	1.73	0.70
1:A:173:GLU:HB3	1:A:202:PRO:HG3	1.73	0.70
1:E:250:GLN:HE22	1:E:330:GLN:NE2	1.88	0.70
1:D:173:GLU:HB3	1:D:202:PRO:HG3	1.73	0.70
1:D:94:ARG:HG3	1:D:169:MET:HB2	1.74	0.69
1:B:107:LEU:HB3	1:B:126:LYS:HE3	1.73	0.69
1:C:51:ILE:HD12	1:F:64:PRO:HB3	1.74	0.69
1:C:173:GLU:HB3	1:C:202:PRO:HG3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ILE:HD12	1:D:64:PRO:HB3	1.73	0.69
1:A:94:ARG:HG3	1:A:169:MET:HB2	1.73	0.69
1:D:91:GLY:HA3	1:D:125:ALA:O	1.93	0.68
1:C:94:ARG:HG3	1:C:169:MET:HB2	1.74	0.68
1:A:250:GLN:HE22	1:A:330:GLN:NE2	1.90	0.68
1:B:250:GLN:HE22	1:B:330:GLN:NE2	1.91	0.68
1:E:91:GLY:HA3	1:E:125:ALA:O	1.92	0.68
3:C:551:NDP:H52N	3:C:551:NDP:H2N	1.74	0.68
1:B:34:THR:HG22	1:B:36:GLU:N	2.09	0.68
1:D:332:THR:N	1:D:335:ASN:HD21	1.90	0.68
1:C:501:THR:HA	1:F:66:ARG:NH2	2.08	0.67
1:C:258:HIS:HD2	1:C:261:ARG:HH11	1.42	0.67
1:F:332:THR:H	1:F:335:ASN:ND2	1.93	0.67
1:E:34:THR:HG22	1:E:36:GLU:N	2.10	0.66
1:C:34:THR:HG22	1:C:36:GLU:N	2.09	0.66
1:F:34:THR:HG22	1:F:36:GLU:N	2.09	0.66
1:C:1:ALA:O	1:C:2:ASP:HB2	1.93	0.66
1:D:34:THR:HG22	1:D:36:GLU:N	2.09	0.66
1:E:112:THR:CG2	1:E:124:GLY:H	2.09	0.66
1:B:112:THR:CG2	1:B:124:GLY:H	2.09	0.66
1:E:255:VAL:HG23	6:E:555:HOH:O	1.95	0.66
1:D:258:HIS:HD2	1:D:261:ARG:HH11	1.45	0.65
3:E:551:NDP:H52N	3:E:551:NDP:H2N	1.78	0.65
1:A:34:THR:HG22	1:A:36:GLU:N	2.10	0.65
1:E:258:HIS:HD2	1:E:261:ARG:HH11	1.43	0.65
1:F:258:HIS:HD2	1:F:261:ARG:HH11	1.44	0.65
1:D:332:THR:H	1:D:335:ASN:ND2	1.89	0.65
1:C:64:PRO:HB3	1:F:51:ILE:HD12	1.78	0.65
1:B:258:HIS:HD2	1:B:261:ARG:HH11	1.45	0.65
1:A:258:HIS:HD2	1:A:261:ARG:HH11	1.44	0.64
1:A:64:PRO:HB3	1:D:51:ILE:HD12	1.80	0.64
1:B:496:ALA:O	1:B:498:VAL:HG23	1.97	0.64
1:D:33:LYS:HD2	1:D:495:GLU:HB2	1.80	0.64
1:D:253:GLY:HA3	3:D:551:NDP:O1A	1.98	0.64
1:E:332:THR:H	1:E:335:ASN:ND2	1.93	0.64
1:F:253:GLY:HA3	3:F:551:NDP:O1A	1.98	0.64
1:C:253:GLY:HA3	3:C:551:NDP:O1A	1.97	0.64
1:E:496:ALA:HA	1:E:500:PHE:HB2	1.80	0.64
1:B:44:ARG:HD3	1:B:499:THR:HA	1.79	0.64
1:A:112:THR:CG2	1:A:124:GLY:H	2.10	0.63
1:E:253:GLY:HA3	3:E:551:NDP:O1A	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:332:THR:N	1:E:335:ASN:HD21	1.94	0.63
1:A:349:ASN:ND2	3:A:551:NDP:O2D	2.31	0.63
1:D:150:MET:HG3	5:D:552:B1T:CLAE	2.36	0.62
1:A:332:THR:H	1:A:335:ASN:ND2	1.94	0.62
1:C:112:THR:CG2	1:C:124:GLY:H	2.12	0.62
1:D:28:LEU:HD22	1:D:490:PHE:CD2	2.34	0.62
1:A:44:ARG:HH22	1:D:66:ARG:HH22	1.47	0.61
1:B:332:THR:H	1:B:335:ASN:ND2	1.94	0.61
1:B:332:THR:N	1:B:335:ASN:HD21	1.94	0.61
1:D:378:VAL:HG23	6:D:554:HOH:O	2.01	0.61
1:A:253:GLY:HA3	3:A:551:NDP:O1A	2.00	0.61
1:E:141:LEU:O	1:E:145:THR:HG23	2.01	0.61
1:F:332:THR:N	1:F:335:ASN:HD21	1.93	0.61
1:D:112:THR:CG2	1:D:124:GLY:H	2.13	0.61
1:D:141:LEU:O	1:D:145:THR:HG23	2.01	0.60
1:F:7:PRO:HD2	1:F:329:LYS:HD2	1.82	0.60
1:C:332:THR:H	1:C:335:ASN:ND2	1.93	0.60
1:F:112:THR:CG2	1:F:124:GLY:H	2.14	0.60
1:C:141:LEU:O	1:C:145:THR:HG23	2.01	0.60
1:C:432:PRO:HB3	1:C:436:PHE:HD2	1.67	0.60
1:F:432:PRO:HB3	1:F:436:PHE:HD2	1.66	0.60
1:A:141:LEU:O	1:A:145:THR:HG23	2.01	0.60
1:C:332:THR:N	1:C:335:ASN:HD21	1.93	0.60
1:E:53:LYS:O	1:E:82:HIS:HE1	1.84	0.60
1:F:53:LYS:O	1:F:82:HIS:HE1	1.85	0.59
1:F:141:LEU:O	1:F:145:THR:HG23	2.02	0.59
1:A:53:LYS:O	1:A:82:HIS:HE1	1.84	0.59
1:A:413:VAL:HG13	1:A:430:ILE:HG13	1.85	0.59
1:B:3:ARG:CG	1:B:3:ARG:HH11	2.08	0.59
1:D:410:LEU:HG	1:D:430:ILE:HG22	1.84	0.59
1:B:141:LEU:O	1:B:145:THR:HG23	2.03	0.58
1:F:410:LEU:HG	1:F:430:ILE:HG22	1.85	0.58
1:D:53:LYS:O	1:D:82:HIS:HE1	1.86	0.58
1:C:53:LYS:O	1:C:82:HIS:HE1	1.86	0.58
1:B:432:PRO:HB3	1:B:436:PHE:HD2	1.68	0.58
1:B:3:ARG:NH1	1:B:3:ARG:HG3	2.05	0.58
1:F:413:VAL:HG13	1:F:430:ILE:HG13	1.85	0.58
1:E:358:LYS:O	1:E:362:GLU:HG3	2.04	0.58
1:C:349:ASN:ND2	3:C:551:NDP:O2D	2.37	0.58
1:F:114:LYS:HD2	1:F:378:VAL:HG21	1.84	0.58
1:E:410:LEU:HG	1:E:430:ILE:HG22	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:THR:OG1	3:C:551:NDP:H42N	2.02	0.58
1:F:5:ASP:OD1	1:F:355:GLU:HB3	2.03	0.58
1:D:413:VAL:HG13	1:D:430:ILE:HG13	1.86	0.58
1:E:413:VAL:HG13	1:E:430:ILE:HG13	1.84	0.57
1:C:413:VAL:HG13	1:C:430:ILE:HG13	1.85	0.57
1:A:410:LEU:O	1:A:413:VAL:HG12	2.05	0.57
1:B:358:LYS:O	1:B:362:GLU:HG3	2.03	0.57
1:D:410:LEU:O	1:D:413:VAL:HG12	2.05	0.57
1:A:205:GLN:HE22	1:B:496:ALA:CB	2.16	0.57
1:A:332:THR:N	1:A:335:ASN:HD21	1.94	0.57
1:A:215:THR:OG1	3:A:551:NDP:H42N	2.04	0.57
1:D:498:VAL:HG22	1:E:146:ARG:NH2	2.19	0.57
1:B:63:PHE:CZ	1:B:75:ILE:HD11	2.40	0.57
1:D:114:LYS:HD2	1:D:378:VAL:HG21	1.87	0.56
1:E:494:ASN:O	1:E:498:VAL:HB	2.04	0.56
1:A:201:LYS:NZ	1:A:388:ASN:HD21	2.03	0.56
1:E:432:PRO:HB3	1:E:436:PHE:HD2	1.70	0.56
1:B:410:LEU:HG	1:B:430:ILE:HG22	1.86	0.56
1:D:358:LYS:O	1:D:362:GLU:HG3	2.06	0.56
2:B:550:GLU:HB3	3:B:551:NDP:H41N	1.88	0.56
1:A:432:PRO:HB3	1:A:436:PHE:HD2	1.71	0.56
1:A:392:VAL:HG13	1:B:386:LEU:HD21	1.88	0.56
1:F:82:HIS:HD2	1:F:112:THR:HG21	1.71	0.56
1:D:432:PRO:HB3	1:D:436:PHE:HD2	1.70	0.56
1:C:20:GLY:O	1:C:24:VAL:HG23	2.06	0.56
1:B:53:LYS:O	1:B:82:HIS:HE1	1.88	0.56
1:E:92:GLY:HA3	2:E:550:GLU:N	2.21	0.56
1:A:410:LEU:HG	1:A:430:ILE:HG22	1.86	0.56
1:F:82:HIS:CD2	1:F:112:THR:HG21	2.41	0.56
1:B:413:VAL:HG13	1:B:430:ILE:HG13	1.87	0.56
1:F:91:GLY:O	1:F:165:PRO:HA	2.06	0.56
1:C:410:LEU:O	1:C:413:VAL:HG12	2.05	0.56
1:C:414:GLN:HG3	1:C:428:ILE:O	2.06	0.56
1:B:201:LYS:NZ	1:B:388:ASN:HD21	2.04	0.56
1:D:215:THR:OG1	3:D:551:NDP:H42N	2.06	0.56
1:A:91:GLY:O	1:A:165:PRO:HA	2.06	0.56
1:B:392:VAL:HG13	1:F:386:LEU:HD21	1.88	0.55
1:C:82:HIS:CD2	1:C:112:THR:HG21	2.42	0.55
1:A:44:ARG:NH2	1:D:66:ARG:HH22	2.03	0.55
1:E:91:GLY:O	1:E:165:PRO:HA	2.07	0.55
1:B:209:HIS:HE1	4:B:553:GTP:O1A	1.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:LYS:O	1:A:362:GLU:HG3	2.06	0.55
1:E:63:PHE:CZ	1:E:75:ILE:HD11	2.42	0.55
1:C:114:LYS:HD2	1:C:378:VAL:HG21	1.88	0.55
1:C:410:LEU:HG	1:C:430:ILE:HG22	1.89	0.55
1:E:349:ASN:CG	3:E:551:NDP:O2D	2.45	0.55
1:B:414:GLN:HG3	1:B:428:ILE:O	2.06	0.55
1:C:358:LYS:O	1:C:362:GLU:HG3	2.06	0.55
1:F:5:ASP:O	1:F:7:PRO:HD3	2.07	0.55
1:A:20:GLY:O	1:A:24:VAL:HG23	2.07	0.55
1:E:414:GLN:HG3	1:E:428:ILE:O	2.07	0.55
1:A:82:HIS:HD2	1:A:112:THR:HG21	1.72	0.55
1:E:410:LEU:O	1:E:413:VAL:HG12	2.07	0.55
1:D:20:GLY:O	1:D:24:VAL:HG23	2.07	0.55
1:C:63:PHE:CZ	1:C:75:ILE:HD11	2.42	0.54
1:D:63:PHE:CZ	1:D:75:ILE:HD11	2.42	0.54
1:D:82:HIS:HD2	1:D:112:THR:HG21	1.73	0.54
1:A:205:GLN:NE2	1:B:496:ALA:HB2	2.20	0.54
1:C:91:GLY:O	1:C:165:PRO:HA	2.07	0.54
1:B:20:GLY:O	1:B:24:VAL:HG23	2.08	0.54
1:F:4:GLU:OE2	1:F:333:LYS:HB3	2.07	0.54
1:C:82:HIS:HD2	1:C:112:THR:HG21	1.71	0.54
1:A:63:PHE:CZ	1:A:75:ILE:HD11	2.42	0.54
5:E:552:B1T:OAB	5:E:552:B1T:OAA	2.26	0.54
1:D:82:HIS:CD2	1:D:112:THR:HG21	2.42	0.54
1:E:82:HIS:CD2	1:E:112:THR:HG21	2.43	0.54
1:E:79:ARG:HH11	1:E:127:ALA:HB2	1.73	0.54
1:E:82:HIS:HD2	1:E:112:THR:HG21	1.72	0.54
1:A:82:HIS:CD2	1:A:112:THR:HG21	2.43	0.54
1:D:91:GLY:O	1:D:165:PRO:HA	2.08	0.54
5:B:552:B1T:OAA	5:B:552:B1T:OAB	2.25	0.54
1:D:459:ARG:NH1	1:D:463:GLN:HE22	2.05	0.54
1:F:358:LYS:O	1:F:362:GLU:HG3	2.08	0.54
1:F:20:GLY:O	1:F:24:VAL:HG23	2.07	0.54
1:A:386:LEU:HD21	1:F:392:VAL:HG13	1.90	0.54
1:B:66:ARG:HH22	1:E:44:ARG:HH22	1.56	0.54
1:B:410:LEU:O	1:B:413:VAL:HG12	2.08	0.53
1:C:366:MET:HB2	1:C:475:LEU:HD22	1.89	0.53
1:F:410:LEU:O	1:F:413:VAL:HG12	2.09	0.53
1:C:392:VAL:HG13	1:E:386:LEU:HD21	1.89	0.53
5:D:552:B1T:OAA	5:D:552:B1T:OAB	2.26	0.53
1:F:63:PHE:CZ	1:F:75:ILE:HD11	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:GLN:HG3	1:A:428:ILE:O	2.09	0.53
1:A:79:ARG:HH11	1:A:127:ALA:HB2	1.73	0.53
1:C:99:VAL:HA	1:C:103:GLU:OE1	2.09	0.53
1:B:82:HIS:HD2	1:B:112:THR:HG21	1.74	0.52
5:A:552:B1T:OAA	5:A:552:B1T:OAB	2.28	0.52
1:B:85:HIS:HB2	1:B:492:VAL:HG11	1.91	0.52
1:B:82:HIS:CD2	1:B:112:THR:HG21	2.45	0.52
1:E:126:LYS:NZ	2:E:550:GLU:N	2.53	0.52
1:F:61:LEU:HD12	1:F:61:LEU:N	2.25	0.52
1:C:61:LEU:N	1:C:61:LEU:HD12	2.25	0.52
1:A:201:LYS:HZ1	1:A:388:ASN:HD21	1.58	0.52
1:C:24:VAL:HG22	1:C:483:VAL:HG22	1.92	0.52
5:A:552:B1T:SAK	1:E:147:ARG:HB2	2.49	0.52
1:B:91:GLY:O	1:B:165:PRO:HA	2.09	0.52
1:F:79:ARG:HH11	1:F:127:ALA:HB2	1.74	0.52
1:B:459:ARG:NH1	1:B:463:GLN:HE22	2.08	0.52
1:E:20:GLY:O	1:E:24:VAL:HG23	2.09	0.52
5:C:552:B1T:OAB	5:C:552:B1T:OAA	2.27	0.51
1:E:61:LEU:HD12	1:E:61:LEU:N	2.25	0.51
1:B:72:TRP:HE1	1:E:499:THR:CG2	2.23	0.51
1:D:499:THR:O	1:D:499:THR:HG23	2.11	0.51
1:A:498:VAL:HB	1:D:72:TRP:CH2	2.45	0.51
1:A:436:PHE:HB2	1:F:408:HIS:HB3	1.92	0.51
1:F:37:THR:HA	1:F:41:LYS:CD	2.40	0.51
5:F:552:B1T:OAA	5:F:552:B1T:OAB	2.28	0.51
1:F:316:GLU:O	1:F:340:LYS:HD3	2.10	0.51
1:C:201:LYS:NZ	1:C:388:ASN:HD21	2.09	0.51
1:B:99:VAL:HA	1:B:103:GLU:OE1	2.10	0.51
1:F:99:VAL:HA	1:F:103:GLU:OE1	2.11	0.51
1:D:79:ARG:HH11	1:D:127:ALA:HB2	1.75	0.51
1:B:37:THR:HA	1:B:41:LYS:CD	2.41	0.51
1:F:414:GLN:HG3	1:F:428:ILE:O	2.10	0.51
1:F:236:LEU:O	1:F:342:LYS:HE2	2.11	0.51
1:C:79:ARG:HH11	1:C:127:ALA:HB2	1.76	0.51
1:B:219:VAL:HG22	1:B:373:LEU:HD13	1.93	0.51
1:F:7:PRO:HD2	1:F:329:LYS:CD	2.41	0.51
1:F:89:CYS:HB3	1:F:125:ALA:HB2	1.93	0.51
1:E:89:CYS:HB3	1:E:125:ALA:HB2	1.93	0.51
1:D:37:THR:HA	1:D:41:LYS:CD	2.41	0.51
1:A:450:HIS:CE1	4:A:553:GTP:O3G	2.64	0.50
1:B:114:LYS:HD2	1:B:378:VAL:HG21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:GLN:HG3	1:D:428:ILE:O	2.10	0.50
1:A:236:LEU:O	1:A:342:LYS:HE2	2.11	0.50
1:C:495:GLU:HG3	1:D:204:SER:OG	2.10	0.50
1:D:236:LEU:O	1:D:342:LYS:HE2	2.10	0.50
