Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:52 PM GMT

PDB ID	:	1R0L
Title	:	1-deoxy-D-xylulose 5-phosphate reductoisomerase from zymomonas mobilis in complex with NADPH
Authors	:	Ricagno, S.; Grolle, S.; Bringer-Meyer, S.; Sahm, H.; Lindqvist, Y.; Schneider, G.
Deposited on	:	2003-09-22
Resolution	:	2.70 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:

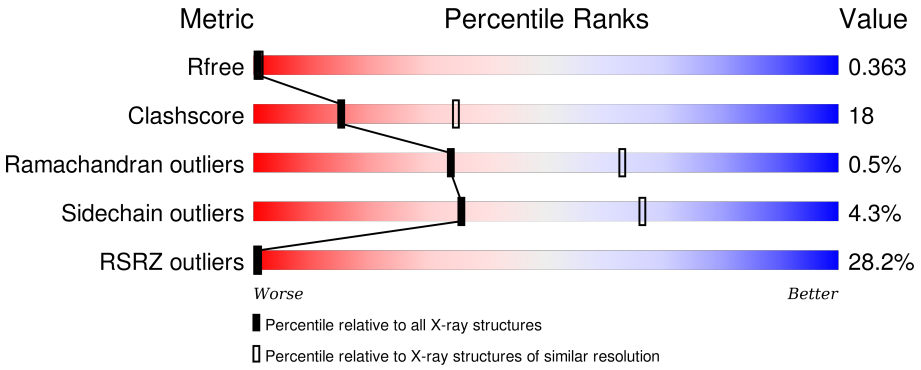
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	388	34% 63% 32%
1	B	388	15% 66% 30%
1	C	388	37% 66% 29%
1	D	388	23% 66% 30%

2 Entry composition

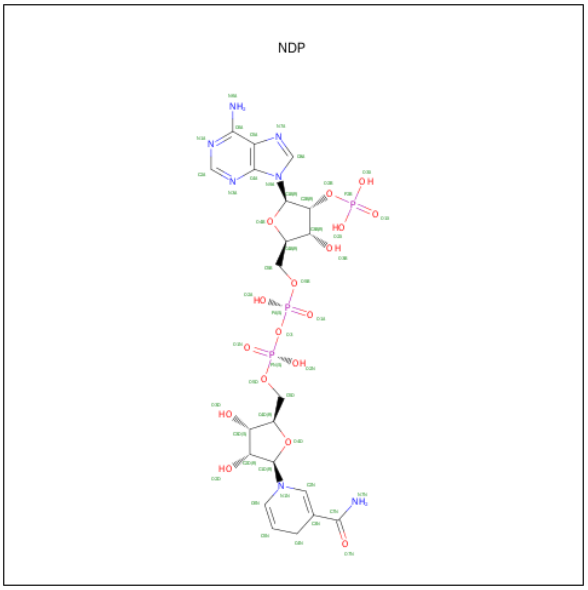
There are 3 unique types of molecules in this entry. The entry contains 11652 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1-deoxy-D-xylulose 5-phosphate reductoisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	0	0
			2854	1798	496	544	16			
1	B	379	Total	C	N	O	S	0	0	0
			2867	1807	499	545	16			
1	C	378	Total	C	N	O	S	0	0	0
			2855	1799	495	544	17			
1	D	378	Total	C	N	O	S	0	0	0
			2860	1802	498	544	16			

- Molecule 2 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
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is water.

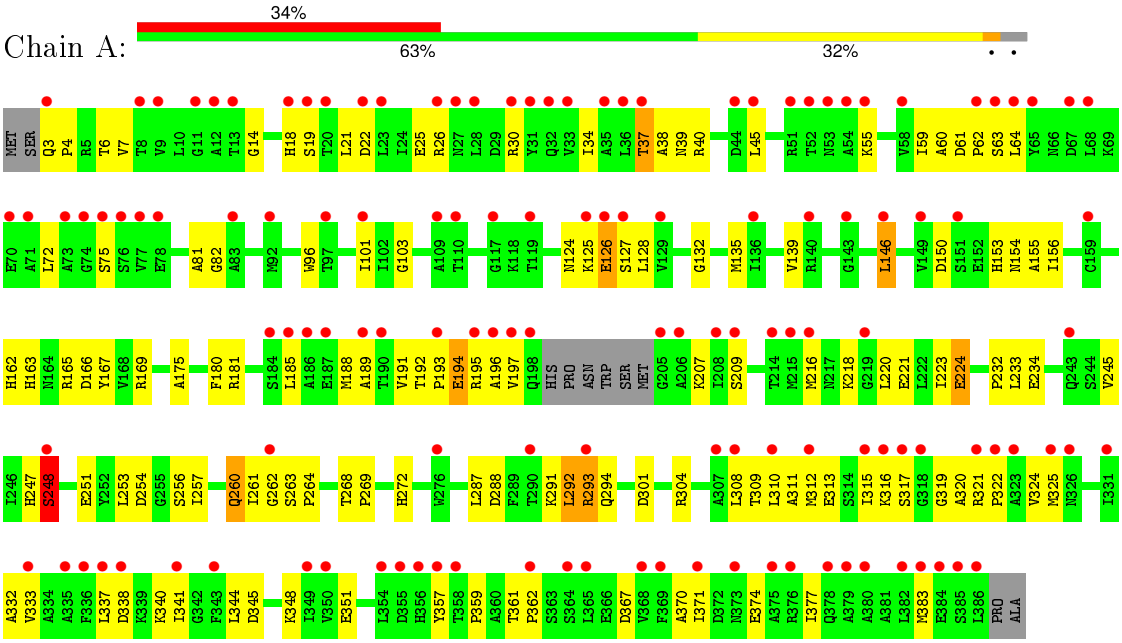
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	B	36	Total	O	0	0
			36	36		
3	C	22	Total	O	0	0
			22	22		
3	D	20	Total	O	0	0
			20	20		

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.

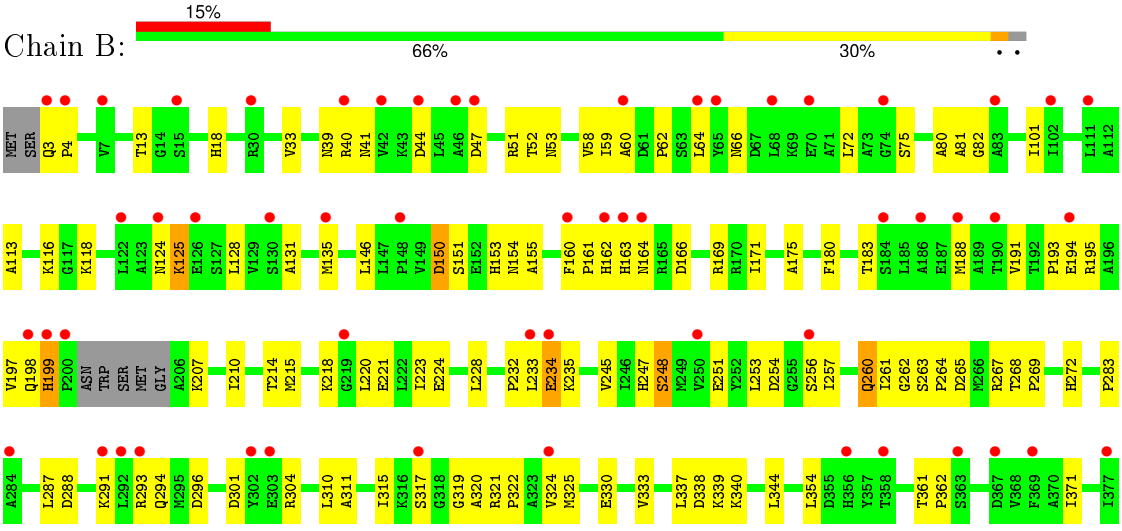
- Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase

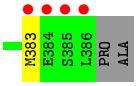
Chain A:



- Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase

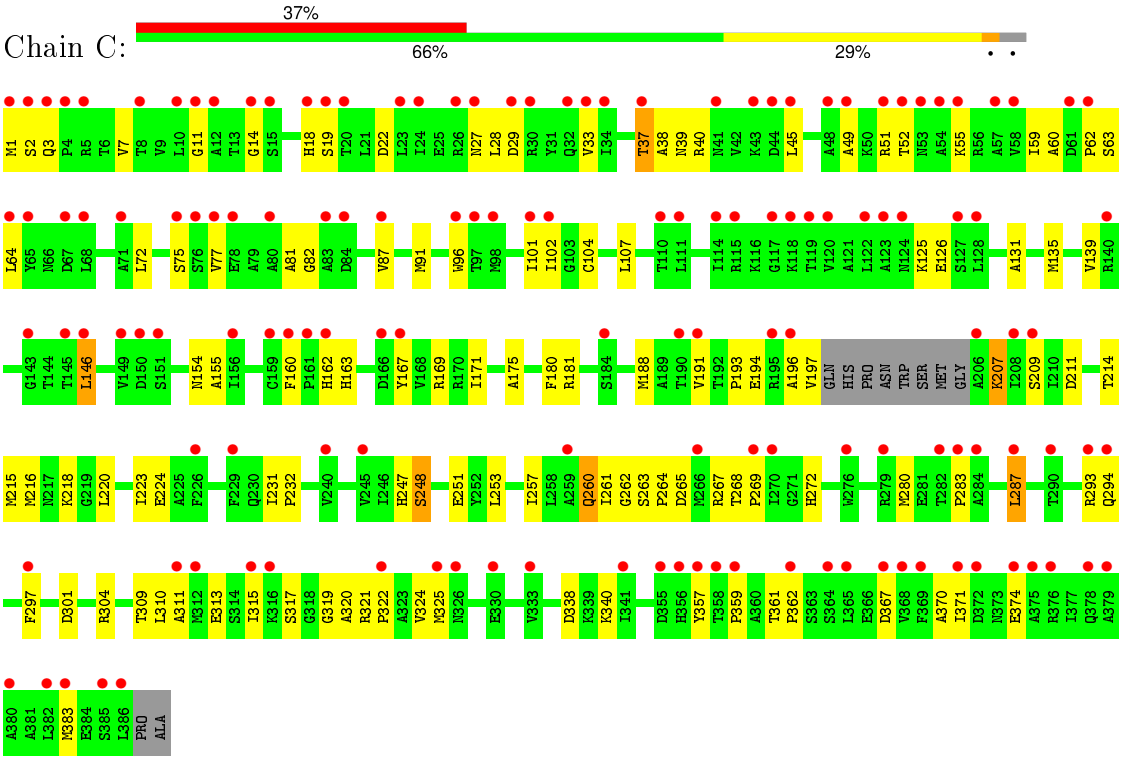
Chain B:





