



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2018 – 10:59 AM EST

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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030736

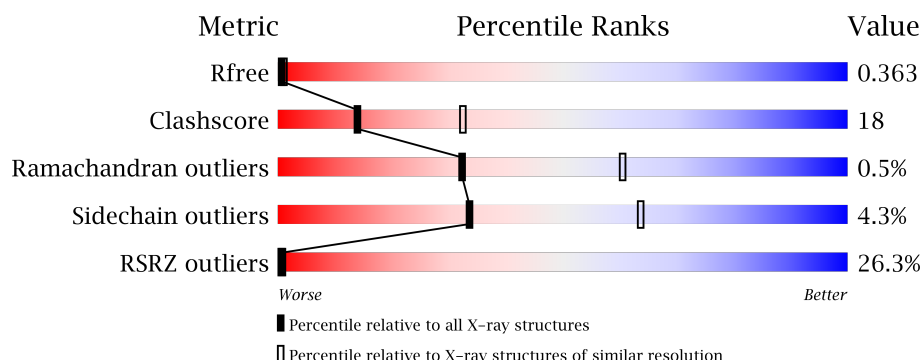
1 Overall quality at a glance

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}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (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 $\leq 5\%$. 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	<div> <div>32%</div> <div>63%</div> <div>32%</div> <div>..</div> </div>
1	B	388	<div> <div>14%</div> <div>66%</div> <div>30%</div> <div>..</div> </div>
1	C	388	<div> <div>35%</div> <div>66%</div> <div>29%</div> <div>..</div> </div>
1	D	388	<div> <div>22%</div> <div>66%</div> <div>30%</div> <div>...</div> </div>

2 Entry composition ⓘ

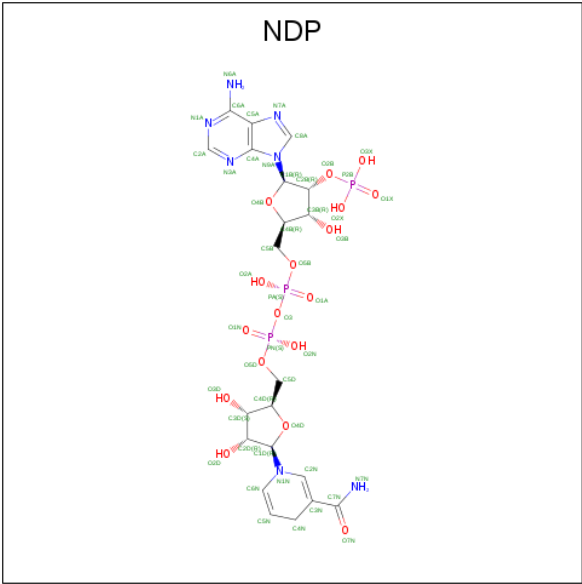
There are 3 unique types of molecules in this entry. The entry contains 11652 atoms, of which 0 are hydrogens and 0 are deuteriums.

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: C₂₁H₃₀N₇O₁₇P₃).



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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		