1:A:61:LEU:HD12	1:A:61:LEU:N	2.26	0.50
1:C:37:THR:HA	1:C:41:LYS:CD	2.41	0.50
1:D:61:LEU:N	1:D:61:LEU:HD12	2.26	0.50
1:C:37:THR:HA	1:C:41:LYS:HD2	1.94	0.50
1:C:174:ARG:HG3	1:E:497:GLY:N	2.27	0.50
1:B:126:LYS:NZ	2:B:550:GLU:N	2.57	0.50
1:E:37:THR:HA	1:E:41:LYS:CD	2.42	0.50
1:C:236:LEU:O	1:C:342:LYS:HE2	2.12	0.50
1:B:236:LEU:O	1:B:342:LYS:HE2	2.11	0.50
1:F:219:VAL:HG22	1:F:373:LEU:HD13	1.93	0.50
1:A:99:VAL:HA	1:A:103:GLU:OE1	2.12	0.49
1:A:316:GLU:O	1:A:340:LYS:HD3	2.12	0.49
1:A:37:THR:HA	1:A:41:LYS:CD	2.42	0.49
1:C:146:ARG:HG2	1:C:182:THR:OG1	2.12	0.49
1:A:367:VAL:HG23	6:A:555:HOH:O	2.12	0.49
1:E:236:LEU:O	1:E:342:LYS:HE2	2.12	0.49
1:D:32:LEU:CD2	1:D:494:ASN:HD21	2.18	0.49
1:D:169:MET:HA	3:D:551:NDP:O1N	2.12	0.49
1:A:498:VAL:HB	1:D:72:TRP:HH2	1.78	0.49
1:E:459:ARG:NH1	1:E:463:GLN:HE22	2.10	0.49
3:B:551:NDP:H2N	3:B:551:NDP:H52N	1.94	0.49
1:A:37:THR:HA	1:A:41:LYS:HD2	1.94	0.49
1:B:79:ARG:HH11	1:B:127:ALA:HB2	1.78	0.49
1:F:169:MET:HA	3:F:551:NDP:O1N	2.13	0.49
1:B:24:VAL:HG22	1:B:483:VAL:HG22	1.94	0.49
1:F:33:LYS:HG3	1:F:494:ASN:OD1	2.13	0.49
1:B:255:VAL:HG11	3:B:551:NDP:O4D	2.13	0.49
1:F:459:ARG:NH1	1:F:463:GLN:HE22	2.11	0.49
1:A:166:ALA:HB3	2:A:550:GLU:HG2	1.95	0.49
1:C:255:VAL:HG23	1:C:256:GLY:H	1.78	0.49
1:B:341:ALA:O	1:B:365:ILE:HD12	2.12	0.49
1:D:341:ALA:O	1:D:365:ILE:HD12	2.13	0.49
1:B:146:ARG:HG2	1:B:182:THR:OG1	2.13	0.49
1:F:255:VAL:HG23	1:F:256:GLY:H	1.78	0.49
1:E:341:ALA:O	1:E:365:ILE:HD12	2.13	0.48
1:D:61:LEU:HD23	1:D:151:GLU:HB3	1.95	0.48
1:D:24:VAL:HG22	1:D:483:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:VAL:HA	1:D:103:GLU:OE1	2.13	0.48
1:A:103:GLU:O	1:A:107:LEU:HD22	2.13	0.48
1:F:24:VAL:HG22	1:F:483:VAL:HG13	1.96	0.48
1:F:5:ASP:O	1:F:353:THR:HG21	2.14	0.48
1:C:150:MET:CG	5:C:552:B1T:CLAE	2.89	0.48
1:C:44:ARG:HH22	1:F:66:ARG:HH22	1.60	0.48
1:E:349:ASN:ND2	3:E:551:NDP:O2D	2.46	0.48
1:E:255:VAL:HG23	1:E:256:GLY:H	1.78	0.48
1:B:61:LEU:N	1:B:61:LEU:HD12	2.28	0.48
1:A:459:ARG:NH1	1:A:463:GLN:HE22	2.11	0.48
1:C:341:ALA:O	1:C:365:ILE:HD12	2.14	0.48
1:D:316:GLU:O	1:D:340:LYS:HD3	2.12	0.48
1:E:499:THR:HG22	1:E:499:THR:O	2.14	0.48
1:B:37:THR:HA	1:B:41:LYS:HD2	1.96	0.48
1:E:401:TYR:O	1:E:405:SER:HB2	2.13	0.48
1:B:423:LYS:HE2	1:B:423:LYS:HA	1.95	0.48
1:C:219:VAL:HG22	1:C:373:LEU:HD13	1.95	0.48
1:D:67:ARG:HD2	1:D:140:GLU:OE2	2.14	0.48
1:A:255:VAL:HG23	1:A:256:GLY:H	1.78	0.48
1:D:423:LYS:HE2	1:D:423:LYS:HA	1.96	0.48
1:B:103:GLU:O	1:B:107:LEU:HD22	2.14	0.48
2:D:550:GLU:HA	3:D:551:NDP:H41N	1.95	0.48
1:E:114:LYS:HD2	1:E:378:VAL:HG21	1.94	0.48
1:C:459:ARG:NH1	1:C:463:GLN:HE22	2.11	0.48
1:F:341:ALA:O	1:F:365:ILE:HD12	2.14	0.48
1:E:252:PHE:CZ	1:E:291:LEU:HD13	2.49	0.48
1:D:369:PRO:HD3	1:D:477:LEU:HB2	1.96	0.48
1:A:366:MET:HB2	1:A:475:LEU:HD22	1.95	0.47
1:F:348:ALA:HA	3:F:551:NDP:H1D	1.96	0.47
1:B:89:CYS:HB3	1:B:125:ALA:HB2	1.95	0.47
1:E:99:VAL:HA	1:E:103:GLU:OE1	2.14	0.47
1:D:255:VAL:HG23	1:D:256:GLY:H	1.77	0.47
1:E:146:ARG:HG2	1:E:182:THR:OG1	2.14	0.47
1:C:118:VAL:O	1:C:118:VAL:HG13	2.14	0.47
1:B:255:VAL:HG23	1:B:256:GLY:H	1.79	0.47
1:D:497:GLY:O	1:D:498:VAL:C	2.52	0.47
1:D:436:PHE:HB2	1:E:408:HIS:HB3	1.96	0.47
1:A:212:ILE:HB	4:A:553:GTP:O2'	2.14	0.47
1:B:252:PHE:CZ	1:B:291:LEU:HD13	2.49	0.47
1:C:252:PHE:CZ	1:C:291:LEU:HD13	2.49	0.47
1:C:89:CYS:HB3	1:C:125:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:GLU:HG2	3:A:551:NDP:O3B	2.14	0.47
1:B:111:MET:SD	1:B:114:LYS:HE3	2.55	0.47
1:D:118:VAL:HG13	1:D:118:VAL:O	2.14	0.47
1:A:444:SER:H	1:A:447:ASP:HB2	1.78	0.47
1:E:201:LYS:NZ	1:E:388:ASN:HD21	2.12	0.47
1:D:219:VAL:HG22	1:D:373:LEU:HD13	1.96	0.47
1:A:349:ASN:HB2	3:A:551:NDP:O2D	2.15	0.47
1:A:24:VAL:CG2	1:A:483:VAL:HG13	2.45	0.47
1:F:369:PRO:HB2	1:F:371:LEU:HD23	1.97	0.47
1:F:201:LYS:NZ	1:F:388:ASN:HD21	2.13	0.47
1:A:423:LYS:HE2	1:A:423:LYS:HA	1.97	0.47
1:A:401:TYR:O	1:A:405:SER:HB2	2.14	0.47
1:E:219:VAL:HG22	1:E:373:LEU:HD13	1.97	0.47
1:C:423:LYS:HE2	1:C:423:LYS:HA	1.96	0.47
1:D:37:THR:HA	1:D:41:LYS:HD2	1.95	0.47
1:E:118:VAL:O	1:E:118:VAL:HG13	2.15	0.47
1:A:114:LYS:HD2	1:A:378:VAL:HG21	1.95	0.47
1:F:335:ASN:HD22	1:F:336:ALA:N	2.13	0.47
1:E:37:THR:HA	1:E:41:LYS:HD2	1.96	0.47
1:B:316:GLU:O	1:B:340:LYS:HD3	2.15	0.47
1:E:423:LYS:HE2	1:E:423:LYS:HA	1.96	0.47
1:F:275:GLU:HG2	3:F:551:NDP:O3B	2.15	0.47
1:A:93:ILE:HG12	1:A:127:ALA:HB3	1.97	0.47
1:B:201:LYS:HZ1	1:B:388:ASN:HD21	1.62	0.47
1:A:341:ALA:O	1:A:365:ILE:HD12	2.14	0.47
1:C:316:GLU:O	1:C:340:LYS:HD3	2.14	0.47
1:F:67:ARG:HD2	1:F:140:GLU:OE2	2.15	0.47
1:D:265:ARG:NH1	4:D:553:GTP:O2G	2.45	0.47
1:F:494:ASN:O	1:F:499:THR:HG22	2.15	0.46
1:F:126:LYS:HZ3	2:F:550:GLU:N	2.12	0.46
1:A:89:CYS:HB3	1:A:125:ALA:HB2	1.96	0.46
1:C:24:VAL:CG2	1:C:483:VAL:HG13	2.46	0.46
1:C:61:LEU:HD23	1:C:151:GLU:HB3	1.98	0.46
1:B:229:GLU:C	1:B:231:SER:H	2.18	0.46
1:C:103:GLU:O	1:C:107:LEU:HD22	2.16	0.46
1:F:37:THR:HA	1:F:41:LYS:HD2	1.96	0.46
1:A:219:VAL:HG22	1:A:373:LEU:HD13	1.97	0.46
1:B:4:GLU:OE1	1:B:333:LYS:HB3	2.16	0.46
1:A:118:VAL:HG13	1:A:118:VAL:O	2.14	0.46
1:B:401:TYR:O	1:B:405:SER:HB2	2.15	0.46
1:D:229:GLU:C	1:D:231:SER:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:335:ASN:N	1:E:335:ASN:HD22	2.13	0.46
1:C:501:THR:O	1:C:501:THR:HG22	2.15	0.46
1:E:369:PRO:HB2	1:E:371:LEU:HD23	1.96	0.46
1:E:369:PRO:HD3	1:E:477:LEU:HB2	1.98	0.46
1:B:496:ALA:C	1:B:498:VAL:H	2.19	0.46
1:F:103:GLU:O	1:F:107:LEU:HD22	2.15	0.46
1:A:369:PRO:HD3	1:A:477:LEU:HB2	1.97	0.46
1:D:252:PHE:CZ	1:D:291:LEU:HD13	2.51	0.46
1:D:93:ILE:HG12	1:D:127:ALA:HB3	1.97	0.46
1:F:24:VAL:HG22	1:F:483:VAL:HG22	1.96	0.46
1:C:401:TYR:O	1:C:405:SER:HB2	2.15	0.46
1:C:369:PRO:HD3	1:C:477:LEU:HB2	1.97	0.46
1:B:335:ASN:HD22	1:B:335:ASN:N	2.14	0.46
1:F:252:PHE:CZ	1:F:291:LEU:HD13	2.51	0.46
1:E:316:GLU:O	1:E:340:LYS:HD3	2.16	0.46
1:A:335:ASN:N	1:A:335:ASN:HD22	2.14	0.46
1:F:339:VAL:O	1:F:340:LYS:HB2	2.16	0.46
1:E:118:VAL:HG22	1:E:456:THR:HG22	1.97	0.46
1:A:65:ILE:O	1:A:65:ILE:HG13	2.16	0.46
2:D:550:GLU:HA	3:D:551:NDP:C5N	2.46	0.46
1:F:118:VAL:HG22	1:F:456:THR:HG22	1.97	0.46
1:D:401:TYR:O	1:D:405:SER:HB2	2.15	0.46
1:F:495:GLU:O	1:F:498:VAL:HB	2.16	0.46
1:E:67:ARG:HD2	1:E:140:GLU:OE2	2.16	0.46
1:A:90:LYS:HD2	1:A:164:VAL:HB	1.98	0.46
1:E:103:GLU:O	1:E:107:LEU:HD22	2.17	0.45
1:D:201:LYS:NZ	1:D:388:ASN:HD21	2.14	0.45
1:A:146:ARG:HG2	1:A:182:THR:OG1	2.15	0.45
1:B:5:ASP:OD2	1:B:332:THR:HB	2.17	0.45
1:E:374:ASN:HB2	3:E:551:NDP:H6N	1.98	0.45
1:A:412:SER:HA	1:B:433:THR:HG23	1.97	0.45
1:F:423:LYS:HA	1:F:423:LYS:HE2	1.98	0.45
1:D:335:ASN:HD22	1:D:336:ALA:N	2.15	0.45
1:C:66:ARG:HH22	1:F:44:ARG:HH22	1.65	0.45
1:C:118:VAL:HG22	1:C:456:THR:HG22	1.97	0.45
1:A:369:PRO:HB2	1:A:371:LEU:HD23	1.99	0.45
1:E:331:LEU:HB2	1:E:352:THR:HG22	1.98	0.45
1:F:61:LEU:HD23	1:F:151:GLU:HB3	1.98	0.45
1:E:118:VAL:HG22	1:E:456:THR:CG2	2.46	0.45
1:F:492:VAL:O	1:F:498:VAL:HG11	2.17	0.45
1:A:252:PHE:CZ	1:A:291:LEU:HD13	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ILE:O	1:B:65:ILE:HG13	2.16	0.45
1:A:4:GLU:OE1	1:A:4:GLU:HA	2.16	0.45
1:C:5:ASP:OD1	1:C:7:PRO:HD3	2.17	0.45
1:E:32:LEU:HD22	1:E:34:THR:OG1	2.17	0.45
2:D:550:GLU:HA	3:D:551:NDP:C4N	2.47	0.45
1:F:287:ASP:HB3	1:F:290:GLU:HG3	1.99	0.45
1:A:2:ASP:O	1:A:6:ASP:HB2	2.16	0.45
1:A:67:ARG:HD2	1:A:140:GLU:OE2	2.17	0.45
1:F:401:TYR:O	1:F:405:SER:HB2	2.17	0.45
1:D:85:HIS:HD2	1:D:492:VAL:HG21	1.82	0.45
1:C:67:ARG:HD2	1:C:140:GLU:OE2	2.17	0.45
1:F:32:LEU:HD22	1:F:34:THR:OG1	2.16	0.45
1:F:118:VAL:O	1:F:118:VAL:HG13	2.16	0.45
1:D:32:LEU:HD22	1:D:34:THR:OG1	2.17	0.45
1:B:93:ILE:HG12	1:B:127:ALA:HB3	1.99	0.45
1:C:93:ILE:HG12	1:C:127:ALA:HB3	1.98	0.45
1:C:229:GLU:C	1:C:231:SER:H	2.20	0.45
1:C:433:THR:HG23	1:D:412:SER:HA	1.98	0.45
1:D:433:THR:HG23	1:E:412:SER:HA	1.99	0.45
1:C:331:LEU:HD23	1:C:352:THR:HG22	1.99	0.45
1:A:229:GLU:O	1:A:231:SER:N	2.44	0.45
1:F:4:GLU:OE2	1:F:5:ASP:N	2.50	0.44
1:D:146:ARG:HD3	5:D:552:B1T:HAI	1.99	0.44
1:D:118:VAL:HG22	1:D:456:THR:HG22	1.98	0.44
1:E:331:LEU:HD23	1:E:352:THR:HG22	1.98	0.44
1:A:331:LEU:HD23	1:A:352:THR:HG22	1.99	0.44
1:E:366:MET:HB2	1:E:475:LEU:HD22	1.99	0.44
1:C:169:MET:HA	3:C:551:NDP:O1N	2.17	0.44
1:A:24:VAL:HG22	1:A:483:VAL:HG13	1.98	0.44
1:F:24:VAL:CG2	1:F:483:VAL:HG13	2.47	0.44
1:C:118:VAL:HG22	1:C:456:THR:CG2	2.47	0.44
1:A:496:ALA:HA	1:A:500:PHE:CG	2.52	0.44
1:A:75:ILE:CD1	1:A:144:ILE:HG23	2.48	0.44
1:B:118:VAL:HG13	1:B:118:VAL:O	2.16	0.44
1:E:24:VAL:HG22	1:E:483:VAL:HG22	2.00	0.44
1:F:331:LEU:HB2	1:F:352:THR:HG22	2.00	0.44
1:B:369:PRO:HB2	1:B:371:LEU:HD23	1.99	0.44
1:F:335:ASN:N	1:F:335:ASN:HD22	2.15	0.44
1:B:32:LEU:HD22	1:B:34:THR:OG1	2.17	0.44
1:B:496:ALA:C	1:B:498:VAL:N	2.70	0.44
1:D:89:CYS:HB3	1:D:125:ALA:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:ASN:N	1:C:335:ASN:HD22	2.14	0.44
1:E:92:GLY:H	2:E:550:GLU:N	2.15	0.44
1:A:24:VAL:HG22	1:A:483:VAL:HG22	1.98	0.44
1:D:65:ILE:O	1:D:65:ILE:HG13	2.17	0.44
1:D:270:CYS:O	1:D:285:GLY:HA2	2.17	0.44
1:C:32:LEU:HD22	1:C:34:THR:OG1	2.18	0.44
1:D:103:GLU:O	1:D:107:LEU:HD22	2.17	0.44
1:C:24:VAL:HG22	1:C:483:VAL:HG13	1.99	0.44
1:D:369:PRO:HB2	1:D:371:LEU:HD23	2.00	0.44
1:C:369:PRO:HB2	1:C:371:LEU:HD23	1.99	0.44
1:F:65:ILE:O	1:F:65:ILE:HG13	2.17	0.44
1:B:335:ASN:HD22	1:B:336:ALA:N	2.15	0.44
1:F:111:MET:SD	1:F:114:LYS:HE3	2.58	0.44
1:C:111:MET:SD	1:C:114:LYS:HE3	2.58	0.44
1:E:229:GLU:C	1:E:231:SER:H	2.21	0.44
1:E:186:THR:OG1	1:E:187:ILE:N	2.50	0.44
1:D:335:ASN:N	1:D:335:ASN:HD22	2.15	0.44