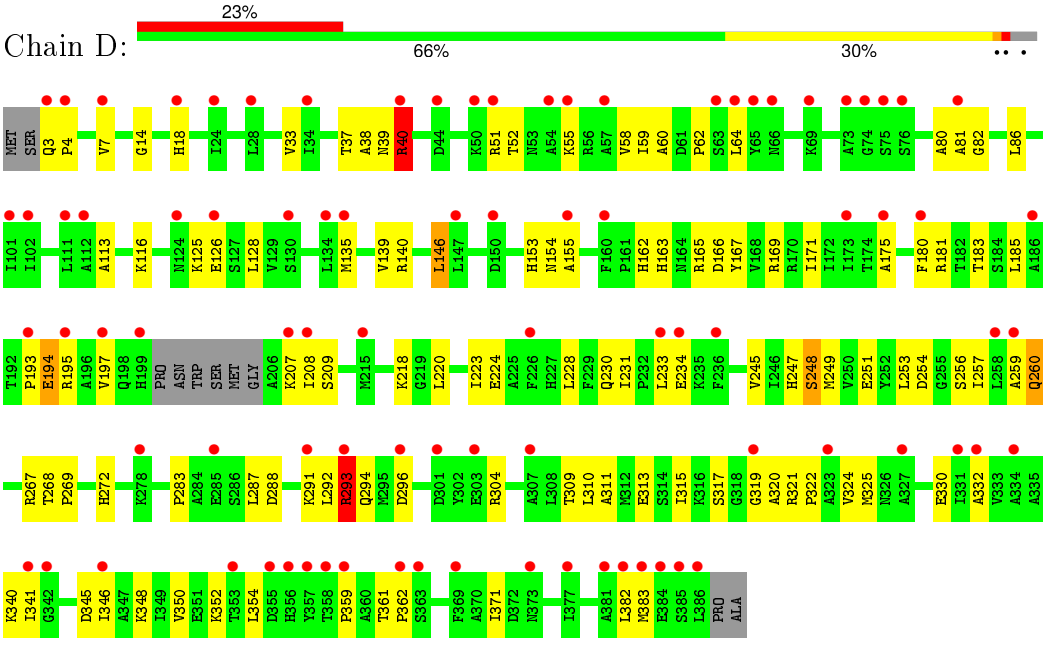
• Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase

Chain C:



• Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.70Å 93.20Å 98.60Å 90.00° 90.50° 90.00°	Depositor
Resolution (Å)	29.63 – 2.70 29.63 – 2.69	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.63-2.70) 98.3 (29.63-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.68Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.249 , 0.269 0.360 , 0.363	Depositor DCC
R_{free} test set	492 reflections (1.14%)	DCC
Wilson B-factor (Å^2)	42.4	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 40.1	EDS
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	3 of 43474 reflections (0.007%)	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	11652	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.88 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.9583e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: 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	0.45	0/2901	0.65	0/3933
1	B	0.46	1/2916 (0.0%)	0.73	2/3955 (0.1%)
1	C	0.41	0/2902	0.62	0/3934
1	D	0.41	0/2908	0.64	2/3943 (0.1%)
All	All	0.43	1/11627 (0.0%)	0.66	4/15765 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	199	HIS	C-O	-5.95	1.12	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	199	HIS	C-N-CD	-17.40	82.32	120.60
1	B	199	HIS	C-N-CA	6.81	150.59	122.00
1	D	40	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	D	126	GLU	CA-CB-CG	-5.09	102.19	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2854	0	2891	113	0
1	B	2867	0	2902	98	14
1	C	2855	0	2897	103	15
1	D	2860	0	2895	101	0
2	A	27	0	11	1	0
2	B	27	0	11	3	0
2	C	27	0	11	1	0
2	D	27	0	11	3	0
3	A	30	0	0	3	0
3	B	36	0	0	6	1
3	C	22	0	0	4	0
3	D	20	0	0	2	0
All	All	11652	0	11629	407	15