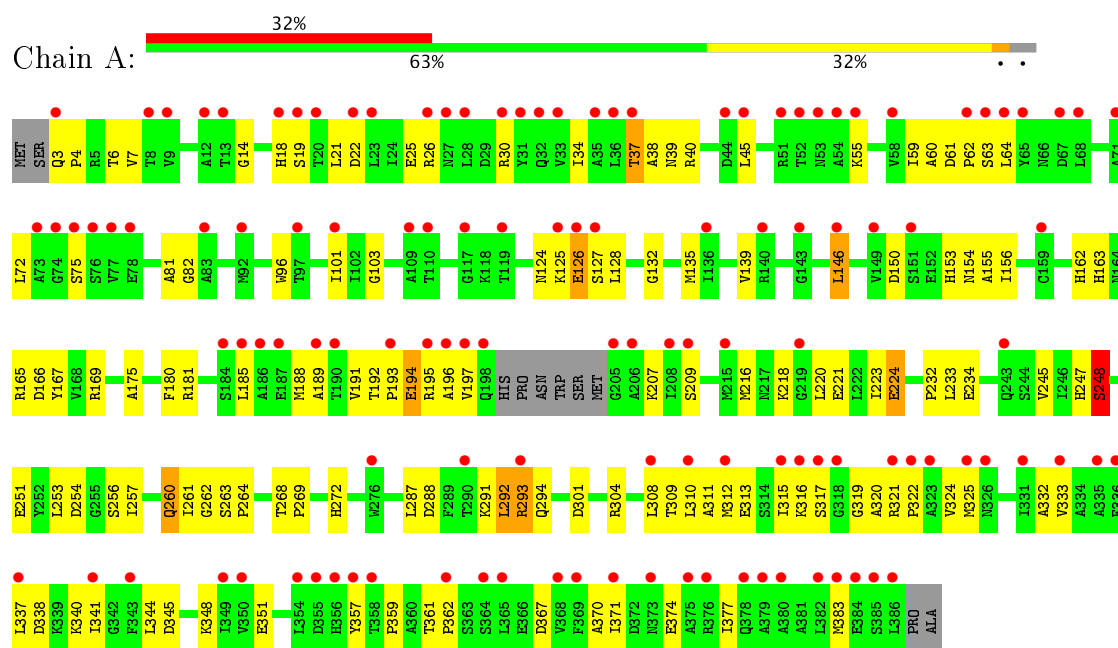
- Molecule 3 is water.

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		

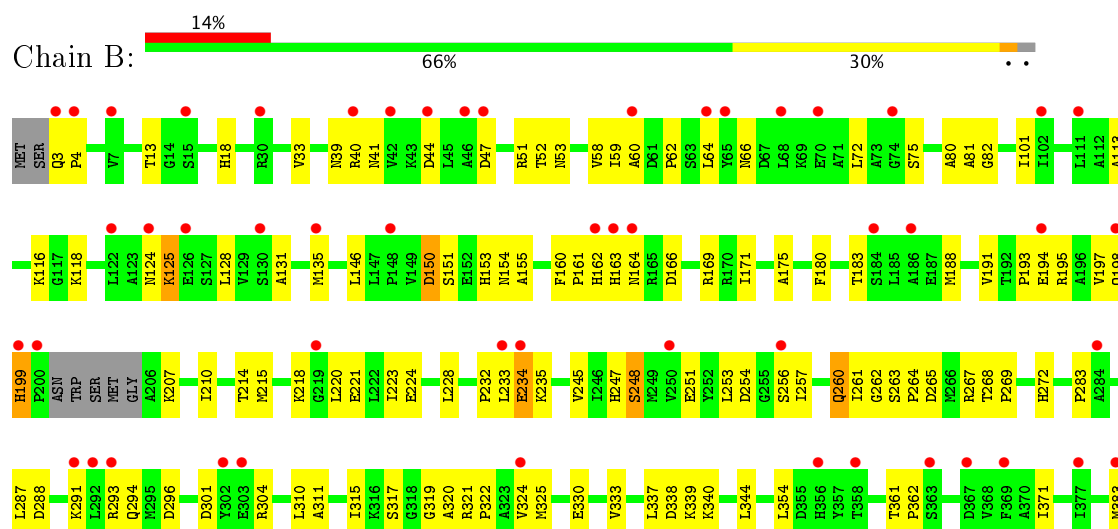
3 Residue-property plots [i](#)

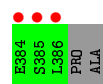
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