1:D:5:ASP:OD2	1:D:332:THR:HB	2.18	0.44
1:C:335:ASN:HD22	1:C:336:ALA:N	2.16	0.44
1:D:496:ALA:HB2	1:E:202:PRO:CB	2.48	0.44
1:C:211:ARG:HH22	3:C:551:NDP:H71N	1.65	0.44
1:C:270:CYS:O	1:C:285:GLY:HA2	2.18	0.44
1:B:287:ASP:HB3	1:B:290:GLU:HG3	2.00	0.44
1:D:339:VAL:O	1:D:340:LYS:HB2	2.18	0.43
1:B:331:LEU:HB2	1:B:352:THR:HG22	2.00	0.43
1:B:487:GLU:OE2	1:B:491:ARG:NH2	2.51	0.43
1:E:93:ILE:HG12	1:E:127:ALA:HB3	1.99	0.43
1:B:414:GLN:O	1:B:418:GLU:HG3	2.19	0.43
1:E:339:VAL:O	1:E:340:LYS:HB2	2.19	0.43
1:B:67:ARG:HD2	1:B:140:GLU:OE2	2.17	0.43
1:C:12:MET:HG3	1:C:354:PRO:HD3	1.99	0.43
1:B:493:TYR:C	1:B:495:GLU:H	2.20	0.43
1:D:349:ASN:ND2	3:D:551:NDP:O2D	2.52	0.43
1:D:90:LYS:HG3	2:D:550:GLU:OE1	2.18	0.43
1:F:25:GLU:O	1:F:29:VAL:HG23	2.19	0.43
1:E:116:ALA:O	1:E:488:LYS:HD2	2.18	0.43
1:B:28:LEU:HD22	1:B:490:PHE:CD2	2.53	0.43
1:C:65:ILE:HG13	1:C:65:ILE:O	2.18	0.43
1:E:270:CYS:O	1:E:285:GLY:HA2	2.18	0.43
1:D:90:LYS:HD2	1:D:164:VAL:HB	1.99	0.43
1:D:496:ALA:HB1	1:E:205:GLN:CG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ASN:CB	3:A:551:NDP:O2D	2.66	0.43
1:C:408:HIS:HB3	1:E:436:PHE:HB2	1.99	0.43
1:F:287:ASP:HA	1:F:288:PRO:HD3	1.92	0.43
1:B:118:VAL:HG22	1:B:456:THR:CG2	2.48	0.43
1:E:287:ASP:HB3	1:E:290:GLU:HG3	2.01	0.43
1:E:335:ASN:HD22	1:E:336:ALA:N	2.16	0.43
1:D:146:ARG:HG2	1:D:182:THR:OG1	2.18	0.43
1:B:491:ARG:HG3	1:B:491:ARG:HH11	1.84	0.43
1:A:32:LEU:HD22	1:A:34:THR:OG1	2.18	0.43
1:E:65:ILE:O	1:E:65:ILE:HG13	2.18	0.43
1:F:9:PHE:O	1:F:12:MET:HB3	2.18	0.43
1:A:335:ASN:HD22	1:A:336:ALA:N	2.16	0.43
1:C:44:ARG:NH2	1:F:66:ARG:HH22	2.17	0.43
1:E:287:ASP:HA	1:E:288:PRO:HD3	1.91	0.43
1:B:90:LYS:HD2	1:B:164:VAL:HB	2.01	0.43
1:E:85:HIS:HD2	1:E:492:VAL:HG21	1.83	0.43
1:D:111:MET:SD	1:D:114:LYS:HE3	2.59	0.43
1:D:201:LYS:HZ1	1:D:388:ASN:HD21	1.67	0.43
1:D:287:ASP:HB3	1:D:290:GLU:HG3	2.00	0.43
1:F:96:SER:O	1:F:130:LYS:HA	2.18	0.43
1:F:186:THR:OG1	1:F:187:ILE:N	2.52	0.43
1:A:501:THR:C	1:F:138:ASP:OD2	2.57	0.43
1:D:24:VAL:CG2	1:D:483:VAL:HG13	2.49	0.43
1:B:61:LEU:HD23	1:B:151:GLU:HB3	2.00	0.43
1:F:331:LEU:HD23	1:F:352:THR:HG22	2.00	0.43
1:B:369:PRO:HD3	1:B:477:LEU:HB2	1.99	0.43
1:A:25:GLU:O	1:A:29:VAL:HG23	2.19	0.43
1:C:287:ASP:HA	1:C:288:PRO:HD3	1.91	0.43
1:E:90:LYS:HD2	1:E:164:VAL:HB	2.00	0.43
1:C:178:TRP:NE1	1:E:497:GLY:O	2.51	0.43
1:C:229:GLU:O	1:C:231:SER:N	2.45	0.43
1:B:118:VAL:HG22	1:B:456:THR:HG22	2.01	0.43
1:B:172:GLY:O	1:B:176:MET:HG2	2.19	0.43
2:E:550:GLU:HB3	3:E:551:NDP:H41N	2.00	0.42
1:C:496:ALA:H	1:C:500:PHE:HE1	1.66	0.42
1:C:496:ALA:C	1:C:498:VAL:H	2.21	0.42
1:C:339:VAL:O	1:C:340:LYS:HB2	2.19	0.42
1:A:229:GLU:C	1:A:231:SER:H	2.19	0.42
1:E:169:MET:HG2	3:E:551:NDP:O1N	2.20	0.42
1:B:408:HIS:HB3	1:F:436:PHE:HB2	2.01	0.42
1:C:287:ASP:HB3	1:C:290:GLU:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:VAL:HG23	1:A:163:ASP:N	2.34	0.42
1:E:61:LEU:HD23	1:E:151:GLU:HB3	2.02	0.42
1:D:118:VAL:HG22	1:D:456:THR:CG2	2.49	0.42
1:F:498:VAL:C	1:F:500:PHE:H	2.23	0.42
1:C:386:LEU:HD21	1:D:392:VAL:HG13	2.00	0.42
1:F:229:GLU:C	1:F:231:SER:H	2.21	0.42
1:E:172:GLY:O	1:E:176:MET:HG2	2.19	0.42
1:B:32:LEU:HD23	1:B:494:ASN:OD1	2.19	0.42
1:C:78:TYR:O	1:C:127:ALA:HA	2.18	0.42
1:C:174:ARG:HG3	1:E:497:GLY:HA2	2.00	0.42
1:E:201:LYS:HZ1	1:E:388:ASN:HD21	1.66	0.42
1:F:369:PRO:HD3	1:F:477:LEU:HB2	2.01	0.42
1:B:339:VAL:O	1:B:340:LYS:HB2	2.19	0.42
1:C:364:ASN:HA	1:C:364:ASN:HD22	1.62	0.42
1:D:33:LYS:HD2	1:D:495:GLU:CB	2.48	0.42
1:A:408:HIS:HB3	1:B:436:PHE:HB2	2.01	0.42
1:D:498:VAL:HA	1:D:500:PHE:CE1	2.54	0.42
1:A:61:LEU:HD23	1:A:151:GLU:HB3	2.01	0.42
1:C:137:THR:OG1	1:C:140:GLU:HG3	2.19	0.42
1:D:335:ASN:ND2	1:D:335:ASN:H	2.18	0.42
1:F:118:VAL:HG22	1:F:456:THR:CG2	2.49	0.42
1:F:172:GLY:O	1:F:176:MET:HG2	2.20	0.42
1:A:172:GLY:O	1:A:176:MET:HG2	2.19	0.42
1:A:186:THR:OG1	1:A:187:ILE:N	2.49	0.42
1:A:490:PHE:O	1:A:493:TYR:N	2.48	0.42
1:D:309:ILE:HD12	1:D:309:ILE:N	2.35	0.42
1:E:75:ILE:CD1	1:E:144:ILE:HG23	2.50	0.42
1:C:331:LEU:HB2	1:C:352:THR:HG22	2.01	0.42
1:A:331:LEU:HB2	1:A:352:THR:HG22	2.01	0.42
1:B:444:SER:H	1:B:447:ASP:HB2	1.84	0.42
1:C:28:LEU:HD22	1:C:490:PHE:CD2	2.54	0.42
1:A:335:ASN:H	1:A:335:ASN:ND2	2.17	0.42
1:D:386:LEU:HD21	1:E:392:VAL:CG1	2.46	0.42
1:B:229:GLU:O	1:B:231:SER:N	2.44	0.42
1:F:146:ARG:HG2	1:F:182:THR:OG1	2.19	0.42
1:F:90:LYS:HD2	1:F:164:VAL:HB	2.02	0.42
1:B:79:ARG:HA	1:B:126:LYS:O	2.20	0.42
1:D:378:VAL:HG22	2:D:550:GLU:HB2	2.02	0.42
1:A:244:ASP:OD2	1:A:244:ASP:N	2.51	0.42
1:F:93:ILE:HG12	1:F:127:ALA:HB3	2.02	0.41
1:D:331:LEU:HD23	1:D:352:THR:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:366:MET:HB2	1:F:475:LEU:HD22	2.01	0.41
1:A:287:ASP:HB3	1:A:290:GLU:HG3	2.01	0.41
1:A:79:ARG:HA	1:A:126:LYS:O	2.20	0.41
1:D:75:ILE:CD1	1:D:144:ILE:HG23	2.50	0.41
1:C:174:ARG:HG3	1:E:497:GLY:CA	2.50	0.41
1:E:281:TRP:CZ2	1:E:283:PRO:HD3	2.54	0.41
1:F:39:GLU:O	1:F:43:ASN:HB2	2.20	0.41
1:A:292:GLU:O	1:A:296:LEU:HB2	2.21	0.41
1:C:333:LYS:HD2	1:C:355:GLU:HG2	2.02	0.41
1:B:309:ILE:N	1:B:309:ILE:HD12	2.35	0.41
1:E:47:GLY:O	1:E:51:ILE:HG12	2.20	0.41
1:F:114:LYS:HD2	1:F:378:VAL:CG2	2.50	0.41
1:B:413:VAL:CG1	1:B:430:ILE:HG21	2.51	0.41
1:D:24:VAL:HG22	1:D:483:VAL:HG13	2.01	0.41
1:E:111:MET:SD	1:E:114:LYS:HE3	2.60	0.41
1:C:90:LYS:HD2	1:C:164:VAL:HB	2.02	0.41
1:E:133:PRO:HG2	1:E:170:SER:HB3	2.02	0.41
1:C:44:ARG:HE	1:C:499:THR:HG22	1.85	0.41
1:D:79:ARG:HA	1:D:126:LYS:O	2.21	0.41
1:D:146:ARG:HD3	5:D:552:B1T:CAI	2.49	0.41
1:F:414:GLN:O	1:F:418:GLU:HG3	2.20	0.41
1:B:133:PRO:HG2	1:B:170:SER:HB3	2.03	0.41
1:F:4:GLU:CD	1:F:5:ASP:N	2.74	0.41
1:E:335:ASN:H	1:E:335:ASN:ND2	2.18	0.41
1:B:169:MET:HG2	3:B:551:NDP:O1N	2.21	0.41
1:A:75:ILE:HD11	1:A:144:ILE:HG23	2.02	0.41
1:C:201:LYS:HZ1	1:C:388:ASN:HD21	1.68	0.41
1:F:371:LEU:H	1:F:371:LEU:HD23	1.86	0.41
1:F:137:THR:OG1	1:F:140:GLU:HG3	2.21	0.41
1:A:1:ALA:N	1:A:6:ASP:OD1	2.50	0.41
1:D:172:GLY:O	1:D:176:MET:HG2	2.20	0.41
1:E:79:ARG:HA	1:E:126:LYS:O	2.20	0.41
1:E:496:ALA:O	1:E:500:PHE:HB2	2.21	0.41
1:E:413:VAL:CG1	1:E:430:ILE:HG21	2.51	0.41
1:C:4:GLU:O	1:C:5:ASP:HB3	2.19	0.41
1:B:317:VAL:HG22	1:B:318:ASP:N	2.36	0.41
1:A:317:VAL:HG22	1:A:318:ASP:N	2.36	0.41
1:E:25:GLU:O	1:E:29:VAL:HG23	2.20	0.41
1:C:492:VAL:O	1:C:496:ALA:HB2	2.21	0.41
1:A:339:VAL:O	1:A:340:LYS:HB2	2.19	0.41
1:B:39:GLU:O	1:B:43:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:ASN:ND2	1:C:335:ASN:H	2.19	0.41
1:E:414:GLN:O	1:E:418:GLU:HG3	2.21	0.41
1:F:211:ARG:HB3	6:F:557:HOH:O	2.21	0.41
1:B:335:ASN:ND2	1:B:335:ASN:H	2.18	0.41
1:A:169:MET:HA	3:A:551:NDP:O1N	2.21	0.41
2:F:550:GLU:HB2	3:F:551:NDP:H41N	2.02	0.41
1:F:349:ASN:N	3:F:551:NDP:O2D	2.54	0.41
1:C:114:LYS:HD2	1:C:378:VAL:CG2	2.51	0.41
1:B:66:ARG:HH22	1:E:44:ARG:NH2	2.19	0.41
1:A:414:GLN:O	1:A:418:GLU:HG3	2.21	0.41
1:E:24:VAL:CG2	1:E:483:VAL:HG13	2.51	0.41
1:A:118:VAL:HG22	1:A:456:THR:HG22	2.02	0.41
1:E:162:VAL:HG23	1:E:163:ASP:N	2.36	0.41
1:C:133:PRO:HG2	1:C:170:SER:HB3	2.03	0.41
1:D:317:VAL:HG22	1:D:318:ASP:N	2.36	0.41
1:A:333:LYS:HD2	1:A:355:GLU:HG2	2.02	0.41
1:E:39:GLU:O	1:E:43:ASN:HB2	2.20	0.41
1:B:25:GLU:O	1:B:29:VAL:HG23	2.21	0.41
1:E:107:LEU:CB	1:E:126:LYS:HG2	2.52	0.40
1:F:79:ARG:HA	1:F:126:LYS:O	2.21	0.40
1:F:47:GLY:O	1:F:51:ILE:HG12	2.22	0.40
1:C:59:LEU:HG	1:C:61:LEU:HD11	2.03	0.40
1:A:401:TYR:CD2	1:B:443:ALA:HB2	2.55	0.40
1:E:137:THR:OG1	1:E:140:GLU:HG3	2.21	0.40
1:D:2:ASP:CG	1:D:3:ARG:H	2.25	0.40
1:F:133:PRO:HG2	1:F:170:SER:HB3	2.02	0.40
1:C:162:VAL:HG23	1:C:163:ASP:N	2.36	0.40
1:C:25:GLU:O	1:C:29:VAL:HG23	2.21	0.40
1:C:309:ILE:N	1:C:309:ILE:HD12	2.36	0.40
1:A:139:ASN:HD22	1:B:501:THR:CG2	2.34	0.40
1:D:47:GLY:O	1:D:51:ILE:HG12	2.21	0.40
1:C:75:ILE:CD1	1:C:144:ILE:HG23	2.51	0.40
1:A:401:TYR:CE2	1:B:443:ALA:HB2	2.57	0.40
1:B:96:SER:O	1:B:130:LYS:HA	2.21	0.40
1:D:39:GLU:O	1:D:43:ASN:HB2	2.21	0.40
1:E:107:LEU:HB3	1:E:126:LYS:HG2	2.02	0.40
1:C:107:LEU:HB3	1:C:126:LYS:HG2	2.03	0.40
1:D:33:LYS:HD2	1:D:495:GLU:HG3	2.03	0.40
1:B:75:ILE:CD1	1:B:144:ILE:HG23	2.51	0.40
1:B:162:VAL:HG23	1:B:163:ASP:N	2.36	0.40
1:B:264:HIS:HA	1:B:268:ALA:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:491:ARG:HG3	1:D:491:ARG:HH11	1.86	0.40
1:A:96:SER:O	1:A:130:LYS:HA	2.20	0.40
1:E:264:HIS:HA	1:E:268:ALA:O	2.21	0.40
1:C:498:VAL:O	1:C:499:THR:CB	2.69	0.40
1:A:413:VAL:CG1	1:A:430:ILE:HG21	2.52	0.40
1:E:59:LEU:HG	1:E:61:LEU:HD11	2.02	0.40
1:B:371:LEU:H	1:B:371:LEU:HD23	1.86	0.40
1:B:287:ASP:HA	1:B:288:PRO:HD3	1.90	0.40
1:A:133:PRO:HG2	1:A:170:SER:HB3	2.02	0.40
1:F:349:ASN:N	3:F:551:NDP:HO2N	2.19	0.40
1:F:349:ASN:HB2	3:F:551:NDP:O2D	2.21	0.40
1:E:24:VAL:HG22	1:E:483:VAL:HG13	2.03	0.40
1:B:331:LEU:HD23	1:B:352:THR:HG22	2.02	0.40
1:D:25:GLU:O	1:D:29:VAL:HG23	2.21	0.40
1:A:39:GLU:O	1:A:43:ASN:HB2	2.22	0.40
1:E:96:SER:O	1:E:130:LYS:HA	2.21	0.40
1:C:244:ASP:OD2	1:C:244:ASP:N	2.51	0.40
1:D:264:HIS:HA	1:D:268:ALA:O	2.22	0.40
1:D:133:PRO:HG2	1:D:170:SER:HB3	2.04	0.40
1:F:162:VAL:HG23	1:F:163:ASP:N	2.36	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%)	464 (93%)	28 (6%)	7 (1%)	14	24
1	B	499/501 (100%)	463 (93%)	30 (6%)	6 (1%)	16	29
1	C	499/501 (100%)	459 (92%)	33 (7%)	7 (1%)	14	24
1	D	499/501 (100%)	462 (93%)	32 (6%)	5 (1%)	19	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	499/501 (100%)	462 (93%)	33 (7%)	4 (1%)	24 41
1	F	499/501 (100%)	462 (93%)	30 (6%)	7 (1%)	14 24
All	All	2994/3006 (100%)	2772 (93%)	186 (6%)	36 (1%)	16 29