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 (407) 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:C:125:LYS:HB2	1:C:224:GLU:OE2	1.50	1.11
1:D:40:ARG:HG2	1:D:64:LEU:HD11	1.48	0.95
1:C:126:GLU:OE1	1:C:126:GLU:HA	1.74	0.87
1:A:3:GLN:HB3	1:A:4:PRO:HD3	1.59	0.84
1:A:247:HIS:HD2	1:A:260:GLN:HE22	1.25	0.82
1:C:207:LYS:HE2	1:C:211:ASP:OD2	1.81	0.80
1:B:47:ASP:CG	1:B:51:ARG:HH22	1.85	0.80
1:D:220:LEU:O	1:D:224:GLU:HG3	1.81	0.79
1:C:251:GLU:HG3	1:C:257:ILE:HG12	1.63	0.79
1:C:294:GLN:NE2	1:D:294:GLN:HE22	1.80	0.79
1:A:125:LYS:HG3	1:A:126:GLU:N	1.95	0.79
1:B:154:ASN:HD21	1:B:272:HIS:CD2	2.03	0.77
1:B:51:ARG:HG3	1:B:51:ARG:HH21	1.49	0.76
1:A:124:ASN:ND2	1:A:126:GLU:HB2	2.01	0.76
1:D:154:ASN:HD21	1:D:272:HIS:CD2	2.04	0.76
1:A:124:ASN:HD21	1:A:126:GLU:HB2	1.51	0.75
1:C:220:LEU:O	1:C:224:GLU:HG3	1.87	0.75
1:B:154:ASN:HD21	1:B:272:HIS:HD2	1.37	0.73
1:A:247:HIS:CD2	1:A:260:GLN:HE22	2.05	0.73
1:B:267:ARG:CZ	1:B:283:PRO:HG2	2.19	0.73
1:C:125:LYS:CB	1:C:224:GLU:OE2	2.36	0.72
1:D:125:LYS:HB3	1:D:224:GLU:OE2	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LEU:O	1:A:25:GLU:HG3	1.90	0.72
1:A:374:GLU:O	1:A:377:ILE:HG12	1.89	0.71
1:D:3:GLN:N	1:D:4:PRO:HD3	2.05	0.71
1:C:223:ILE:HG12	1:C:315:ILE:HG12	1.72	0.71
1:B:207:LYS:HE3	1:B:330:GLU:OE1	1.90	0.71
1:B:223:ILE:HG12	1:B:315:ILE:HG12	1.71	0.70
1:C:297:PHE:O	1:D:293:ARG:HG2	1.93	0.69
1:D:309:THR:O	1:D:313:GLU:HG3	1.92	0.69
1:D:362:PRO:HG3	1:D:371:ILE:HD12	1.76	0.68
1:D:39:ASN:HD22	1:D:60:ALA:HB3	1.59	0.68
1:C:319:GLY:HA2	1:C:361:THR:HG22	1.76	0.68
1:A:362:PRO:HG3	1:A:371:ILE:HD12	1.75	0.68
1:D:7:VAL:HG13	1:D:96:TRP:HE3	1.59	0.68
1:A:154:ASN:HD21	1:A:272:HIS:CD2	2.10	0.68
1:A:223:ILE:HG12	1:A:315:ILE:CG1	2.24	0.68
1:A:301:ASP:OD2	1:A:304:ARG:HD3	1.93	0.67
1:B:40:ARG:HH11	1:B:40:ARG:HG2	1.60	0.67
1:B:39:ASN:HB2	2:B:401:NDP:C4A	2.24	0.67
1:C:37:THR:HG21	1:C:101:ILE:HD11	1.77	0.67
1:C:180:PHE:HZ	1:C:191:VAL:HG11	1.58	0.66
1:D:59:ILE:O	1:D:81:ALA:HA	1.95	0.66
1:D:233:LEU:HD21	1:D:315:ILE:HG21	1.78	0.66
1:C:319:GLY:CA	1:C:361:THR:HG22	2.26	0.66
1:C:126:GLU:CA	1:C:126:GLU:OE1	2.43	0.66
1:D:154:ASN:HD21	1:D:272:HIS:HD2	1.43	0.66
1:B:362:PRO:HG3	1:B:371:ILE:HD12	1.78	0.65
1:D:251:GLU:HG3	1:D:257:ILE:HG12	1.78	0.65
1:A:317:SER:HB3	1:A:321:ARG:HG3	1.77	0.65
1:C:267:ARG:CZ	1:C:283:PRO:HG2	2.25	0.65
1:B:47:ASP:CG	1:B:51:ARG:NH2	2.50	0.65
1:A:223:ILE:CG1	1:A:315:ILE:HD11	2.26	0.65
1:C:338:ASP:OD1	1:C:340:LYS:HE3	1.97	0.65
1:B:233:LEU:HD21	1:B:315:ILE:HG21	1.80	0.64
1:A:7:VAL:HG13	1:A:96:TRP:HE3	1.63	0.64
1:A:357:TYR:CZ	1:A:374:GLU:HG2	2.31	0.64
1:A:223:ILE:HG12	1:A:315:ILE:HD11	1.78	0.64
1:A:207:LYS:HD2	1:A:333:VAL:HG11	1.79	0.64
1:C:311:ALA:N	1:C:325:MET:HE1	2.13	0.64
1:B:338:ASP:OD1	1:B:340:LYS:HE3	1.97	0.64
1:A:309:THR:O	1:A:313:GLU:HG3	1.98	0.64
1:C:301:ASP:OD2	1:C:304:ARG:HD3	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:HIS:ND1	3:B:434:HOH:O	2.30	0.63
1:C:39:ASN:HA	1:C:60:ALA:HB3	1.79	0.63
1:B:223:ILE:HG12	1:B:315:ILE:CG1	2.28	0.63
1:B:59:ILE:O	1:B:81:ALA:HA	1.99	0.63
1:B:267:ARG:NH1	1:B:283:PRO:HG2	2.14	0.62
1:A:125:LYS:HD3	3:A:407:HOH:O	1.98	0.62
1:C:55:LYS:NZ	1:C:55:LYS:HB3	2.14	0.62
1:B:51:ARG:NH2	1:B:51:ARG:HG3	2.13	0.62
1:C:223:ILE:HG12	1:C:315:ILE:CG1	2.29	0.62
1:A:268:THR:HB	1:A:269:PRO:CD	2.30	0.62
1:D:39:ASN:HB2	2:D:403:NDP:C4A	2.30	0.62
1:C:197:VAL:HA	1:C:209:SER:HB3	1.82	0.62
1:C:180:PHE:CZ	1:C:191:VAL:HG11	2.35	0.61
1:A:345:ASP:HA	1:A:348:LYS:HD2	1.82	0.61
1:A:62:PRO:HG3	1:A:82:GLY:HA2	1.81	0.61
1:B:194:GLU:OE1	1:B:194:GLU:N	2.34	0.61
1:A:207:LYS:CD	1:A:333:VAL:HG11	2.31	0.61
1:A:338:ASP:OD1	1:A:340:LYS:HE3	2.00	0.61
1:A:125:LYS:CG	1:A:126:GLU:N	2.63	0.61
1:D:86:LEU:HD11	2:D:403:NDP:H2A	1.82	0.60
1:D:345:ASP:HA	1:D:348:LYS:HD2	1.83	0.60
1:A:311:ALA:N	1:A:325:MET:HE1	2.17	0.60
1:D:39:ASN:HA	1:D:60:ALA:HB3	1.83	0.60
1:B:251:GLU:HG3	1:B:257:ILE:HG12	1.84	0.60
1:A:103:GLY:HA2	1:A:126:GLU:HG3	1.83	0.60
1:B:193:PRO:O	1:B:197:VAL:HG22	2.02	0.60
1:D:193:PRO:O	1:D:197:VAL:HG22	2.02	0.60
1:B:150:ASP:OD2	1:B:153:HIS:ND1	2.35	0.60
1:A:221:GLU:HA	1:A:224:GLU:HG3	1.83	0.60
1:B:47:ASP:OD2	1:B:51:ARG:NH2	2.30	0.59
1:A:30:ARG:HB2	3:A:404:HOH:O	2.02	0.59
1:C:362:PRO:HG3	1:C:371:ILE:HD12	1.84	0.59
1:A:294:GLN:NE2	1:B:294:GLN:NE2	2.50	0.59
1:B:118:LYS:HE3	3:B:430:HOH:O	2.03	0.59
1:A:162:HIS:O	1:A:163:HIS:HB2	2.03	0.59
1:A:135:MET:O	1:A:139:VAL:HG23	2.03	0.59
1:A:223:ILE:HG12	1:A:315:ILE:CD1	2.33	0.59
1:A:220:LEU:O	1:A:224:GLU:CG	2.51	0.59
1:C:7:VAL:HG13	1:C:96:TRP:HE3	1.68	0.59
1:B:3:GLN:HB2	1:B:4:PRO:HD3	1.85	0.59
1:A:223:ILE:HG12	1:A:315:ILE:HG12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:ALA:CB	1:C:218:LYS:HE3	2.33	0.58
1:D:185:LEU:HA	1:D:188:MET:HE2	1.85	0.58
1:C:62:PRO:HG3	1:C:82:GLY:HA2	1.85	0.58
1:D:223:ILE:HG12	1:D:315:ILE:HG12	1.86	0.57
1:A:207:LYS:HE2	1:A:333:VAL:HG21	1.85	0.57
1:C:72:LEU:O	1:C:75:SER:HB3	2.03	0.57
1:B:40:ARG:HA	1:B:64:LEU:CD1	2.34	0.57
1:A:319:GLY:HA2	1:A:361:THR:HG22	1.85	0.57
1:D:58:VAL:HG22	1:D:80:ALA:HB3	1.86	0.57
1:C:223:ILE:HG12	1:C:315:ILE:CD1	2.34	0.57
1:D:267:ARG:CZ	1:D:283:PRO:HG2	2.34	0.57
1:D:207:LYS:HE3	1:D:330:GLU:OE1	2.05	0.57
1:B:47:ASP:OD1	1:B:51:ARG:NH2	2.37	0.56
1:D:338:ASP:OD1	1:D:340:LYS:HE3	2.05	0.56
1:D:40:ARG:HA	1:D:64:LEU:CD1	2.35	0.56
1:B:311:ALA:O	1:B:315:ILE:HG13	2.05	0.56
1:A:180:PHE:CZ	1:A:191:VAL:HG11	2.40	0.56
1:A:216:MET:SD	1:A:325:MET:HE2	2.46	0.56
1:D:175:ALA:CB	1:D:218:LYS:HE3	2.36	0.56
1:A:220:LEU:O	1:A:224:GLU:HG3	2.06	0.56
1:C:309:THR:O	1:C:313:GLU:HG3	2.05	0.56
1:B:39:ASN:HA	1:B:60:ALA:HB3	1.88	0.56
1:B:220:LEU:O	1:B:224:GLU:HG3	2.07	0.55
1:C:40:ARG:HA	1:C:64:LEU:CD1	2.35	0.55
1:D:362:PRO:HG3	1:D:371:ILE:CD1	2.37	0.55
1:D:325:MET:HB2	1:D:354:LEU:HD21	1.88	0.55
1:B:320:ALA:O	1:B:324:VAL:HG23	2.07	0.55
1:D:310:LEU:CB	1:D:325:MET:HE3	2.36	0.55
1:A:332:ALA:O	1:A:341:ILE:HD11	2.06	0.55
1:D:268:THR:HB	1:D:269:PRO:CD	2.37	0.54
1:C:311:ALA:O	1:C:315:ILE:HG13	2.07	0.54
1:C:162:HIS:O	1:C:163:HIS:HB2	2.08	0.54
1:D:3:GLN:N	1:D:4:PRO:CD	2.71	0.54
1:D:223:ILE:HG12	1:D:315:ILE:CG1	2.38	0.54
1:B:338:ASP:HA	3:B:409:HOH:O	2.06	0.54
1:C:154:ASN:HD21	1:C:272:HIS:CD2	2.26	0.54
1:B:311:ALA:N	1:B:325:MET:HE3	2.23	0.53
1:C:59:ILE:O	1:C:81:ALA:HA	2.09	0.53
1:C:317:SER:HB3	1:C:321:ARG:HG3	1.90	0.53
1:A:175:ALA:HB2	1:A:218:LYS:HE2	1.89	0.53
1:A:292:LEU:HD22	1:A:294:GLN:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:GLY:CA	1:A:361:THR:HG22	2.39	0.53
1:C:155:ALA:HB1	1:C:260:GLN:HB3	1.89	0.53
1:B:39:ASN:ND2	1:B:40:ARG:HG3	2.24	0.53
1:B:58:VAL:HG22	1:B:80:ALA:HB3	1.90	0.53
1:C:294:GLN:NE2	1:D:294:GLN:NE2	2.52	0.53
1:B:254:ASP:OD1	1:B:256:SER:HB3	2.09	0.53
1:D:332:ALA:O	1:D:341:ILE:HD11	2.08	0.53
1:C:223:ILE:HG12	1:C:315:ILE:HD11	1.91	0.53
1:B:234:GLU:H	1:B:234:GLU:CD	2.11	0.52
1:A:154:ASN:HD21	1:A:272:HIS:HD2	1.55	0.52
1:B:188:MET:HA	1:B:191:VAL:HG23	1.90	0.52
1:A:59:ILE:O	1:A:81:ALA:HA	2.09	0.52
1:C:51:ARG:HG2	1:C:51:ARG:HH21	1.75	0.52
1:A:234:GLU:H	1:A:234:GLU:CD	2.13	0.52
1:D:311:ALA:O	1:D:315:ILE:HG13	2.09	0.52
1:A:294:GLN:HG2	1:B:296:ASP:OD1	2.10	0.52
1:D:254:ASP:OD1	1:D:256:SER:HB3	2.10	0.52
1:D:55:LYS:NZ	1:D:55:LYS:HB3	2.25	0.52
1:C:27:ASN:C	1:C:29:ASP:H	2.11	0.52
1:C:197:VAL:HG12	1:C:197:VAL:O	2.10	0.51
1:A:175:ALA:CB	1:A:218:LYS:HE2	2.40	0.51
1:A:40:ARG:HA	1:A:64:LEU:CD1	2.40	0.51
1:A:169:ARG:NH2	1:A:253:LEU:O	2.43	0.51
1:A:39:ASN:HA	1:A:60:ALA:HB3	1.91	0.51
1:C:135:MET:O	1:C:139:VAL:HG23	2.10	0.51
1:C:362:PRO:HG3	1:C:371:ILE:CD1	2.39	0.51
1:A:180:PHE:HZ	1:A:191:VAL:HG11	1.74	0.51
1:A:40:ARG:HA	1:A:64:LEU:HD12	1.92	0.51
1:B:268:THR:HB	1:B:269:PRO:CD	2.41	0.51
1:D:263:SER:HB2	1:D:264:PRO:HD2	1.91	0.51
1:C:251:GLU:HG3	1:C:257:ILE:CG1	2.39	0.51
1:D:223:ILE:HG12	1:D:315:ILE:HD11	1.93	0.51
1:A:188:MET:HA	1:A:191:VAL:HG23	1.92	0.51
1:D:188:MET:HA	1:D:191:VAL:HG23	1.92	0.51
1:C:27:ASN:C	1:C:29:ASP:N	2.63	0.51
1:B:310:LEU:HB2	1:B:325:MET:HE3	1.92	0.50
1:C:33:VAL:HG21	1:C:52:THR:HB	1.93	0.50
1:D:319:GLY:HA2	1:D:361:THR:HG22	1.93	0.50
1:A:245:VAL:O	1:A:261:ILE:HG23	2.11	0.50
1:A:254:ASP:OD1	1:A:256:SER:HB3	2.11	0.50
1:B:162:HIS:O	1:B:163:HIS:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:ARG:HG2	1:D:51:ARG:HH21	1.77	0.50
1:C:55:LYS:HZ3	1:C:55:LYS:HB3	1.75	0.50
1:B:221:GLU:HA	1:B:224:GLU:OE1	2.11	0.50
1:A:357:TYR:CE1	1:A:359:PRO:HD3	2.46	0.50
1:B:310:LEU:CB	1:B:325:MET:HE3	2.42	0.50
1:D:320:ALA:O	1:D:324:VAL:HG23	2.12	0.50
1:A:126:GLU:HA	1:A:126:GLU:OE1	2.11	0.49
1:C:40:ARG:HA	1:C:64:LEU:HD12	1.94	0.49
1:C:125:LYS:HE2	1:C:224:GLU:OE1	2.12	0.49
1:A:34:ILE:O	1:A:55:LYS:HB2	2.13	0.49
1:C:223:ILE:CG1	1:C:315:ILE:HD11	2.41	0.49
1:D:162:HIS:O	1:D:163:HIS:HB2	2.12	0.49
1:A:357:TYR:CE1	1:A:374:GLU:HG2	2.47	0.49
1:B:223:ILE:HG12	1:B:315:ILE:CD1	2.41	0.49
1:B:66:ASN:ND2	3:B:429:HOH:O	2.40	0.49
1:D:153:HIS:HE1	1:D:224:GLU:OE1	1.96	0.49