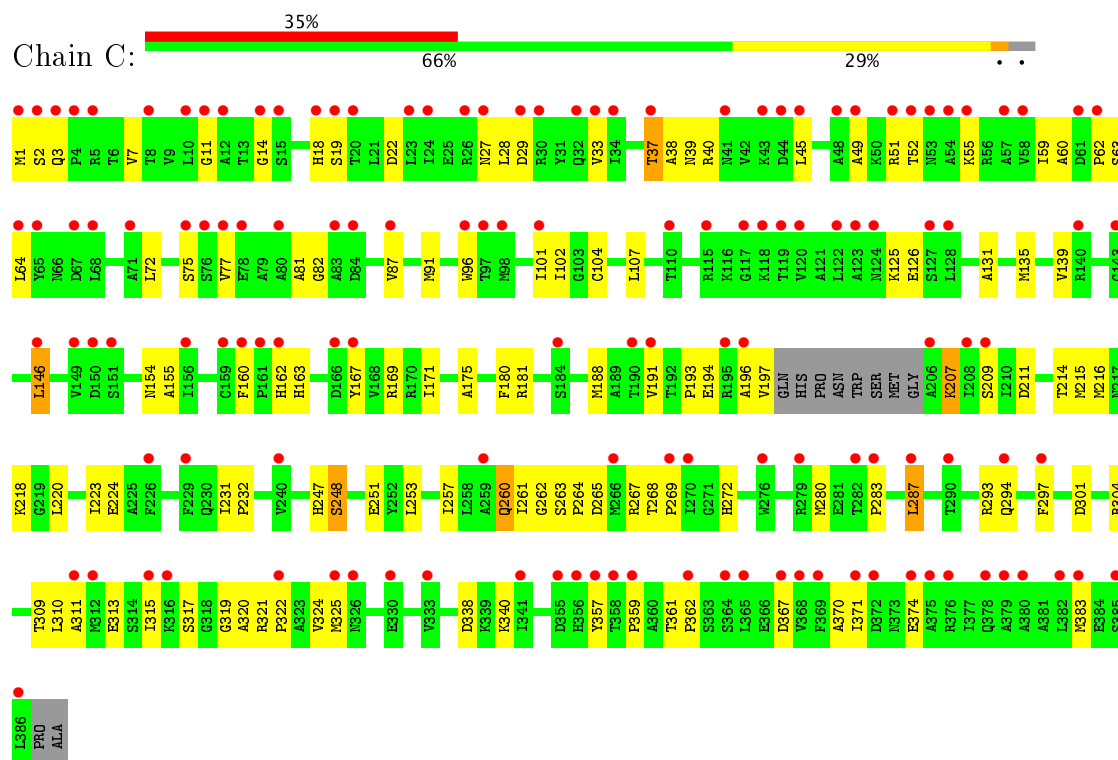


- Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase





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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	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 $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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(°)	Ideal(°)
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:A:124:ASN:ND2	1:A:126:GLU:HB2	2.01	0.76
1:B:51:ARG:HG3	1:B:51:ARG:HH21	1.49	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:C:319:GLY:HA2	1:C:361:THR:HG22	1.76	0.68
1:D:39:ASN:HD22	1:D:60:ALA:HB3	1.59	0.68
1:A:362:PRO:HG3	1:A:371:ILE:HD12	1.75	0.68
1:A:154:ASN:HD21	1:A:272:HIS:CD2	2.10	0.68
1:D:7:VAL:HG13	1:D:96:TRP:HE3	1.59	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:A:317:SER:HB3	1:A:321:ARG:HG3	1.77	0.65
1:D:251:GLU:HG3	1:D:257:ILE:HG12	1.78	0.65
1:C:267:ARG:CZ	1:C:283:PRO:HG2	2.25	0.65
1:A:223:ILE:CG1	1:A:315:ILE:HD11	2.26	0.65
1:B:47:ASP:CG	1:B:51:ARG:NH2	2.50	0.65
1:C:338:ASP:OD1	1:C:340:LYS:HE3	1.97	0.65
1:A:7:VAL:HG13	1:A:96:TRP:HE3	1.63	0.64
1:B:233:LEU:HD21	1:B:315:ILE:HG21	1.80	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:A:357:TYR:CZ	1:A:374:GLU:HG2	2.31	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:C:197:VAL:HA	1:C:209:SER:HB3	1.82	0.62
1:D:39:ASN:HB2	2:D:403:NDP:C4A	2.30	0.62
1:A:345:ASP:HA	1:A:348:LYS:HD2	1.82	0.61
1:C:180:PHE:CZ	1:C:191:VAL:HG11	2.35	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:B:251:GLU:HG3	1:B:257:ILE:HG12	1.84	0.60
1:D:39:ASN:HA	1:D:60:ALA:HB3	1.83	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:B:150:ASP:OD2	1:B:153:HIS:ND1	2.35	0.60
1:D:193:PRO:O	1:D:197:VAL:HG22	2.02	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:A:162:HIS:O	1:A:163:HIS:HB2	2.03	0.59
1:B:118:LYS:HE3	3:B:430:HOH:O	2.03	0.59
1:A:135:MET:O	1:A:139:VAL:HG23	2.03	0.59
1:A:220:LEU:O	1:A:224:GLU:CG	2.51	0.59
1:A:223:ILE:HG12	1:A:315:ILE:CD1	2.33	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:A:207:LYS:HE2	1:A:333:VAL:HG21	1.85	0.57
1:D:223:ILE:HG12	1:D:315:ILE:HG12	1.86	0.57
1:C:72:LEU:O	1:C:75:SER:HB3	2.03	0.57
1:A:319:GLY:HA2	1:A:361:THR:HG22	1.85	0.57
1:B:40:ARG:HA	1:B:64:LEU:CD1	2.34	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:207:LYS:HE3	1:D:330:GLU:OE1	2.05	0.57
1:D:267:ARG:CZ	1:D:283:PRO:HG2	2.34	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:A:180:PHE:CZ	1:A:191:VAL:HG11	2.40	0.56
1:B:311:ALA:O	1:B:315:ILE:HG13	2.05	0.56
1:D:40:ARG:HA	1:D:64:LEU:CD1	2.35	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:B:320:ALA:O	1:B:324:VAL:HG23	2.07	0.55
1:D:325:MET:HB2	1:D:354:LEU:HD21	1.88	0.55
1:A:332:ALA:O	1:A:341:ILE:HD11	2.06	0.55
1:D:310:LEU:CB	1:D:325:MET:HE3	2.36	0.55