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	SER
1	A	496	ALA
1	B	3	ARG
1	B	313	SER
1	C	2	ASP
1	C	5	ASP
1	C	313	SER
1	C	494	ASN
1	C	495	GLU
1	D	313	SER
1	D	498	VAL
1	E	313	SER
1	F	313	SER
1	F	495	GLU
1	A	312	GLY
1	A	422	GLY
1	A	497	GLY
1	B	312	GLY
1	B	422	GLY
1	B	495	GLU
1	C	312	GLY
1	C	422	GLY
1	D	312	GLY
1	D	422	GLY
1	D	499	THR
1	E	312	GLY
1	E	422	GLY
1	E	494	ASN
1	F	312	GLY
1	F	422	GLY
1	F	494	ASN
1	A	500	PHE
1	B	2	ASP
1	F	2	ASP

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Mol	Chain	Res	Type
1	F	498	VAL
1	A	498	VAL

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%)	394 (94%)	23 (6%)	27	48
1	B	417/417 (100%)	393 (94%)	24 (6%)	25	45
1	C	417/417 (100%)	392 (94%)	25 (6%)	24	43
1	D	417/417 (100%)	393 (94%)	24 (6%)	25	45
1	E	417/417 (100%)	393 (94%)	24 (6%)	25	45
1	F	417/417 (100%)	395 (95%)	22 (5%)	28	50
All	All	2502/2502 (100%)	2360 (94%)	142 (6%)	25	46