1:C:11:GLY:H	1:C:37:THR:HG22	1.78	0.49
1:D:249:MET:HG2	1:D:259:ALA:HB2	1.94	0.49
1:B:267:ARG:NH1	1:B:283:PRO:CG	2.76	0.49
1:D:39:ASN:ND2	1:D:60:ALA:HB3	2.28	0.49
1:A:357:TYR:CD1	1:A:359:PRO:HD3	2.48	0.48
1:C:357:TYR:CE1	1:C:374:GLU:HG2	2.49	0.48
1:C:216:MET:SD	1:C:325:MET:HE2	2.53	0.48
1:B:40:ARG:HA	1:B:64:LEU:HD12	1.93	0.48
1:C:101:ILE:HB	3:C:411:HOH:O	2.13	0.48
1:A:7:VAL:HG13	1:A:96:TRP:CE3	2.47	0.48
1:A:189:ALA:HB2	1:A:344:LEU:HD12	1.93	0.48
1:C:207:LYS:CE	1:C:211:ASP:OD2	2.57	0.48
1:B:261:ILE:HG22	1:B:262:GLY:N	2.28	0.48
1:D:180:PHE:HB3	1:D:183:THR:HB	1.96	0.48
1:B:101:ILE:O	1:B:124:ASN:ND2	2.46	0.48
1:B:321:ARG:HB2	1:B:322:PRO:CD	2.43	0.48
1:A:362:PRO:HG3	1:A:371:ILE:CD1	2.43	0.48
1:B:362:PRO:HG3	1:B:371:ILE:CD1	2.42	0.48
1:D:139:VAL:HG21	1:D:146:LEU:HD12	1.96	0.48
1:A:196:ALA:O	1:A:209:SER:HB3	2.14	0.48
1:A:155:ALA:HB1	1:A:260:GLN:HB3	1.95	0.48
1:D:169:ARG:NH2	1:D:253:LEU:O	2.46	0.48
1:D:175:ALA:HA	1:D:218:LYS:HE3	1.96	0.48
1:B:175:ALA:HB1	3:B:417:HOH:O	2.14	0.48
1:C:160:PHE:HE1	1:C:171:ILE:HD11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:HIS:ND1	1:B:260:GLN:NE2	2.59	0.48
1:B:265:ASP:OD1	1:B:267:ARG:HB2	2.14	0.48
1:C:37:THR:HG23	3:C:424:HOH:O	2.13	0.48
1:D:62:PRO:HG3	1:D:82:GLY:HA2	1.94	0.47
1:A:193:PRO:HB3	1:A:337:LEU:HD23	1.95	0.47
1:C:39:ASN:HB2	2:C:402:NDP:C4A	2.45	0.47
1:D:317:SER:HB3	1:D:321:ARG:HG3	1.95	0.47
1:A:3:GLN:HA	1:A:3:GLN:OE1	2.14	0.47
1:D:223:ILE:HG12	1:D:315:ILE:CD1	2.44	0.47
1:C:154:ASN:HD21	1:C:272:HIS:HD2	1.63	0.47
1:B:263:SER:HB2	1:B:264:PRO:HD2	1.95	0.47
1:D:167:TYR:O	1:D:253:LEU:HG	2.15	0.47
1:C:357:TYR:CZ	1:C:374:GLU:HG2	2.48	0.47
1:D:319:GLY:CA	1:D:361:THR:HG22	2.45	0.47
1:D:7:VAL:HG13	1:D:96:TRP:CE3	2.44	0.47
1:D:251:GLU:HG3	1:D:257:ILE:CG1	2.45	0.47
1:A:220:LEU:O	1:A:224:GLU:HG2	2.13	0.47
1:A:245:VAL:HG21	1:A:292:LEU:HD11	1.97	0.47
1:C:27:ASN:O	1:C:29:ASP:N	2.48	0.47
1:A:4:PRO:HA	1:A:30:ARG:O	2.14	0.47
1:C:214:THR:O	1:C:215:MET:HB2	2.14	0.47
1:B:180:PHE:CZ	1:B:191:VAL:HG11	2.50	0.47
1:C:251:GLU:CG	1:C:257:ILE:HG12	2.41	0.47
1:A:223:ILE:HA	1:A:315:ILE:CD1	2.45	0.47
1:C:181:ARG:C	1:C:304:ARG:HH22	2.15	0.47
1:C:7:VAL:HG13	1:C:96:TRP:CE3	2.48	0.47
1:B:160:PHE:HE1	1:B:171:ILE:HD11	1.80	0.47
1:A:223:ILE:HA	1:A:315:ILE:HD13	1.95	0.46
1:C:247:HIS:O	1:C:248:SER:CB	2.62	0.46
1:D:247:HIS:ND1	1:D:260:GLN:NE2	2.52	0.46
1:A:310:LEU:HB2	1:A:325:MET:HE1	1.97	0.46
1:A:367:ASP:O	1:A:370:ALA:HB3	2.15	0.46
1:A:320:ALA:O	1:A:324:VAL:HG23	2.16	0.46
1:A:167:TYR:O	1:A:253:LEU:HG	2.14	0.46
1:C:265:ASP:OD1	1:C:267:ARG:HB2	2.15	0.46
1:C:38:ALA:HB3	1:C:45:LEU:HD22	1.96	0.46
1:B:232:PRO:HD2	1:B:235:LYS:HD2	1.96	0.46
1:B:72:LEU:O	1:B:75:SER:HB3	2.16	0.46
1:B:125:LYS:HB2	1:B:224:GLU:OE2	2.16	0.46
1:B:40:ARG:HG2	1:B:40:ARG:NH1	2.28	0.46
1:B:169:ARG:HD2	1:B:251:GLU:OE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:LEU:HB2	1:D:325:MET:HE3	1.98	0.46
1:A:251:GLU:HG3	1:A:257:ILE:HG12	1.98	0.46
1:C:131:ALA:O	1:C:135:MET:HG2	2.16	0.46
1:A:195:ARG:O	1:A:195:ARG:HG2	2.15	0.46
1:B:223:ILE:HG12	1:B:315:ILE:HD11	1.97	0.46
1:A:294:GLN:HE22	1:B:294:GLN:NE2	2.14	0.46
1:B:155:ALA:HB1	1:B:260:GLN:HB3	1.97	0.46
1:D:249:MET:HG2	1:D:259:ALA:CB	2.46	0.45
1:C:310:LEU:C	1:C:325:MET:HE1	2.37	0.45
1:C:359:PRO:HG3	1:C:371:ILE:HG23	1.98	0.45
1:D:128:LEU:HD13	1:D:228:LEU:HG	1.99	0.45
1:C:268:THR:HB	1:C:269:PRO:CD	2.47	0.45
1:B:169:ARG:NH2	1:B:253:LEU:O	2.49	0.45
1:B:125:LYS:CB	1:B:224:GLU:OE2	2.65	0.45
1:C:193:PRO:O	1:C:197:VAL:HG23	2.16	0.45
1:A:128:LEU:HA	1:A:132:GLY:HA2	1.98	0.45
1:C:191:VAL:HG11	1:C:196:ALA:HB2	1.99	0.45
1:D:169:ARG:HD2	1:D:251:GLU:OE2	2.17	0.45
1:B:223:ILE:CG1	1:B:315:ILE:HD11	2.47	0.45
1:A:139:VAL:HG21	1:A:146:LEU:HD12	1.99	0.45
1:D:171:ILE:HD11	1:D:231:ILE:HD12	1.99	0.45
1:B:223:ILE:HD13	1:B:322:PRO:HB3	1.99	0.45
1:D:207:LYS:HD2	1:D:207:LYS:O	2.16	0.45
1:A:357:TYR:CZ	1:A:374:GLU:CG	2.99	0.45
1:C:263:SER:HB2	1:C:264:PRO:HD2	1.98	0.45
1:B:175:ALA:CB	1:B:218:LYS:HE3	2.47	0.45
1:A:6:THR:HG21	3:A:410:HOH:O	2.15	0.45
1:B:33:VAL:HG21	1:B:52:THR:HB	1.99	0.44
1:B:62:PRO:HG3	1:B:82:GLY:HA2	1.99	0.44
1:C:59:ILE:HG23	1:C:59:ILE:O	2.17	0.44
1:C:321:ARG:HB2	1:C:322:PRO:CD	2.47	0.44
1:D:269:PRO:O	1:D:272:HIS:HB3	2.17	0.44
1:B:317:SER:HB3	1:B:321:ARG:HG3	1.99	0.44
1:C:139:VAL:HG21	1:C:146:LEU:HD12	1.98	0.44
1:B:245:VAL:O	1:B:261:ILE:HG23	2.17	0.44
1:D:245:VAL:O	1:D:261:ILE:HG23	2.17	0.44
1:C:261:ILE:HG22	1:C:262:GLY:N	2.33	0.44
1:A:247:HIS:O	1:A:248:SER:CB	2.64	0.44
1:A:233:LEU:HD21	1:A:315:ILE:HG21	1.98	0.44
1:B:198:GLN:O	1:B:199:HIS:HB3	2.17	0.44
1:C:231:ILE:HG23	1:C:232:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:HIS:ND1	3:D:411:HOH:O	2.36	0.44
1:B:210:ILE:HG21	1:B:333:VAL:HG13	2.00	0.44
1:D:288:ASP:CG	1:D:291:LYS:HG2	2.38	0.44
1:C:14:GLY:O	1:C:18:HIS:HB2	2.18	0.44
1:A:321:ARG:HB2	1:A:322:PRO:CD	2.48	0.43
1:C:167:TYR:O	1:C:253:LEU:HG	2.18	0.43
1:D:165:ARG:HD2	1:D:230:GLN:O	2.19	0.43
1:C:367:ASP:O	1:C:370:ALA:HB3	2.17	0.43
1:C:19:SER:O	1:C:22:ASP:HB3	2.18	0.43
1:A:59:ILE:HG23	1:A:59:ILE:O	2.18	0.43
1:B:319:GLY:HA2	1:B:361:THR:HG22	2.00	0.43
1:B:128:LEU:HD13	1:B:228:LEU:HG	2.00	0.43
1:A:3:GLN:HB3	1:A:4:PRO:CD	2.41	0.43
1:C:175:ALA:HA	1:C:218:LYS:HE3	2.01	0.43
1:A:22:ASP:O	1:A:26:ARG:HG3	2.19	0.43
1:A:288:ASP:CG	1:A:291:LYS:HG3	2.39	0.43
1:A:192:THR:OG1	1:A:194:GLU:HG2	2.18	0.43
1:B:288:ASP:CG	1:B:291:LYS:HG2	2.39	0.43
1:D:310:LEU:C	1:D:325:MET:HE3	2.39	0.43
1:C:169:ARG:NH2	1:C:253:LEU:O	2.52	0.43
1:B:113:ALA:O	1:B:116:LYS:HB2	2.19	0.43
1:D:292:LEU:O	1:D:294:GLN:N	2.48	0.42
1:C:320:ALA:O	1:C:324:VAL:HG23	2.19	0.42
1:C:104:CYS:HA	1:C:107:LEU:HG	2.00	0.42
1:C:218:LYS:HD3	1:C:218:LYS:HA	1.86	0.42
1:A:39:ASN:HB2	2:A:400:NDP:C4A	2.49	0.42
1:A:37:THR:HG21	1:A:101:ILE:HD11	2.01	0.42
1:C:293:ARG:O	1:D:296:ASP:HA	2.18	0.42
1:D:194:GLU:HG2	1:D:194:GLU:H	1.26	0.42
1:C:37:THR:CG2	3:C:424:HOH:O	2.66	0.42
1:C:261:ILE:HG22	1:C:287:LEU:HD12	2.01	0.42
1:A:19:SER:O	1:A:22:ASP:HB3	2.19	0.42
1:B:337:LEU:C	1:B:339:LYS:H	2.21	0.42
1:D:185:LEU:HD23	1:D:188:MET:HE3	2.02	0.42
1:A:216:MET:O	1:A:220:LEU:HG	2.19	0.42
1:A:294:GLN:NE2	1:B:294:GLN:CD	2.73	0.42
1:D:33:VAL:HG21	1:D:52:THR:HB	2.02	0.42
1:C:1:MET:O	1:C:2:SER:HB2	2.19	0.42
1:D:165:ARG:CD	1:D:230:GLN:O	2.68	0.42
1:B:214:THR:O	1:B:215:MET:HB2	2.20	0.42
1:D:293:ARG:HB3	1:D:293:ARG:HE	1.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:ARG:O	1:C:304:ARG:NH2	2.42	0.42
1:A:268:THR:HB	1:A:269:PRO:HD2	2.02	0.42
1:A:232:PRO:HB3	1:A:234:GLU:OE2	2.19	0.42
1:A:308:LEU:O	1:A:312:MET:HG3	2.20	0.42
1:A:150:ASP:OD2	1:A:153:HIS:ND1	2.36	0.42
1:A:181:ARG:C	1:A:304:ARG:HH22	2.24	0.42
1:B:319:GLY:CA	1:B:361:THR:HG22	2.50	0.42
1:A:261:ILE:HG22	1:A:262:GLY:N	2.34	0.42
1:D:14:GLY:O	1:D:18:HIS:HB2	2.20	0.42
1:C:188:MET:HA	1:C:191:VAL:HG23	2.02	0.41
1:B:160:PHE:CG	1:B:161:PRO:HD2	2.55	0.41
1:D:346:ILE:O	1:D:350:VAL:HG23	2.20	0.41
1:B:41:ASN:ND2	1:B:44:ASP:OD2	2.53	0.41
1:D:352:LYS:HB3	1:D:382:LEU:HD13	2.02	0.41
1:A:263:SER:HB2	1:A:264:PRO:HD2	2.01	0.41
1:B:325:MET:HB2	1:B:354:LEU:HD21	2.02	0.41
1:B:13:THR:HG1	2:B:401:NDP:P2B	2.43	0.41
1:B:39:ASN:HB2	2:B:401:NDP:C5A	2.50	0.41
1:D:128:LEU:CD1	1:D:228:LEU:HG	2.50	0.41
1:D:261:ILE:HG22	1:D:262:GLY:N	2.35	0.41
1:A:313:GLU:O	1:A:316:LYS:HB3	2.20	0.41
1:D:181:ARG:C	1:D:304:ARG:HH22	2.23	0.41
1:D:218:LYS:HA	1:D:218:LYS:HD3	1.87	0.41
1:D:321:ARG:HB2	1:D:322:PRO:CD	2.50	0.41
1:D:113:ALA:O	1:D:116:LYS:HB2	2.21	0.41
1:D:359:PRO:HG3	1:D:371:ILE:HG23	2.02	0.41
1:A:38:ALA:HB3	1:A:45:LEU:HD22	2.03	0.41
1:D:208:ILE:HG23	1:D:209:SER:N	2.36	0.41
1:D:38:ALA:HB1	2:D:403:NDP:O3X	2.20	0.41
1:B:344:LEU:HB2	3:B:428:HOH:O	2.19	0.41
1:D:224:GLU:OE2	3:D:404:HOH:O	2.22	0.41
1:D:223:ILE:CG1	1:D:315:ILE:HD11	2.50	0.41
1:D:251:GLU:CG	1:D:257:ILE:HG12	2.49	0.41
1:A:345:ASP:O	1:A:348:LYS:HB2	2.21	0.41
1:D:267:ARG:NH1	1:D:283:PRO:HG2	2.35	0.41
1:D:91:MET:O	1:D:116:LYS:HE3	2.21	0.41
1:A:72:LEU:O	1:A:75:SER:HB3	2.20	0.41
1:B:131:ALA:O	1:B:135:MET:HG2	2.21	0.41
1:C:280:MET:HG2	3:C:406:HOH:O	2.21	0.41
1:A:156:ILE:HG13	1:A:248:SER:HB3	2.02	0.41
1:B:310:LEU:C	1:B:325:MET:HE3	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LEU:O	1:A:293:ARG:CB	2.66	0.41
1:A:14:GLY:O	1:A:18:HIS:HB2	2.20	0.41
1:D:155:ALA:HB3	1:D:248:SER:HB2	2.03	0.40
1:C:49:ALA:HB1	1:C:77:VAL:HG11	2.03	0.40
1:C:87:VAL:O	1:C:91:MET:HG3	2.21	0.40
1:B:51:ARG:NH2	1:B:51:ARG:CG	2.76	0.40
1:B:180:PHE:HB3	1:B:183:THR:HB	2.02	0.40
1:C:223:ILE:HA	1:C:315:ILE:HD13	2.03	0.40
1:D:361:THR:HA	1:D:362:PRO:HD3	1.93	0.40
1:C:319:GLY:HA3	1:C:361:THR:HG22	1.99	0.40
1:D:135:MET:O	1:D:139:VAL:HG23	2.22	0.40
1:B:301:ASP:OD2	1:B:304:ARG:HD3	2.21	0.40
1:D:40:ARG:HA	1:D:64:LEU:HD12	2.02	0.40
1:C:361:THR:HA	1:C:362:PRO:HD3	1.91	0.40
1:B:361:THR:HA	1:B:362:PRO:HD3	1.92	0.40
1:C:102:ILE:O	1:C:102:ILE:HD12	2.22	0.40