1:D:268:THR:HB	1:D:269:PRO:CD	2.37	0.54
1:C:162:HIS:O	1:C:163:HIS:HB2	2.08	0.54
1:C:311:ALA:O	1:C:315:ILE:HG13	2.07	0.54
1:D:3:GLN:N	1:D:4:PRO:CD	2.71	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:D:223:ILE:HG12	1:D:315:ILE:CG1	2.38	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:B:254:ASP:OD1	1:B:256:SER:HB3	2.09	0.53
1:C:294:GLN:NE2	1:D:294:GLN:NE2	2.52	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:A:59:ILE:O	1:A:81:ALA:HA	2.09	0.52
1:B:188:MET:HA	1:B:191:VAL:HG23	1.90	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:A:294:GLN:HG2	1:B:296:ASP:OD1	2.10	0.52
1:D:311:ALA:O	1:D:315:ILE:HG13	2.09	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:A:169:ARG:NH2	1:A:253:LEU:O	2.43	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:C:197:VAL:HG12	1:C:197:VAL:O	2.10	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: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:C:362:PRO:HG3	1:C:371:ILE:CD1	2.39	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:A:188:MET:HA	1:A:191:VAL:HG23	1.92	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:C:27:ASN:C	1:C:29:ASP:N	2.63	0.51
1:D:188:MET:HA	1:D:191:VAL:HG23	1.92	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: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:D:319:GLY:HA2	1:D:361:THR:HG22	1.93	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:B:221:GLU:HA	1:B:224:GLU:OE1	2.11	0.50
1:C:55:LYS:HZ3	1:C:55:LYS:HB3	1.75	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:A:34:ILE:O	1:A:55:LYS:HB2	2.13	0.49
1:C:125:LYS:HE2	1:C:224:GLU:OE1	2.12	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:A:189:ALA:HB2	1:A:344:LEU:HD12	1.93	0.48
1:A:7:VAL:HG13	1:A:96:TRP:CE3	2.47	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:C:216:MET:SD	1:C:325:MET:HE2	2.53	0.48
1:B:101:ILE:O	1:B:124:ASN:ND2	2.46	0.48
1:B:261:ILE:HG22	1:B:262:GLY:N	2.28	0.48
1:C:207:LYS:CE	1:C:211:ASP:OD2	2.57	0.48
1:D:180:PHE:HB3	1:D:183:THR:HB	1.96	0.48
1:A:196:ALA:O	1:A:209:SER:HB3	2.14	0.48
1:A:362:PRO:HG3	1:A:371:ILE:CD1	2.43	0.48
1:B:321:ARG:HB2	1:B:322:PRO:CD	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: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:B:247:HIS:ND1	1:B:260:GLN:NE2	2.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:PHE:HE1	1:C:171:ILE:HD11	1.78	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:B:263:SER:HB2	1:B:264:PRO:HD2	1.95	0.47
1:C:154:ASN:HD21	1:C:272:HIS:HD2	1.63	0.47
1:D:223:ILE:HG12	1:D:315:ILE:CD1	2.44	0.47
1:C:357:TYR:CZ	1:C:374:GLU:HG2	2.48	0.47
1:D:167:TYR:O	1:D:253:LEU:HG	2.15	0.47
1:C:27:ASN:O	1:C:29:ASP:N	2.48	0.47
1:D:319:GLY:CA	1:D:361:THR:HG22	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:D:251:GLU:HG3	1:D:257:ILE:CG1	2.45	0.47