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	PHE
1	A	24	VAL
1	A	32	LEU
1	A	37	THR
1	A	43	ASN
1	A	107	LEU
1	A	112	THR
1	A	118	VAL
1	A	132	ASN
1	A	145	THR
1	A	255	VAL
1	A	279	SER
1	A	291	LEU
1	A	296	LEU
1	A	331	LEU
1	A	335	ASN

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Mol	Chain	Res	Type
1	A	363	ARG
1	A	364	ASN
1	A	373	LEU
1	A	386	LEU
1	A	392	VAL
1	A	410	LEU
1	A	500	PHE
1	B	3	ARG
1	B	9	PHE
1	B	24	VAL
1	B	32	LEU
1	B	37	THR
1	B	43	ASN
1	B	64	PRO
1	B	107	LEU
1	B	112	THR
1	B	118	VAL
1	B	132	ASN
1	B	145	THR
1	B	255	VAL
1	B	279	SER
1	B	291	LEU
1	B	296	LEU
1	B	331	LEU
1	B	335	ASN
1	B	363	ARG
1	B	373	LEU
1	B	378	VAL
1	B	386	LEU
1	B	392	VAL
1	B	410	LEU
1	C	2	ASP
1	C	4	GLU
1	C	9	PHE
1	C	24	VAL
1	C	32	LEU
1	C	37	THR
1	C	43	ASN
1	C	107	LEU
1	C	112	THR
1	C	118	VAL
1	C	132	ASN

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Mol	Chain	Res	Type
1	C	145	THR
1	C	255	VAL
1	C	271	VAL
1	C	279	SER
1	C	291	LEU
1	C	296	LEU
1	C	331	LEU
1	C	335	ASN
1	C	363	ARG
1	C	373	LEU
1	C	386	LEU
1	C	392	VAL
1	C	410	LEU
1	C	499	THR
1	D	4	GLU
1	D	9	PHE
1	D	24	VAL
1	D	32	LEU
1	D	37	THR
1	D	43	ASN
1	D	107	LEU
1	D	112	THR
1	D	118	VAL
1	D	132	ASN
1	D	145	THR
1	D	255	VAL
1	D	279	SER
1	D	291	LEU
1	D	296	LEU
1	D	331	LEU
1	D	335	ASN
1	D	363	ARG
1	D	373	LEU
1	D	386	LEU
1	D	392	VAL
1	D	410	LEU
1	D	499	THR
1	D	500	PHE
1	E	3	ARG
1	E	9	PHE
1	E	24	VAL
1	E	32	LEU

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Mol	Chain	Res	Type
1	E	37	THR
1	E	43	ASN
1	E	64	PRO
1	E	107	LEU
1	E	112	THR
1	E	118	VAL
1	E	132	ASN
1	E	145	THR
1	E	255	VAL
1	E	279	SER
1	E	291	LEU
1	E	296	LEU
1	E	331	LEU
1	E	335	ASN
1	E	363	ARG
1	E	373	LEU
1	E	386	LEU
1	E	392	VAL
1	E	410	LEU
1	E	494	ASN
1	F	24	VAL
1	F	32	LEU
1	F	37	THR
1	F	43	ASN
1	F	107	LEU
1	F	112	THR
1	F	118	VAL
1	F	132	ASN
1	F	145	THR
1	F	255	VAL
1	F	279	SER
1	F	291	LEU
1	F	296	LEU
1	F	331	LEU
1	F	335	ASN
1	F	363	ARG
1	F	373	LEU
1	F	386	LEU
1	F	392	VAL
1	F	410	LEU
1	F	491	ARG
1	F	495	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	82	HIS
1	A	132	ASN
1	A	195	HIS
1	A	205	GLN
1	A	254	ASN
1	A	258	HIS
1	A	330	GLN
1	A	335	ASN
1	A	364	ASN
1	A	388	ASN
1	A	406	ASN
1	A	450	HIS
1	B	56	ASN
1	B	82	HIS
1	B	132	ASN
1	B	195	HIS
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	364	ASN
1	B	388	ASN
1	B	406	ASN
1	C	56	ASN
1	C	82	HIS
1	C	132	ASN
1	C	195	HIS
1	C	254	ASN
1	C	258	HIS
1	C	330	GLN
1	C	335	ASN
1	C	364	ASN
1	C	388	ASN
1	C	406	ASN
1	C	494	ASN
1	D	56	ASN
1	D	82	HIS
1	D	132	ASN

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Mol	Chain	Res	Type
1	D	195	HIS
1	D	254	ASN
1	D	258	HIS
1	D	330	GLN
1	D	335	ASN
1	D	364	ASN
1	D	388	ASN
1	D	406	ASN
1	D	494	ASN
1	E	56	ASN
1	E	82	HIS
1	E	132	ASN
1	E	195	HIS
1	E	254	ASN
1	E	258	HIS
1	E	330	GLN
1	E	335	ASN
1	E	364	ASN
1	E	388	ASN
1	E	390	ASN
1	E	406	ASN
1	E	494	ASN
1	F	56	ASN
1	F	82	HIS
1	F	132	ASN
1	F	195	HIS
1	F	254	ASN
1	F	258	HIS
1	F	330	GLN
1	F	335	ASN
1	F	364	ASN
1	F	388	ASN
1	F	406	ASN
1	F	450	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 (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	0.64	0	3,9,11	1.19	1 (33%)
3	NDP	A	551	-	42,52,52	1.55	6 (14%)	55,80,80	3.69	24 (43%)
5	B1T	A	552	-	20,20,20	0.78	0	29,29,29	0.90	0
4	GTP	A	553	-	25,34,34	1.68	3 (12%)	34,54,54	4.41	14 (41%)
2	GLU	B	550	-	4,8,9	0.65	0	3,9,11	1.36	1 (33%)
3	NDP	B	551	-	42,52,52	1.53	3 (7%)	55,80,80	3.58	21 (38%)
5	B1T	B	552	-	20,20,20	0.75	0	29,29,29	0.76	0
4	GTP	B	553	-	25,34,34	1.52	5 (20%)	34,54,54	4.61	15 (44%)
2	GLU	C	550	-	4,8,9	0.34	0	3,9,11	1.02	0
3	NDP	C	551	-	42,52,52	1.47	5 (11%)	55,80,80	3.68	22 (40%)
5	B1T	C	552	-	20,20,20	0.76	0	29,29,29	0.78	0
4	GTP	C	553	-	25,34,34	1.92	4 (16%)	34,54,54	2.04	9 (26%)
2	GLU	D	550	-	4,8,9	0.60	0	3,9,11	1.25	1 (33%)
3	NDP	D	551	-	42,52,52	1.54	4 (9%)	55,80,80	3.63	21 (38%)
5	B1T	D	552	-	20,20,20	0.81	0	29,29,29	0.77	0
4	GTP	D	553	-	25,34,34	1.93	3 (12%)	34,54,54	4.88	15 (44%)
2	GLU	E	550	-	4,8,9	0.49	0	3,9,11	1.29	1 (33%)
3	NDP	E	551	-	42,52,52	1.44	5 (11%)	55,80,80	3.44	18 (32%)
5	B1T	E	552	-	20,20,20	0.79	0	29,29,29	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GTP	E	553	-	25,34,34	1.57	5 (20%)	34,54,54	3.75	17 (50%)
2	GLU	F	550	-	4,8,9	1.64	1 (25%)	3,9,11	0.82	0
3	NDP	F	551	-	42,52,52	1.58	6 (14%)	55,80,80	3.47	22 (40%)
5	B1T	F	552	-	20,20,20	0.82	1 (5%)	29,29,29	0.86	0
4	GTP	F	553	-	25,34,34	3.05	8 (32%)	34,54,54	4.75	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	B1T	A	552	-	-	0/4/4/4	0/2/2/2
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	B1T	B	552	-	-	0/4/4/4	0/2/2/2
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	B1T	C	552	-	-	0/4/4/4	0/2/2/2
4	GTP	C	553	-	-	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	B1T	D	552	-	-	0/4/4/4	0/2/2/2
4	GTP	D	553	-	-	0/18/38/38	0/3/3/3
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	B1T	E	552	-	-	0/4/4/4	0/2/2/2
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	B1T	F	552	-	-	0/4/4/4	0/2/2/2
4	GTP	F	553	-	-	0/18/38/38	0/3/3/3