All (15) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ASN:N	1:C:1:MET:O[2_656]	0.73	1.47
1:B:164:ASN:N	1:C:1:MET:C[2_656]	1.46	0.74
1:B:163:HIS:C	1:C:1:MET:C[2_656]	1.50	0.70
1:B:164:ASN:CA	1:C:1:MET:O[2_656]	1.55	0.65
1:B:163:HIS:N	1:C:1:MET:CA[2_656]	1.59	0.61
1:B:163:HIS:CA	1:C:1:MET:CA[2_656]	1.81	0.39
1:B:163:HIS:C	1:C:1:MET:O[2_656]	1.82	0.38
1:B:162:HIS:CA	1:C:1:MET:SD[2_656]	1.85	0.35
1:B:163:HIS:C	1:C:2:SER:N[2_656]	1.87	0.33
1:B:163:HIS:O	1:C:2:SER:N[2_656]	1.99	0.21
1:B:163:HIS:CA	1:C:1:MET:C[2_656]	2.06	0.14
1:B:163:HIS:O	1:C:2:SER:CA[2_656]	2.08	0.12
1:B:163:HIS:CA	1:C:1:MET:N[2_656]	2.14	0.06
1:B:164:ASN:C	1:C:1:MET:O[2_656]	2.15	0.05
1:C:3:GLN:N	3:B:412:HOH:O[2_646]	2.16	0.04