1:D:7:VAL:HG13	1:D:96:TRP:CE3	2.44	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:A:223:ILE:HA	1:A:315:ILE:CD1	2.45	0.47
1:B:160:PHE:HE1	1:B:171:ILE:HD11	1.80	0.47
1:C:251:GLU:CG	1:C:257:ILE:HG12	2.41	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: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:320:ALA:O	1:A:324:VAL:HG23	2.16	0.46
1:A:367:ASP:O	1:A:370:ALA:HB3	2.15	0.46
1:A:167:TYR:O	1:A:253:LEU:HG	2.14	0.46
1:B:232:PRO:HD2	1:B:235:LYS:HD2	1.96	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: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:169:ARG:HD2	1:B:251:GLU:OE2	2.15	0.46
1:B:40:ARG:HG2	1:B:40:ARG:NH1	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:GLU:HG3	1:A:257:ILE:HG12	1.98	0.46
1:D:310:LEU:HB2	1:D:325:MET:HE3	1.98	0.46
1:A:195:ARG:O	1:A:195:ARG:HG2	2.15	0.46
1:C:131:ALA:O	1:C:135:MET:HG2	2.16	0.46
1:B:155:ALA:HB1	1:B:260:GLN:HB3	1.97	0.46
1:A:294:GLN:HE22	1:B:294:GLN:NE2	2.14	0.46
1:B:223:ILE:HG12	1:B:315:ILE:HD11	1.97	0.46
1:D:249:MET:HG2	1:D:259:ALA:CB	2.46	0.45
1:C:268:THR:HB	1:C:269:PRO:CD	2.47	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:B:125:LYS:CB	1:B:224:GLU:OE2	2.65	0.45
1:B:169:ARG:NH2	1:B:253:LEU:O	2.49	0.45
1:A:128:LEU:HA	1:A:132:GLY:HA2	1.98	0.45
1:C:193:PRO:O	1:C:197:VAL:HG23	2.16	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:A:139:VAL:HG21	1:A:146:LEU:HD12	1.99	0.45
1:B:223:ILE:CG1	1:B:315:ILE:HD11	2.47	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:A:6:THR:HG21	3:A:410:HOH:O	2.15	0.45
1:B:175:ALA:CB	1:B:218:LYS:HE3	2.47	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:321:ARG:HB2	1:C:322:PRO:CD	2.47	0.44
1:C:59:ILE:O	1:C:59:ILE:HG23	2.17	0.44
1:B:245:VAL:O	1:B:261:ILE:HG23	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:C:261:ILE:HG22	1:C:262:GLY:N	2.33	0.44
1:D:245:VAL:O	1:D:261:ILE:HG23	2.17	0.44
1:D:269:PRO:O	1:D:272:HIS:HB3	2.17	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:B:210:ILE:HG21	1:B:333:VAL:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ILE:HG23	1:C:232:PRO:HD2	2.00	0.44
1:D:18:HIS:ND1	3:D:411:HOH:O	2.36	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:C:367:ASP:O	1:C:370:ALA:HB3	2.17	0.43
1:D:165:ARG:HD2	1:D:230:GLN:O	2.19	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:128:LEU:HD13	1:B:228:LEU:HG	2.00	0.43
1:B:319:GLY:HA2	1:B:361:THR:HG22	2.00	0.43
1:A:3:GLN:HB3	1:A:4:PRO:CD	2.41	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:C:175:ALA:HA	1:C:218:LYS:HE3	2.01	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:B:113:ALA:O	1:B:116:LYS:HB2	2.19	0.43
1:C:169:ARG:NH2	1:C:253:LEU:O	2.52	0.43
1:D:310:LEU:C	1:D:325:MET:HE3	2.39	0.43
1:C:104:CYS:HA	1:C:107:LEU:HG	2.00	0.42
1:C:320:ALA:O	1:C:324:VAL:HG23	2.19	0.42
1:D:292:LEU:O	1:D:294:GLN:N	2.48	0.42