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	553	GTP	C8-N7	-2.32	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	552	B1T	CAR-SAK	-2.25	1.75	1.78
4	A	553	GTP	C8-N7	-2.07	1.30	1.34
4	C	553	GTP	C8-N7	-2.05	1.30	1.34
3	C	551	NDP	C8A-N7A	-2.01	1.30	1.34
3	B	551	NDP	O4D-C4D	2.05	1.49	1.45
4	F	553	GTP	PG-O3G	2.05	1.62	1.54
4	B	553	GTP	PG-O2G	2.07	1.62	1.54
3	A	551	NDP	PA-O5B	2.08	1.68	1.59
4	D	553	GTP	PG-O2G	2.11	1.62	1.54
4	F	553	GTP	PB-O2B	2.11	1.64	1.54
4	C	553	GTP	C6-N1	2.13	1.37	1.33
3	F	551	NDP	PN-O2N	2.14	1.64	1.54
3	E	551	NDP	C2N-C3N	2.15	1.39	1.34
4	F	553	GTP	C5-C4	2.15	1.45	1.40
3	D	551	NDP	P2B-O3X	2.16	1.62	1.54
4	B	553	GTP	O4'-C1'	2.16	1.43	1.41
3	A	551	NDP	P2B-O3X	2.19	1.62	1.54
3	A	551	NDP	P2B-O2X	2.20	1.62	1.54
3	C	551	NDP	P2B-O2X	2.20	1.62	1.54
3	D	551	NDP	C1D-N1N	2.21	1.53	1.46
4	E	553	GTP	PG-O2G	2.22	1.62	1.54
3	E	551	NDP	P2B-O2X	2.23	1.62	1.54
4	C	553	GTP	PG-O2G	2.24	1.62	1.54
4	F	553	GTP	PA-O2A	2.25	1.64	1.54
3	F	551	NDP	P2B-O3X	2.25	1.62	1.54
4	E	553	GTP	C3'-C4'	2.26	1.59	1.53
3	F	551	NDP	P2B-O2X	2.30	1.63	1.54
4	E	553	GTP	C6-N1	2.40	1.37	1.33
4	F	553	GTP	C6-C5	2.47	1.46	1.41
3	E	551	NDP	P2B-O3X	2.48	1.63	1.54
4	B	553	GTP	C6-N1	2.48	1.37	1.33
3	F	551	NDP	C2N-C3N	2.49	1.40	1.34
3	A	551	NDP	C2N-C3N	2.50	1.40	1.34
4	E	553	GTP	O4'-C4'	2.57	1.51	1.45
4	A	553	GTP	C6-N1	2.60	1.37	1.33
4	D	553	GTP	C6-N1	2.77	1.38	1.33
3	C	551	NDP	C2N-C3N	2.87	1.41	1.34
4	B	553	GTP	C2'-C3'	2.92	1.61	1.53
3	B	551	NDP	O4D-C1D	2.96	1.49	1.42
2	F	550	GLU	CB-CA	3.00	1.56	1.53
4	E	553	GTP	O4'-C1'	3.00	1.45	1.41
4	F	553	GTP	C6-N1	3.02	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	551	NDP	O4D-C1D	3.06	1.49	1.42
3	D	551	NDP	O4D-C1D	3.09	1.49	1.42
3	A	551	NDP	O4D-C1D	3.24	1.50	1.42
3	C	551	NDP	O4D-C1D	3.30	1.50	1.42
3	E	551	NDP	O4D-C1D	3.42	1.50	1.42
3	E	551	NDP	O4B-C1B	4.15	1.46	1.41
4	F	553	GTP	C3'-C4'	4.72	1.65	1.53
3	C	551	NDP	O4B-C1B	5.09	1.47	1.41
3	A	551	NDP	O4B-C1B	5.31	1.47	1.41
4	A	553	GTP	O4'-C1'	5.53	1.48	1.41
3	B	551	NDP	O4B-C1B	5.74	1.48	1.41
3	F	551	NDP	O4B-C1B	5.90	1.48	1.41
3	D	551	NDP	O4B-C1B	5.96	1.48	1.41
4	C	553	GTP	O4'-C1'	7.03	1.50	1.41
4	D	553	GTP	O4'-C1'	7.20	1.50	1.41
4	F	553	GTP	O4'-C1'	12.28	1.56	1.41