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	374/388 (96%)	355 (95%)	17 (4%)	2 (0%)	34	63
1	B	375/388 (97%)	355 (95%)	19 (5%)	1 (0%)	46	75
1	C	374/388 (96%)	353 (94%)	19 (5%)	2 (0%)	34	63
1	D	374/388 (96%)	360 (96%)	12 (3%)	2 (0%)	34	63
All	All	1497/1552 (96%)	1423 (95%)	67 (4%)	7 (0%)	34	63

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	248	SER
1	B	248	SER
1	C	248	SER
1	D	248	SER
1	D	293	ARG
1	A	127	SER
1	C	28	LEU

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	299/308 (97%)	281 (94%)	18 (6%)	24	50
1	B	301/308 (98%)	287 (95%)	14 (5%)	32	63
1	C	300/308 (97%)	292 (97%)	8 (3%)	52	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	300/308 (97%)	288 (96%)	12 (4%)	38 69
All	All	1200/1232 (97%)	1148 (96%)	52 (4%)	35 66

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	THR
1	A	61	ASP
1	A	63	SER
1	A	126	GLU
1	A	146	LEU
1	A	165	ARG
1	A	166	ASP
1	A	185	LEU
1	A	194	GLU
1	A	197	VAL
1	A	224	GLU
1	A	248	SER
1	A	260	GLN
1	A	287	LEU
1	A	292	LEU
1	A	293	ARG
1	A	351	GLU
1	A	383	MET
1	B	18	HIS
1	B	53	ASN
1	B	125	LYS
1	B	146	LEU
1	B	150	ASP
1	B	151	SER
1	B	166	ASP
1	B	195	ARG
1	B	234	GLU
1	B	248	SER
1	B	260	GLN
1	B	287	LEU
1	B	293	ARG
1	B	383	MET
1	C	37	THR
1	C	63	SER
1	C	146	LEU
1	C	194	GLU

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Mol	Chain	Res	Type
1	C	207	LYS
1	C	260	GLN
1	C	287	LEU
1	C	383	MET
1	D	37	THR
1	D	40	ARG
1	D	140	ARG
1	D	146	LEU
1	D	166	ASP
1	D	194	GLU
1	D	195	ARG
1	D	234	GLU
1	D	260	GLN
1	D	287	LEU
1	D	293	ARG
1	D	383	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	247	HIS
1	A	260	GLN
1	A	272	HIS
1	A	294	GLN
1	B	53	ASN
1	B	260	GLN
1	B	272	HIS
1	B	294	GLN
1	C	53	ASN
1	C	260	GLN
1	C	272	HIS
1	C	294	GLN
1	D	39	ASN
1	D	53	ASN
1	D	142	HIS
1	D	153	HIS
1	D	260	GLN
1	D	272	HIS

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

4 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	NDP	A	400	-	24,29,52	1.76	8 (33%)	29,45,80	3.01	13 (44%)
2	NDP	B	401	-	24,29,52	1.74	5 (20%)	29,45,80	3.04	12 (41%)
2	NDP	C	402	-	24,29,52	1.60	3 (12%)	29,45,80	1.89	7 (24%)
2	NDP	D	403	-	24,29,52	3.68	11 (45%)	29,45,80	4.43	17 (58%)

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	NDP	A	400	-	-	0/11/31/77	0/3/3/5
2	NDP	B	401	-	-	0/11/31/77	0/3/3/5
2	NDP	C	402	-	-	0/11/31/77	0/3/3/5
2	NDP	D	403	-	-	0/11/31/77	0/3/3/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	403	NDP	O5B-C5B	-7.33	1.14	1.44
2	D	403	NDP	C3B-C4B	-6.86	1.34	1.53
2	D	403	NDP	C8A-N7A	-5.67	1.23	1.34
2	D	403	NDP	C5B-C4B	-5.61	1.33	1.51
2	C	402	NDP	PA-O1A	-3.64	1.39	1.51
2	B	401	NDP	PA-O1A	-3.46	1.39	1.51
2	A	400	NDP	PA-O1A	-3.04	1.41	1.51
2	B	401	NDP	C8A-N7A	-2.90	1.29	1.34
2	C	402	NDP	C8A-N7A	-2.72	1.29	1.34
2	B	401	NDP	C5B-C4B	-2.56	1.43	1.51
2	A	400	NDP	C8A-N7A	-2.41	1.30	1.34
2	A	400	NDP	P2B-O2B	-2.38	1.52	1.60
2	D	403	NDP	PA-O1A	-2.11	1.44	1.51
2	A	400	NDP	C5B-C4B	-2.11	1.44	1.51
2	D	403	NDP	C2A-N1A	2.04	1.37	1.33
2	A	400	NDP	C3B-C4B	2.09	1.58	1.53
2	A	400	NDP	C2A-N3A	2.38	1.36	1.32
2	A	400	NDP	O4B-C1B	2.68	1.44	1.41
2	D	403	NDP	O4B-C4B	3.06	1.52	1.45
2	D	403	NDP	C2A-N3A	3.18	1.37	1.32
2	D	403	NDP	O3B-C3B	3.20	1.50	1.43
2	B	401	NDP	C3B-C4B	3.26	1.61	1.53
2	D	403	NDP	PA-O5B	3.28	1.71	1.60
2	B	401	NDP	O3B-C3B	3.42	1.51	1.43
2	C	402	NDP	O3B-C3B	3.77	1.52	1.43
2	A	400	NDP	O3B-C3B	4.53	1.53	1.43
2	D	403	NDP	O4B-C1B	10.01	1.53	1.41