1:A:37:THR:HG21	1:A:101:ILE:HD11	2.01	0.42
1:A:39:ASN:HB2	2:A:400:NDP:C4A	2.49	0.42
1:C:218:LYS:HD3	1:C:218:LYS:HA	1.86	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: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:C:261:ILE:HG22	1:C:287:LEU:HD12	2.01	0.42
1:C:37:THR:CG2	3:C:424:HOH:O	2.66	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:C:1:MET:O	1:C:2:SER:HB2	2.19	0.42
1:D:33:VAL:HG21	1:D:52:THR:HB	2.02	0.42
1:B:214:THR:O	1:B:215:MET:HB2	2.20	0.42
1:D:165:ARG:CD	1:D:230:GLN:O	2.68	0.42
1:A:150:ASP:OD2	1:A:153:HIS:ND1	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:PRO:HB3	1:A:234:GLU:OE2	2.19	0.42
1:A:268:THR:HB	1:A:269:PRO:HD2	2.02	0.42
1:A:308:LEU:O	1:A:312:MET:HG3	2.20	0.42
1:C:181:ARG:O	1:C:304:ARG:NH2	2.42	0.42
1:D:293:ARG:HB3	1:D:293:ARG:HE	1.28	0.42
1:A:261:ILE:HG22	1:A:262:GLY:N	2.34	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:D:14:GLY:O	1:D:18:HIS:HB2	2.20	0.42
1:A:263:SER:HB2	1:A:264:PRO:HD2	2.01	0.41
1:B:160:PHE:CG	1:B:161:PRO:HD2	2.55	0.41
1:B:41:ASN:ND2	1:B:44:ASP:OD2	2.53	0.41
1:C:188:MET:HA	1:C:191:VAL:HG23	2.02	0.41
1:D:346:ILE:O	1:D:350:VAL:HG23	2.20	0.41
1:D:352:LYS:HB3	1:D:382:LEU:HD13	2.02	0.41
1:B:13:THR:HG1	2:B:401:NDP:P2B	2.43	0.41
1:B:325:MET:HB2	1:B:354:LEU:HD21	2.02	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:113:ALA:O	1:D:116:LYS:HB2	2.21	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: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:359:PRO:HG3	1:D:371:ILE:HG23	2.02	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:A:72:LEU:O	1:A:75:SER:HB3	2.20	0.41
1:D:224:GLU:OE2	3:D:404:HOH:O	2.22	0.41
1:D:251:GLU:CG	1:D:257:ILE:HG12	2.49	0.41
1:D:267:ARG:NH1	1:D:283:PRO:HG2	2.35	0.41
1:D:223:ILE:CG1	1:D:315:ILE:HD11	2.50	0.41
1:A:345:ASP:O	1:A:348:LYS:HB2	2.21	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:D:91:MET:O	1:D:116:LYS:HE3	2.21	0.41
1:A:14:GLY:O	1:A:18:HIS:HB2	2.20	0.41
1:A:156:ILE:HG13	1:A:248:SER:HB3	2.02	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:B:310:LEU:C	1:B:325:MET:HE3	2.42	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:180:PHE:HB3	1:B:183:THR:HB	2.02	0.40
1:B:51:ARG:NH2	1:B:51:ARG:CG	2.76	0.40
1:B:301:ASP:OD2	1:B:304:ARG:HD3	2.21	0.40
1:C:223:ILE:HA	1:C:315:ILE:HD13	2.03	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:D:361:THR:HA	1:D:362:PRO:HD3	1.93	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
1:C:361:THR:HA	1:C:362:PRO:HD3	1.91	0.40
1:D:40:ARG:HA	1:D:64:LEU:HD12	2.02	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%)	32	60
1	B	375/388 (97%)	355 (95%)	19 (5%)	1 (0%)	44	73
1	C	374/388 (96%)	353 (94%)	19 (5%)	2 (0%)	32	60
1	D	374/388 (96%)	360 (96%)	12 (3%)	2 (0%)	32	60
All	All	1497/1552 (96%)	1423 (95%)	67 (4%)	7 (0%)	32	60