All (220) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	553	GTP	C4'-O4'-C1'	-21.30	86.32	109.72
4	F	553	GTP	O3A-PA-O5'	-13.36	67.49	102.94
4	D	553	GTP	PA-O3A-PB	-12.67	97.15	132.73
3	A	551	NDP	O3-PA-O5B	-12.56	69.61	102.94
3	C	551	NDP	O3-PA-O5B	-12.50	69.79	102.94
3	D	551	NDP	O3-PA-O5B	-12.17	70.65	102.94
3	B	551	NDP	O3-PA-O5B	-12.10	70.84	102.94
4	F	553	GTP	O4'-C4'-C3'	-11.86	81.25	105.15
4	A	553	GTP	PA-O3A-PB	-11.39	100.75	132.73
3	C	551	NDP	PN-O3-PA	-10.70	102.67	132.73
3	F	551	NDP	O3-PA-O5B	-10.64	74.71	102.94
3	E	551	NDP	O3-PA-O5B	-10.63	74.74	102.94
3	A	551	NDP	PN-O3-PA	-10.09	104.40	132.73
3	D	551	NDP	PN-O3-PA	-9.87	105.01	132.73
3	B	551	NDP	PN-O3-PA	-9.84	105.11	132.73
4	F	553	GTP	O4'-C4'-C5'	-9.77	74.38	109.32
3	E	551	NDP	PN-O3-PA	-9.77	105.30	132.73
3	F	551	NDP	PN-O3-PA	-9.49	106.09	132.73
3	E	551	NDP	N3A-C2A-N1A	-9.12	121.91	128.89
3	A	551	NDP	O3-PN-O5D	-9.04	78.94	102.94
3	F	551	NDP	O3-PN-O5D	-9.02	79.02	102.94
3	C	551	NDP	O3-PN-O5D	-8.99	79.08	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	551	NDP	N3A-C2A-N1A	-8.95	122.04	128.89
3	A	551	NDP	N3A-C2A-N1A	-8.91	122.07	128.89
3	C	551	NDP	N3A-C2A-N1A	-8.90	122.08	128.89
3	D	551	NDP	O3-PN-O5D	-8.84	79.48	102.94
3	B	551	NDP	N3A-C2A-N1A	-8.80	122.16	128.89
3	F	551	NDP	N3A-C2A-N1A	-8.53	122.36	128.89
3	B	551	NDP	O3-PN-O5D	-8.38	80.71	102.94
4	E	553	GTP	O4'-C4'-C5'	-8.33	79.52	109.32
4	A	553	GTP	O5'-PA-O1A	-7.98	78.63	109.62
4	A	553	GTP	PB-O3B-PG	-7.44	107.71	132.67
4	D	553	GTP	PB-O3B-PG	-7.31	108.17	132.67
3	E	551	NDP	P2B-O2B-C2B	-7.25	104.18	121.56
3	A	551	NDP	C4B-O4B-C1B	-7.14	101.88	109.72
3	E	551	NDP	O3-PN-O5D	-7.12	84.06	102.94
3	F	551	NDP	P2B-O2B-C2B	-6.89	105.05	121.56
3	C	551	NDP	P2B-O2B-C2B	-6.86	105.12	121.56
4	E	553	GTP	O4'-C4'-C3'	-6.79	91.46	105.15
3	D	551	NDP	P2B-O2B-C2B	-6.53	105.89	121.56
3	B	551	NDP	P2B-O2B-C2B	-6.33	106.38	121.56
3	C	551	NDP	C4B-O4B-C1B	-6.26	102.84	109.72
4	C	553	GTP	PA-O3A-PB	-6.15	115.45	132.73
3	E	551	NDP	O5D-PN-O1N	-6.10	85.95	109.62
3	D	551	NDP	O4B-C1B-C2B	-5.96	95.83	106.60
3	D	551	NDP	C4B-O4B-C1B	-5.76	103.39	109.72
3	B	551	NDP	C4B-O4B-C1B	-5.76	103.39	109.72
4	D	553	GTP	O5'-PA-O1A	-5.59	87.91	109.62
3	B	551	NDP	O5B-PA-O1A	-5.56	88.04	109.62
3	E	551	NDP	C4B-O4B-C1B	-5.53	103.64	109.72
3	E	551	NDP	O5B-PA-O1A	-5.49	88.30	109.62
4	D	553	GTP	O2A-PA-O5'	-5.36	81.43	108.46
3	C	551	NDP	O5B-PA-O1A	-5.36	88.81	109.62
3	A	551	NDP	P2B-O2B-C2B	-5.36	108.72	121.56
3	A	551	NDP	O4B-C1B-C2B	-5.35	96.92	106.60
3	D	551	NDP	O2N-PN-O5D	-5.35	81.49	108.46
4	B	553	GTP	O3A-PA-O5'	-5.31	88.85	102.94
3	F	551	NDP	O5B-PA-O1A	-5.26	89.21	109.62
4	F	553	GTP	PB-O3B-PG	-5.25	115.05	132.67
4	C	553	GTP	PB-O3B-PG	-5.25	115.06	132.67
3	F	551	NDP	O5D-PN-O1N	-5.21	89.40	109.62
3	B	551	NDP	O2N-PN-O5D	-5.19	82.28	108.46
3	B	551	NDP	O5D-PN-O1N	-5.16	89.59	109.62
4	F	553	GTP	O5'-PA-O1A	-5.15	89.63	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	551	NDP	O4B-C1B-C2B	-5.10	97.38	106.60
4	D	553	GTP	O2A-PA-O3A	-5.09	81.98	105.09
3	C	551	NDP	O2N-PN-O5D	-5.01	83.22	108.46
3	A	551	NDP	O2N-PN-O5D	-5.01	83.22	108.46
3	A	551	NDP	O5B-PA-O1A	-4.99	90.26	109.62
3	C	551	NDP	O5D-PN-O1N	-4.99	90.26	109.62
3	B	551	NDP	O4B-C1B-C2B	-4.99	97.58	106.60
3	F	551	NDP	O2N-PN-O5D	-4.98	83.35	108.46
3	A	551	NDP	O5D-PN-O1N	-4.90	90.59	109.62
3	D	551	NDP	O5D-PN-O1N	-4.85	90.81	109.62
3	E	551	NDP	O2N-PN-O5D	-4.84	84.03	108.46
4	B	553	GTP	O5'-C5'-C4'	-4.82	91.34	109.12
3	C	551	NDP	O4B-C1B-C2B	-4.67	98.16	106.60
3	D	551	NDP	O5B-PA-O1A	-4.66	91.54	109.62
3	F	551	NDP	C4B-O4B-C1B	-4.61	104.66	109.72
4	E	553	GTP	PB-O3B-PG	-4.50	117.57	132.67
3	E	551	NDP	O4B-C1B-C2B	-4.31	98.80	106.60
4	A	553	GTP	O2A-PA-O5'	-4.18	87.38	108.46
4	B	553	GTP	PB-O3B-PG	-4.17	118.69	132.67
3	F	551	NDP	O2A-PA-O5B	-4.15	87.54	108.46
4	F	553	GTP	O5'-C5'-C4'	-4.08	94.08	109.12
4	E	553	GTP	O3A-PA-O5'	-3.97	92.40	102.94
4	A	553	GTP	O2A-PA-O3A	-3.97	87.09	105.09
3	E	551	NDP	O2A-PA-O5B	-3.91	88.75	108.46
3	D	551	NDP	O2A-PA-O5B	-3.82	89.21	108.46
4	A	553	GTP	N3-C2-N1	-3.82	121.63	127.44
4	E	553	GTP	N3-C2-N1	-3.80	121.66	127.44
4	B	553	GTP	N3-C2-N1	-3.75	121.74	127.44
4	D	553	GTP	N3-C2-N1	-3.64	121.90	127.44
4	D	553	GTP	C5-C6-N1	-3.64	118.62	123.59
4	F	553	GTP	C5-C6-N1	-3.58	118.69	123.59
4	C	553	GTP	C5-C6-N1	-3.57	118.71	123.59
4	F	553	GTP	O2A-PA-O5'	-3.54	90.60	108.46
4	A	553	GTP	C5-C6-N1	-3.46	118.86	123.59
4	C	553	GTP	N3-C2-N1	-3.40	122.26	127.44
3	A	551	NDP	O2A-PA-O5B	-3.36	91.50	108.46
3	B	551	NDP	C2D-C1D-N1N	-3.35	104.28	113.34
3	B	551	NDP	O2A-PA-O5B	-3.34	91.63	108.46
4	E	553	GTP	C5-C6-N1	-3.30	119.08	123.59
3	C	551	NDP	O2A-PA-O5B	-3.28	91.95	108.46
4	E	553	GTP	O2B-PB-O3A	-3.26	90.31	105.09
4	F	553	GTP	PA-O3A-PB	-3.22	123.68	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	551	NDP	C4A-C5A-N7A	-3.21	106.52	109.48
4	B	553	GTP	C2'-C3'-C4'	-3.16	96.11	102.61
3	D	551	NDP	O4D-C4D-C5D	-3.12	98.16	109.32
4	F	553	GTP	N3-C2-N1	-3.09	122.74	127.44
4	B	553	GTP	C5-C6-N1	-3.06	119.41	123.59
4	B	553	GTP	O2B-PB-O3A	-2.94	91.75	105.09
3	A	551	NDP	C2D-C1D-N1N	-2.90	105.52	113.34
4	F	553	GTP	C4-C5-N7	-2.82	106.89	109.48
4	D	553	GTP	C4-C5-N7	-2.75	106.95	109.48
3	A	551	NDP	C4A-C5A-N7A	-2.71	106.99	109.48
4	D	553	GTP	C6-C5-C4	-2.67	117.71	120.90
3	B	551	NDP	O4D-C4D-C5D	-2.64	99.89	109.32
4	A	553	GTP	C6-C5-C4	-2.53	117.87	120.90
3	F	551	NDP	C2D-C1D-N1N	-2.52	106.52	113.34
3	B	551	NDP	C4A-C5A-N7A	-2.52	107.16	109.48
3	C	551	NDP	C2D-C1D-N1N	-2.51	106.55	113.34
3	D	551	NDP	C4A-C5A-N7A	-2.49	107.19	109.48
3	E	551	NDP	C4A-C5A-N7A	-2.47	107.20	109.48
4	E	553	GTP	C6-C5-C4	-2.46	117.96	120.90
4	F	553	GTP	C2'-C1'-N9	-2.44	110.56	114.29
3	A	551	NDP	C1D-N1N-C6N	-2.42	115.39	120.81
3	C	551	NDP	C5D-C4D-C3D	-2.39	105.73	115.21
3	F	551	NDP	C1D-N1N-C6N	-2.37	115.51	120.81
2	B	550	GLU	O-C-CA	-2.34	119.40	125.49
4	E	553	GTP	C4-C5-N7	-2.30	107.36	109.48
3	D	551	NDP	C1D-N1N-C6N	-2.26	115.75	120.81
4	E	553	GTP	PA-O3A-PB	-2.24	126.44	132.73
2	E	550	GLU	O-C-CA	-2.24	119.66	125.49
4	D	553	GTP	C5'-C4'-C3'	-2.23	106.35	115.21
3	C	551	NDP	C1D-N1N-C6N	-2.20	115.88	120.81
3	C	551	NDP	C4A-C5A-N7A	-2.20	107.45	109.48
3	E	551	NDP	C2D-C1D-N1N	-2.19	107.42	113.34
3	A	551	NDP	C3N-C2N-N1N	-2.17	120.03	123.14
4	A	553	GTP	C4-C5-N7	-2.17	107.48	109.48
4	A	553	GTP	C5'-C4'-C3'	-2.16	106.64	115.21
3	D	551	NDP	C2D-C1D-N1N	-2.15	107.52	113.34
4	E	553	GTP	O5'-C5'-C4'	-2.14	101.25	109.12
3	B	551	NDP	C1D-N1N-C6N	-2.13	116.03	120.81
3	F	551	NDP	C3N-C2N-N1N	-2.09	120.15	123.14
2	D	550	GLU	O-C-CA	-2.08	120.07	125.49
4	C	553	GTP	C4-C5-N7	-2.08	107.57	109.48
3	C	551	NDP	C3N-C2N-N1N	-2.06	120.19	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	551	NDP	C5B-C4B-C3B	-2.03	107.14	115.21
3	A	551	NDP	C5D-C4D-C3D	-2.03	107.15	115.21
3	C	551	NDP	C5B-C4B-C3B	-2.03	107.16	115.21
2	A	550	GLU	O-C-CA	-2.01	120.24	125.49
3	C	551	NDP	C1D-N1N-C2N	2.01	124.40	120.91
3	A	551	NDP	O5D-C5D-C4D	2.01	116.54	109.12
3	C	551	NDP	O2A-PA-O3	2.03	114.32	105.09
3	A	551	NDP	O2B-C2B-C3B	2.04	119.45	111.51
4	B	553	GTP	O2B-PB-O3B	2.06	114.45	105.09
3	A	551	NDP	C1D-N1N-C2N	2.07	124.51	120.91
3	B	551	NDP	C3D-C2D-C1D	2.07	105.56	101.40
3	F	551	NDP	O2B-C2B-C1B	2.08	118.14	110.02
4	C	553	GTP	C2'-C3'-C4'	2.09	106.92	102.61
4	A	553	GTP	C2'-C3'-C4'	2.14	107.02	102.61
3	F	551	NDP	C1D-N1N-C2N	2.18	124.71	120.91
3	E	551	NDP	O2N-PN-O3	2.20	115.08	105.09
3	F	551	NDP	O2A-PA-O3	2.21	115.12	105.09
4	E	553	GTP	O2B-PB-O3B	2.22	115.16	105.09
4	F	553	GTP	O2B-PB-O3A	2.24	115.27	105.09
3	D	551	NDP	C1D-N1N-C2N	2.27	124.86	120.91
4	D	553	GTP	O4'-C1'-N9	2.28	112.87	108.10
4	D	553	GTP	C2'-C3'-C4'	2.30	107.33	102.61
3	E	551	NDP	O4B-C1B-N9A	2.34	113.00	108.10
4	C	553	GTP	O4'-C1'-N9	2.36	113.04	108.10
3	A	551	NDP	O2N-PN-O3	2.39	115.92	105.09
3	B	551	NDP	O2A-PA-O3	2.43	116.12	105.09
3	F	551	NDP	O2N-PN-O3	2.45	116.22	105.09
3	D	551	NDP	O2N-PN-O3	2.50	116.42	105.09
3	B	551	NDP	O2N-PN-O3	2.52	116.52	105.09
4	B	553	GTP	C5'-C4'-C3'	2.56	125.37	115.21
4	C	553	GTP	C1'-N9-C4	2.59	130.84	126.94
3	C	551	NDP	O2N-PN-O3	2.60	116.91	105.09
3	B	551	NDP	O4B-C1B-N9A	2.68	113.71	108.10
3	E	551	NDP	O2A-PA-O3	2.75	117.56	105.09
3	D	551	NDP	O4B-C1B-N9A	2.83	114.02	108.10
3	D	551	NDP	O2A-PA-O3	2.84	117.99	105.09
4	F	553	GTP	O2A-PA-O3A	2.96	118.53	105.09
4	B	553	GTP	C6-N1-C2	2.98	120.07	115.94
4	F	553	GTP	C6-N1-C2	3.00	120.10	115.94
4	A	553	GTP	O5'-C5'-C4'	3.01	120.22	109.12
4	C	553	GTP	C6-N1-C2	3.13	120.29	115.94
3	F	551	NDP	O4B-C1B-N9A	3.27	114.95	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	553	GTP	C6-N1-C2	3.28	120.49	115.94
4	D	553	GTP	C6-N1-C2	3.28	120.49	115.94
3	A	551	NDP	O4B-C1B-N9A	3.33	115.07	108.10
4	A	553	GTP	C6-N1-C2	3.35	120.58	115.94
4	E	553	GTP	C4'-O4'-C1'	3.37	113.42	109.72
3	E	551	NDP	O4D-C1D-N1N	3.57	115.61	108.07
3	B	551	NDP	C2D-C3D-C4D	3.72	110.27	102.61
3	D	551	NDP	C2D-C3D-C4D	3.80	110.43	102.61
3	F	551	NDP	C2D-C3D-C4D	3.92	110.68	102.61
4	B	553	GTP	O4'-C4'-C5'	3.94	123.42	109.32
3	A	551	NDP	C2D-C3D-C4D	3.98	110.80	102.61
3	E	551	NDP	C2D-C3D-C4D	4.08	110.99	102.61
4	B	553	GTP	C1'-N9-C4	4.11	133.14	126.94
4	E	553	GTP	C2'-C3'-C4'	4.16	111.17	102.61
3	C	551	NDP	C2D-C3D-C4D	4.18	111.21	102.61
3	F	551	NDP	O4D-C1D-N1N	4.26	117.06	108.07
3	C	551	NDP	O4D-C1D-N1N	4.45	117.46	108.07
4	D	553	GTP	O5'-C5'-C4'	4.55	125.90	109.12
3	A	551	NDP	O4D-C1D-N1N	4.75	118.09	108.07
3	B	551	NDP	O4D-C1D-N1N	4.81	118.23	108.07
3	D	551	NDP	O4D-C1D-N1N	5.23	119.11	108.07
4	E	553	GTP	O4'-C1'-N9	5.94	120.53	108.10
4	B	553	GTP	C2'-C1'-N9	6.22	123.79	114.29
4	B	553	GTP	O4'-C1'-N9	6.74	122.21	108.10
4	F	553	GTP	C2'-C3'-C4'	6.77	116.52	102.61
4	F	553	GTP	C5'-C4'-C3'	7.82	146.23	115.21
4	F	553	GTP	O4'-C1'-N9	8.88	126.70	108.10
4	E	553	GTP	C5'-C4'-C3'	13.24	167.75	115.21
4	A	553	GTP	O3A-PA-O5'	17.09	148.26	102.94
4	D	553	GTP	O3A-PA-O5'	20.25	156.65	102.94

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	553	GTP	C4'

There are no torsion outliers.

There are no ring outliers.