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	403	NDP	O3-PA-O2A	-9.95	69.50	107.38
2	B	401	NDP	O3X-P2B-O1X	-9.15	81.14	110.58
2	A	400	NDP	O3X-P2B-O1X	-9.10	81.30	110.58
2	D	403	NDP	O3X-P2B-O1X	-8.55	83.07	110.58
2	D	403	NDP	N3A-C2A-N1A	-7.12	123.44	128.89
2	D	403	NDP	O5B-PA-O1A	-7.05	89.20	107.14
2	A	400	NDP	N3A-C2A-N1A	-6.83	123.66	128.89
2	B	401	NDP	O3X-P2B-O2X	-6.48	82.69	107.38
2	D	403	NDP	C4B-O4B-C1B	-6.30	102.79	109.72
2	D	403	NDP	O3X-P2B-O2X	-5.75	85.48	107.38
2	C	402	NDP	N3A-C2A-N1A	-5.44	124.73	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	400	NDP	O3X-P2B-O2X	-5.26	87.35	107.38
2	B	401	NDP	N3A-C2A-N1A	-5.00	125.07	128.89
2	C	402	NDP	O4B-C4B-C5B	-3.69	96.13	109.32
2	A	400	NDP	O4B-C4B-C5B	-3.63	96.34	109.32
2	B	401	NDP	O5B-C5B-C4B	-3.44	96.42	109.12
2	B	401	NDP	O4B-C4B-C5B	-3.34	97.38	109.32
2	C	402	NDP	O5B-C5B-C4B	-3.18	97.40	109.12
2	A	400	NDP	O5B-C5B-C4B	-2.64	99.37	109.12
2	D	403	NDP	O3B-C3B-C4B	-2.52	103.49	111.05
2	D	403	NDP	C3B-C2B-C1B	-2.32	98.23	102.73
2	B	401	NDP	O2A-PA-O5B	-2.27	100.01	106.56
2	A	400	NDP	O2A-PA-O5B	-2.16	100.34	106.56
2	A	400	NDP	C3B-C2B-C1B	-2.08	98.70	102.73
2	C	402	NDP	C3B-C2B-C1B	-2.02	98.82	102.73
2	C	402	NDP	O2B-C2B-C3B	2.04	119.44	111.51
2	D	403	NDP	C2B-C3B-C4B	2.07	106.76	101.85
2	A	400	NDP	O2B-C2B-C3B	2.12	119.76	111.51
2	C	402	NDP	O2B-C2B-C1B	2.22	118.68	110.02
2	B	401	NDP	O2B-C2B-C1B	2.24	118.75	110.02
2	A	400	NDP	O2B-C2B-C1B	2.26	118.83	110.02
2	B	401	NDP	O2B-C2B-C3B	2.42	120.92	111.51
2	B	401	NDP	C1B-N9A-C4A	2.54	130.78	126.94
2	A	400	NDP	C1B-N9A-C4A	2.56	130.80	126.94
2	D	403	NDP	O5B-C5B-C4B	3.23	121.03	109.12
2	D	403	NDP	O2B-P2B-O1X	3.68	116.30	107.11
2	C	402	NDP	O2A-PA-O1A	3.81	122.84	110.58
2	A	400	NDP	O2B-P2B-O1X	3.89	116.82	107.11
2	B	401	NDP	O2A-PA-O1A	3.92	123.21	110.58
2	A	400	NDP	O2A-PA-O1A	4.00	123.45	110.58
2	B	401	NDP	O2B-P2B-O1X	4.02	117.14	107.11
2	D	403	NDP	O2X-P2B-O1X	4.09	123.75	110.58
2	A	400	NDP	O2X-P2B-O1X	4.19	124.07	110.58
2	B	401	NDP	O2X-P2B-O1X	4.51	125.11	110.58
2	D	403	NDP	O2A-PA-O5B	4.65	119.94	106.56
2	D	403	NDP	O3-PA-O5B	4.79	120.35	106.56
2	D	403	NDP	C1B-N9A-C4A	5.01	134.50	126.94
2	D	403	NDP	O2A-PA-O1A	5.65	128.77	110.58
2	D	403	NDP	O3-PA-O1A	7.07	133.33	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	NDP	1	0
2	B	401	NDP	3	0
2	C	402	NDP	1	0
2	D	403	NDP	3	0

5.7 Other polymers

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	378/388 (97%)	1.76	132 (34%) 0 0	16, 43, 87, 104	0
1	B	379/388 (97%)	1.12	60 (15%) 3 2	17, 35, 63, 88	0
1	C	378/388 (97%)	1.92	143 (37%) 0 0	22, 44, 69, 94	0
1	D	378/388 (97%)	1.48	91 (24%) 1 1	22, 45, 74, 107	0
All	All	1513/1552 (97%)	1.57	426 (28%) 1 0	16, 41, 75, 107	0