21 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	550	GLU	1	0
3	A	551	NDP	8	0
5	A	552	B1T	2	0
4	A	553	GTP	2	0
2	B	550	GLU	3	0
3	B	551	NDP	5	0
5	B	552	B1T	2	0
4	B	553	GTP	1	0
3	C	551	NDP	6	0
5	C	552	B1T	3	0
4	C	553	GTP	1	0
2	D	550	GLU	5	0
3	D	551	NDP	8	0
5	D	552	B1T	4	0
4	D	553	GTP	1	0
2	E	550	GLU	5	0
3	E	551	NDP	8	0
5	E	552	B1T	1	0
2	F	550	GLU	2	0
3	F	551	NDP	9	0
5	F	552	B1T	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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%)	0.80	58 (11%) 6 6	36, 60, 90, 105	0
1	B	501/501 (100%)	0.62	39 (7%) 16 17	36, 61, 90, 104	0
1	C	501/501 (100%)	0.56	34 (6%) 20 23	34, 59, 90, 107	0
1	D	501/501 (100%)	0.69	43 (8%) 13 14	36, 60, 91, 105	0
1	E	501/501 (100%)	0.72	48 (9%) 10 11	36, 60, 90, 105	0
1	F	501/501 (100%)	0.85	81 (16%) 3 2	37, 61, 90, 105	0
All	All	3006/3006 (100%)	0.71	303 (10%) 9 9	34, 60, 91, 107	0

All (303) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	ALA	13.3
1	E	1	ALA	12.3
1	A	501	THR	10.1
1	C	1	ALA	10.0
1	D	1	ALA	9.9
1	D	424	HIS	9.9
1	A	498	VAL	9.3
1	F	1	ALA	9.2
1	A	500	PHE	8.8
1	B	499	THR	7.9
1	A	424	HIS	7.7
1	C	501	THR	7.5
1	D	498	VAL	7.2
1	F	339	VAL	7.1
1	A	499	THR	7.1
1	A	497	GLY	7.0
1	A	1	ALA	6.6
1	B	424	HIS	6.6
1	E	4	GLU	6.5

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Mol	Chain	Res	Type	RSRZ
1	D	35	ARG	6.4
1	C	426	GLY	6.1
1	E	424	HIS	6.0
1	D	39	GLU	6.0
1	D	496	ALA	5.9
1	B	501	THR	5.9
1	F	3	ARG	5.7
1	E	501	THR	5.7
1	E	496	ALA	5.6
1	F	32	LEU	5.6
1	A	425	GLY	5.4
1	F	501	THR	5.4
1	E	425	GLY	5.3
1	F	500	PHE	5.3
1	E	3	ARG	5.3
1	B	425	GLY	5.3
1	B	500	PHE	5.2
1	D	497	GLY	5.2
1	C	424	HIS	5.2
1	F	2	ASP	5.0
1	B	497	GLY	4.9
1	D	499	THR	4.8
1	F	365	ILE	4.8
1	A	421	PHE	4.8
1	E	497	GLY	4.7
1	A	32	LEU	4.7
1	F	227	ILE	4.7
1	F	286	ILE	4.7
1	F	496	ALA	4.7
1	F	242	PHE	4.6
1	E	190	TYR	4.5
1	A	423	LYS	4.5
1	F	426	GLY	4.5
1	E	35	ARG	4.5
1	F	499	THR	4.5
1	B	32	LEU	4.4
1	A	190	TYR	4.4
1	C	190	TYR	4.4
1	A	3	ARG	4.4
1	A	35	ARG	4.4
1	B	498	VAL	4.3
1	F	190	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	426	GLY	4.2
1	E	426	GLY	4.2
1	F	33	LYS	4.2
1	D	425	GLY	4.2
1	E	2	ASP	4.2
1	C	2	ASP	4.1
1	D	190	TYR	4.1
1	C	425	GLY	4.1
1	A	40	GLN	4.0
1	A	426	GLY	4.0
1	F	35	ARG	4.0
1	F	475	LEU	4.0
1	D	281	TRP	4.0
1	F	302	LEU	4.0
1	B	88	PRO	3.9
1	C	339	VAL	3.9
1	E	499	THR	3.9
1	E	72	TRP	3.9
1	F	230	ALA	3.8
1	B	190	TYR	3.8
1	E	421	PHE	3.8
1	F	34	THR	3.8
1	A	417	LEU	3.8
1	F	4	GLU	3.8
1	E	500	PHE	3.7
1	D	40	GLN	3.7
1	B	39	GLU	3.7
1	A	389	LEU	3.7
1	F	315	LEU	3.7
1	D	87	THR	3.6
1	D	3	ARG	3.6
1	D	88	PRO	3.6
1	F	366	MET	3.6
1	C	35	ARG	3.6
1	E	87	THR	3.5
1	B	3	ARG	3.5
1	F	310	TYR	3.5
1	D	44	ARG	3.5
1	A	29	VAL	3.5
1	B	23	ILE	3.5
1	B	2	ASP	3.5
1	D	501	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	285	GLY	3.5
1	A	33	LYS	3.5
1	E	281	TRP	3.5
1	F	270	CYS	3.5
1	D	32	LEU	3.5
1	D	36	GLU	3.4
1	F	243	GLY	3.4
1	C	87	THR	3.4
1	B	35	ARG	3.3
1	C	3	ARG	3.3
1	B	496	ALA	3.3
1	D	308	LYS	3.3
1	A	39	GLU	3.3
1	A	34	THR	3.3
1	F	312	GLY	3.2
1	B	389	LEU	3.2
1	F	303	GLY	3.2
1	B	87	THR	3.2
1	F	424	HIS	3.2
1	A	36	GLU	3.1
1	E	302	LEU	3.1
1	C	496	ALA	3.1
1	D	4	GLU	3.1
1	F	232	TYR	3.0
1	C	66	ARG	3.0
1	A	390	ASN	3.0
1	A	45	VAL	3.0
1	E	308	LYS	3.0
1	A	2	ASP	2.9
1	D	440	ILE	2.9
1	F	301	ILE	2.9
1	F	316	GLU	2.9
1	D	306	LYS	2.9
1	E	32	LEU	2.9
1	C	39	GLU	2.9
1	A	88	PRO	2.9
1	C	360	PHE	2.9
1	B	297	GLN	2.9
1	F	268	ALA	2.9
1	E	423	LYS	2.8
1	E	339	VAL	2.8
1	F	238	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	39	GLU	2.8
1	D	33	LYS	2.8
1	E	236	LEU	2.8
1	C	498	VAL	2.8
1	A	87	THR	2.8
1	F	241	GLY	2.8
1	F	236	LEU	2.8
1	B	36	GLU	2.8
1	D	339	VAL	2.8
1	D	431	VAL	2.8
1	C	421	PHE	2.8
1	F	228	ASN	2.8
1	F	281	TRP	2.7
1	A	188	GLY	2.7
1	D	426	GLY	2.7
1	A	339	VAL	2.7
1	D	28	LEU	2.7
1	C	500	PHE	2.7
1	F	321	ILE	2.7
1	A	38	GLU	2.7
1	B	38	GLU	2.7
1	F	263	LEU	2.7
1	C	38	GLU	2.7
1	A	388	ASN	2.7
1	F	87	THR	2.7
1	A	267	GLY	2.7
1	F	237	GLY	2.7
1	E	33	LYS	2.7
1	C	361	LEU	2.6
1	D	428	ILE	2.6
1	F	333	LYS	2.6
1	F	251	GLY	2.6
1	F	252	PHE	2.6
1	A	311	GLU	2.6
1	D	34	THR	2.6
1	F	38	GLU	2.6
1	A	496	ALA	2.6
1	E	417	LEU	2.6
1	C	499	THR	2.6
1	F	364	ASN	2.6
1	A	66	ARG	2.5
1	F	362	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	269	LYS	2.5
1	F	498	VAL	2.5
1	D	495	GLU	2.5
1	F	423	LYS	2.5
1	C	238	MET	2.5
1	F	36	GLU	2.5
1	F	334	SER	2.5
1	D	42	ARG	2.5
1	B	33	LYS	2.5
1	F	340	LYS	2.5
1	F	233	MET	2.5
1	F	390	ASN	2.5
1	E	88	PRO	2.5
1	A	386	LEU	2.5
1	B	161	GLY	2.5
1	F	497	GLY	2.5
1	C	36	GLU	2.5
1	E	378	VAL	2.4
1	A	385	TRP	2.4
1	D	473	LEU	2.4
1	F	277	ASP	2.4
1	E	66	ARG	2.4
1	A	189	HIS	2.4
1	A	28	LEU	2.4
1	B	296	LEU	2.4
1	A	391	HIS	2.4
1	F	342	LYS	2.4
1	A	392	VAL	2.4
1	E	498	VAL	2.4
1	C	33	LYS	2.4
1	B	89	CYS	2.4
1	B	283	PRO	2.4
1	F	88	PRO	2.4
1	F	305	PRO	2.4
1	A	9	PHE	2.4
1	C	312	GLY	2.3
1	C	423	LYS	2.3
1	E	11	LYS	2.3
1	F	341	ALA	2.3
1	C	281	TRP	2.3
1	F	296	LEU	2.3
1	D	66	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	38	GLU	2.3
1	B	421	PHE	2.3
1	F	226	PHE	2.3
1	E	188	GLY	2.3
1	E	187	ILE	2.3
1	F	6	ASP	2.3
1	F	308	LYS	2.3
1	E	271	VAL	2.3
1	B	4	GLU	2.3
1	E	95	TYR	2.3
1	E	409	LEU	2.3
1	C	34	THR	2.3
1	A	180	ALA	2.3
1	A	462	ARG	2.3
1	A	302	LEU	2.3
1	F	273	VAL	2.3
1	C	462	ARG	2.3
1	C	365	ILE	2.2
1	E	495	GLU	2.2
1	C	475	LEU	2.2
1	A	427	THR	2.2
1	F	192	ILE	2.2
1	F	428	ILE	2.2
1	F	244	ASP	2.2
1	B	42	ARG	2.2
1	A	23	ILE	2.2
1	F	359	ILE	2.2
1	A	192	ILE	2.2
1	D	286	ILE	2.2
1	F	223	ILE	2.2
1	A	19	ARG	2.2
1	D	243	GLY	2.2
1	D	239	THR	2.2
1	F	311	GLU	2.2
1	D	242	PHE	2.2
1	D	490	PHE	2.2
1	A	193	ASN	2.2
1	C	403	ARG	2.1
1	F	42	ARG	2.1
1	F	389	LEU	2.1
1	A	393	SER	2.1
1	B	230	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	37	THR	2.1
1	C	88	PRO	2.1
1	E	215	THR	2.1
1	E	39	GLU	2.1
1	A	283	PRO	2.1
1	C	427	THR	2.1
1	B	435	GLU	2.1
1	A	491	ARG	2.1
1	E	243	GLY	2.1
1	B	281	TRP	2.1
1	E	24	VAL	2.1
1	B	428	ILE	2.1
1	E	389	LEU	2.1
1	F	421	PHE	2.1
1	E	75	ILE	2.1
1	E	47	GLY	2.1
1	D	419	ARG	2.0
1	E	380	VAL	2.0
1	B	385	TRP	2.0
1	E	305	PRO	2.0
1	A	419	ARG	2.0
1	A	24	VAL	2.0
1	B	392	VAL	2.0
1	F	367	VAL	2.0
1	B	5	ASP	2.0
1	F	284	ASP	2.0
1	D	500	PHE	2.0
1	D	269	LYS	2.0
1	E	469	MET	2.0
1	A	309	ILE	2.0
1	A	490	PHE	2.0
1	E	186	THR	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	B1T	A	552	19/19	0.59	0.47	10.37	106,110,114,117	0
4	GTP	B	553	32/32	0.51	0.50	9.65	105,112,119,119	0
5	B1T	B	552	19/19	0.57	0.36	8.18	103,109,112,113	0
4	GTP	A	553	32/32	0.65	0.42	8.10	111,116,125,126	0
4	GTP	C	553	32/32	0.66	0.33	6.79	104,113,129,131	0
5	B1T	C	552	19/19	0.67	0.33	6.27	104,108,114,115	0
4	GTP	F	553	32/32	0.51	0.56	6.25	116,119,134,135	0
4	GTP	D	553	32/32	0.65	0.31	5.68	105,111,117,118	0
2	GLU	E	550	9/10	0.78	0.39	5.41	68,73,74,75	0
4	GTP	E	553	32/32	0.64	0.31	3.54	100,110,124,125	0
3	NDP	D	551	48/48	0.86	0.26	3.20	52,63,74,79	0
2	GLU	A	550	9/10	0.89	0.27	2.54	58,61,62,63	0
5	B1T	F	552	19/19	0.81	0.24	2.36	93,95,99,100	0
2	GLU	B	550	9/10	0.91	0.25	1.91	54,58,60,60	0
5	B1T	E	552	19/19	0.56	0.38	1.53	105,108,114,116	0
3	NDP	C	551	48/48	0.90	0.21	1.48	43,55,66,72	0
2	GLU	F	550	9/10	0.91	0.19	1.41	67,68,70,71	0
3	NDP	E	551	48/48	0.83	0.23	1.25	67,81,86,87	0
3	NDP	A	551	48/48	0.88	0.20	1.21	59,66,73,77	0
3	NDP	B	551	48/48	0.84	0.22	1.10	64,71,80,85	0
2	GLU	C	550	9/10	0.94	0.18	0.96	52,55,56,57	0
2	GLU	D	550	9/10	0.93	0.21	0.64	41,46,50,51	0
5	B1T	D	552	19/19	0.69	0.30	0.61	104,107,112,113	0
3	NDP	F	551	48/48	0.85	0.22	0.57	74,83,85,87	0

6.5 Other polymers (i)

There are no such residues in this entry.