All (426) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	10.8
1	C	2	SER	10.5
1	C	68	LEU	9.6
1	C	71	ALA	8.7
1	C	365	LEU	7.9
1	A	68	LEU	7.5
1	A	365	LEU	7.5
1	D	4	PRO	6.7
1	C	65	TYR	6.5
1	C	362	PRO	6.3
1	C	356	HIS	6.1
1	B	200	PRO	6.1
1	A	362	PRO	6.0
1	D	356	HIS	6.0
1	A	356	HIS	5.9
1	C	44	ASP	5.7
1	B	199	HIS	5.6
1	C	45	LEU	5.5
1	C	209	SER	5.5
1	C	386	LEU	5.5
1	A	375	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	76	SER	5.1
1	C	385	SER	4.9
1	C	161	PRO	4.8
1	A	209	SER	4.7
1	B	293	ARG	4.7
1	C	52	THR	4.6
1	C	368	VAL	4.6
1	D	303	GLU	4.6
1	C	143	GLY	4.6
1	A	205	GLY	4.5
1	A	140	ARG	4.4
1	D	355	ASP	4.3
1	D	126	GLU	4.3
1	A	379	ALA	4.3
1	A	64	LEU	4.3
1	A	185	LEU	4.2
1	A	71	ALA	4.2
1	A	73	ALA	4.2
1	C	375	ALA	4.2
1	A	385	SER	4.2
1	C	357	TYR	4.2
1	C	312	MET	4.1
1	C	76	SER	4.1
1	C	374	GLU	4.1
1	B	383	MET	4.1
1	C	78	GLU	4.1
1	C	64	LEU	4.0
1	D	64	LEU	4.0
1	D	373	ASN	4.0
1	D	74	GLY	4.0
1	D	233	LEU	4.0
1	C	41	ASN	4.0
1	C	315	ILE	4.0
1	C	326	ASN	3.9
1	A	364	SER	3.9
1	C	27	ASN	3.9
1	A	368	VAL	3.9
1	C	62	PRO	3.9
1	A	333	VAL	3.9
1	C	3	GLN	3.9
1	C	34	ILE	3.8
1	C	18	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	126	GLU	3.8
1	A	349	ILE	3.8
1	A	196	ALA	3.8
1	A	117	GLY	3.8
1	B	124	ASN	3.8
1	C	58	VAL	3.8
1	C	287	LEU	3.8
1	A	27	ASN	3.8
1	A	378	GLN	3.8
1	A	190	THR	3.7
1	A	197	VAL	3.7
1	C	371	ILE	3.7
1	A	386	LEU	3.7
1	A	317	SER	3.7
1	A	44	ASP	3.7
1	D	197	VAL	3.6
1	C	8	THR	3.6
1	D	102	ILE	3.6
1	C	369	PHE	3.6
1	D	75	SER	3.6
1	D	383	MET	3.6
1	C	276	TRP	3.6
1	A	52	THR	3.6
1	C	149	VAL	3.6
1	B	384	GLU	3.6
1	B	46	ALA	3.6
1	D	3	GLN	3.6
1	D	386	LEU	3.6
1	C	55	LYS	3.6
1	A	67	ASP	3.5
1	D	384	GLU	3.5
1	A	312	MET	3.5
1	C	208	ILE	3.5
1	D	180	PHE	3.5
1	C	190	THR	3.5
1	C	140	ARG	3.5
1	A	293	ARG	3.5
1	B	164	ASN	3.5
1	C	53	ASN	3.5
1	A	35	ALA	3.5
1	C	24	ILE	3.4
1	C	117	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	358	THR	3.4
1	D	18	HIS	3.4
1	C	355	ASP	3.4
1	D	63	SER	3.4
1	A	189	ALA	3.4
1	A	371	ILE	3.4
1	C	383	MET	3.4
1	B	163	HIS	3.3
1	D	293	ARG	3.3
1	C	341	ILE	3.3
1	C	67	ASP	3.3
1	B	4	PRO	3.3
1	B	386	LEU	3.3
1	D	359	PRO	3.3
1	B	40	ARG	3.3
1	A	18	HIS	3.3
1	D	199	HIS	3.3
1	C	30	ARG	3.3
1	D	135	MET	3.3
1	C	98	MET	3.3
1	D	377	ILE	3.3
1	B	68	LEU	3.2
1	C	325	MET	3.2
1	B	356	HIS	3.2
1	D	341	ILE	3.2
1	C	378	GLN	3.2
1	A	13	THR	3.2
1	C	297	PHE	3.2
1	A	125	LYS	3.2
1	C	11	GLY	3.2
1	C	316	LYS	3.2
1	A	208	ILE	3.1
1	D	363	SER	3.1
1	C	115	ARG	3.1
1	D	186	ALA	3.1
1	A	12	ALA	3.1
1	A	376	ARG	3.1
1	A	383	MET	3.1
1	A	290	THR	3.1
1	C	29	ASP	3.1
1	C	57	ALA	3.1
1	C	196	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	112	ALA	3.1
1	A	380	ALA	3.1
1	D	327	ALA	3.1
1	D	332	ALA	3.1
1	A	126	GLU	3.1
1	B	219	GLY	3.1
1	B	385	SER	3.1
1	A	8	THR	3.1
1	A	19	SER	3.1
1	C	49	ALA	3.1
1	D	111	LEU	3.1
1	A	341	ILE	3.1
1	B	15	SER	3.1
1	B	3	GLN	3.1
1	C	96	TRP	3.1
1	C	372	ASP	3.1
1	C	77	VAL	3.0
1	D	73	ALA	3.0
1	C	159	CYS	3.0
1	A	350	VAL	3.0
1	C	51	ARG	3.0
1	D	57	ALA	3.0
1	D	76	SER	3.0
1	C	290	THR	3.0
1	A	325	MET	3.0
1	C	150	ASP	3.0
1	D	124	ASN	3.0
1	A	54	ALA	3.0
1	C	15	SER	3.0
1	A	143	GLY	3.0
1	B	70	GLU	3.0
1	A	357	TYR	2.9
1	C	20	THR	2.9
1	D	381	ALA	2.9
1	C	87	VAL	2.9
1	D	160	PHE	2.9
1	B	162	HIS	2.9
1	B	233	LEU	2.9
1	B	30	ARG	2.9
1	C	54	ALA	2.9
1	D	334	ALA	2.9
1	D	130	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	311	ALA	2.9
1	C	195	ARG	2.9
1	C	75	SER	2.9
1	C	330	GLU	2.9
1	B	42	VAL	2.9
1	C	191	VAL	2.9
1	C	48	ALA	2.9
1	C	80	ALA	2.9
1	A	326	ASN	2.9
1	A	127	SER	2.8
1	A	337	LEU	2.8
1	A	331	ILE	2.8
1	A	322	PRO	2.8
1	B	148	PRO	2.8
1	C	118	LYS	2.8
1	B	102	ILE	2.8
1	C	97	THR	2.8
1	A	75	SER	2.8
1	C	151	SER	2.8
1	C	37	THR	2.8
1	D	291	LYS	2.7
1	A	321	ARG	2.7
1	C	101	ILE	2.7
1	C	240	VAL	2.7
1	C	322	PRO	2.7
1	D	307	ALA	2.7
1	A	318	GLY	2.7
1	A	28	LEU	2.7
1	A	198	GLN	2.7
1	D	385	SER	2.7
1	B	291	LYS	2.7
1	B	135	MET	2.7
1	A	30	ARG	2.7
1	C	119	THR	2.7
1	A	215	MET	2.7
1	C	61	ASP	2.7
1	C	84	ASP	2.7
1	D	319	GLY	2.7
1	D	353	THR	2.7
1	A	373	ASN	2.7
1	C	167	TYR	2.7
1	A	23	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	364	SER	2.7
1	B	111	LEU	2.6
1	A	276	TRP	2.6
1	C	162	HIS	2.6
1	A	37	THR	2.6
1	B	64	LEU	2.6
1	C	23	LEU	2.6
1	B	44	ASP	2.6
1	A	159	CYS	2.6
1	C	333	VAL	2.6
1	A	31	TYR	2.6
1	C	270	ILE	2.6
1	D	357	TYR	2.6
1	A	187	GLU	2.6
1	A	55	LYS	2.6
1	A	369	PHE	2.6
1	B	377	ILE	2.6
1	B	60	ALA	2.6
1	B	186	ALA	2.6
1	D	234	GLU	2.6
1	D	40	ARG	2.6
1	C	184	SER	2.6
1	B	47	ASP	2.6
1	B	363	SER	2.6
1	A	206	ALA	2.5
1	C	12	ALA	2.5
1	C	294	GLN	2.5
1	A	63	SER	2.5
1	A	53	ASN	2.5
1	C	26	ARG	2.5
1	D	69	LYS	2.5
1	C	122	LEU	2.5
1	D	278	LYS	2.5
1	A	184	SER	2.5
1	B	256	SER	2.5
1	C	127	SER	2.5
1	A	74	GLY	2.5
1	A	343	PHE	2.5
1	C	120	VAL	2.5
1	A	119	THR	2.5
1	B	65	TYR	2.5
1	D	51	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	160	PHE	2.5
1	C	266	MET	2.5
1	C	367	ASP	2.5
1	D	44	ASP	2.5
1	C	382	LEU	2.5
1	C	359	PRO	2.5
1	D	296	ASP	2.4
1	A	36	LEU	2.4
1	A	9	VAL	2.4
1	A	26	ARG	2.4
1	A	354	LEU	2.4
1	C	269	PRO	2.4
1	A	33	VAL	2.4
1	A	149	VAL	2.4
1	A	358	THR	2.4
1	D	338	ASP	2.4
1	D	134	LEU	2.4
1	A	136	ILE	2.4
1	D	323	ALA	2.4
1	D	346	ILE	2.4
1	D	147	LEU	2.4
1	C	379	ALA	2.4
1	C	380	ALA	2.4
1	A	22	ASP	2.4
1	A	109	ALA	2.4
1	C	83	ALA	2.4
1	C	206	ALA	2.4
1	A	195	ARG	2.4
1	A	78	GLU	2.4
1	C	5	ARG	2.4
1	B	303	GLU	2.3
1	B	250	VAL	2.3
1	D	81	ALA	2.3
1	A	110	THR	2.3
1	A	32	GLN	2.3
1	C	124	ASN	2.3
1	B	234	GLU	2.3
1	A	51	ARG	2.3
1	A	101	ILE	2.3
1	B	194	GLU	2.3
1	A	3	GLN	2.3
1	C	259	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	58	VAL	2.3
1	A	77	VAL	2.3
1	A	193	PRO	2.3
1	C	10	LEU	2.3
1	B	130	SER	2.3
1	B	74	GLY	2.3
1	A	323	ALA	2.3
1	D	50	LYS	2.3
1	A	384	GLU	2.3
1	B	302	TYR	2.3
1	D	226	PHE	2.3
1	C	43	LYS	2.3
1	A	335	ALA	2.3
1	C	123	ALA	2.3
1	D	65	TYR	2.3
1	A	308	LEU	2.3
1	B	122	LEU	2.3
1	C	146	LEU	2.3
1	D	382	LEU	2.3
1	A	219	GLY	2.3
1	A	315	ILE	2.3
1	C	166	ASP	2.2
1	C	226	PHE	2.2
1	A	83	ALA	2.2
1	B	198	GLN	2.2
1	B	358	THR	2.2
1	A	355	ASP	2.2
1	B	367	ASP	2.2
1	A	146	LEU	2.2
1	A	336	PHE	2.2
1	B	369	PHE	2.2
1	C	19	SER	2.2
1	B	7	VAL	2.2
1	D	208	ILE	2.2
1	C	279	ARG	2.2
1	C	33	VAL	2.2
1	C	156	ILE	2.2
1	D	28	LEU	2.2
1	D	150	ASP	2.2
1	C	4	PRO	2.2
1	D	342	GLY	2.2
1	D	55	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	34	ILE	2.2
1	D	362	PRO	2.2
1	C	128	LEU	2.2
1	D	236	PHE	2.2
1	A	316	LYS	2.2
1	C	32	GLN	2.1
1	C	110	THR	2.2
1	D	24	ILE	2.1
1	D	331	ILE	2.1
1	C	14	GLY	2.1
1	D	175	ALA	2.1
1	A	92	MET	2.1
1	B	324	VAL	2.1
1	C	282	THR	2.1
1	A	151	SER	2.1
1	D	66	ASN	2.1
1	A	65	TYR	2.1
1	A	20	THR	2.1
1	A	45	LEU	2.1
1	D	358	THR	2.1
1	A	186	ALA	2.1
1	B	184	SER	2.1
1	B	292	LEU	2.1
1	A	243	GLN	2.1
1	D	301	ASP	2.1
1	D	258	LEU	2.1
1	A	97	THR	2.1
1	D	215	MET	2.1
1	D	261	ILE	2.1
1	D	193	PRO	2.1
1	B	284	ALA	2.1
1	D	155	ALA	2.1
1	D	207	LYS	2.1
1	A	338	ASP	2.1
1	C	376	ARG	2.1
1	D	259	ALA	2.1
1	D	285	GLU	2.1
1	D	7	VAL	2.1
1	B	188	MET	2.1
1	C	229	PHE	2.1
1	C	283	PRO	2.1
1	D	336	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	54	ALA	2.1
1	A	62	PRO	2.0
1	D	101	ILE	2.0
1	A	262	GLY	2.0
1	B	83	ALA	2.0
1	A	310	LEU	2.0
1	A	382	LEU	2.0
1	B	317	SER	2.0
1	C	284	ALA	2.0
1	A	129	VAL	2.0
1	A	214	THR	2.0
1	B	190	THR	2.0
1	C	114	ILE	2.0
1	D	195	ARG	2.0
1	A	216	MET	2.0
1	A	11	GLY	2.0
1	A	248	SER	2.0
1	A	307	ALA	2.0
1	C	111	LEU	2.0
1	A	70	GLU	2.0
1	C	145	THR	2.0
1	C	245	VAL	2.0
1	B	160	PHE	2.0
1	C	102	ILE	2.0
1	D	173	ILE	2.0
1	C	293	ARG	2.0
1	D	369	PHE	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
2	NDP	C	402	27/48	0.69	0.33	0.22	74,76,99,101	0
2	NDP	A	400	27/48	0.74	0.27	-0.42	61,63,89,95	0
2	NDP	B	401	27/48	0.81	0.20	-0.60	41,53,88,96	0
2	NDP	D	403	27/48	0.84	0.20	-0.96	51,55,75,78	0

6.5 Other polymers (i)

There are no such residues in this entry.