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%)	22	48
1	B	301/308 (98%)	287 (95%)	14 (5%)	30	60
1	C	300/308 (97%)	292 (97%)	8 (3%)	50	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	300/308 (97%)	288 (96%)	12 (4%)	36	67
All	All	1200/1232 (97%)	1148 (96%)	52 (4%)	33	64

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	-	25,29,52	1.83	8 (32%)	32,45,80	2.80	15 (46%)
2	NDP	B	401	-	25,29,52	1.76	7 (28%)	32,45,80	2.87	14 (43%)
2	NDP	C	402	-	25,29,52	1.56	3 (12%)	32,45,80	1.95	9 (28%)
2	NDP	D	403	-	25,29,52	3.58	10 (40%)	32,45,80	4.26	19 (59%)

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 (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	403	NDP	O5B-C5B	-7.55	1.14	1.44
2	D	403	NDP	C3B-C4B	-7.07	1.34	1.53
2	D	403	NDP	C8A-N7A	-5.84	1.23	1.34
2	D	403	NDP	C5B-C4B	-5.74	1.33	1.51
2	A	400	NDP	P2B-O2B	-3.89	1.52	1.59
2	C	402	NDP	PA-O1A	-3.40	1.39	1.50
2	B	401	NDP	PA-O1A	-3.22	1.39	1.50
2	B	401	NDP	C8A-N7A	-3.01	1.29	1.34
2	A	400	NDP	PA-O1A	-2.82	1.41	1.50
2	C	402	NDP	C8A-N7A	-2.82	1.29	1.34
2	B	401	NDP	C5B-C4B	-2.62	1.43	1.51
2	B	401	NDP	P2B-O2B	-2.59	1.55	1.59
2	A	400	NDP	C8A-N7A	-2.50	1.30	1.34
2	A	400	NDP	C5B-C4B	-2.15	1.44	1.51
2	B	401	NDP	O5B-C5B	-2.02	1.36	1.44
2	D	403	NDP	C2A-N1A	2.07	1.37	1.33
2	A	400	NDP	C3B-C4B	2.16	1.58	1.53
2	A	400	NDP	O4B-C1B	2.41	1.44	1.41
2	A	400	NDP	C2A-N3A	2.53	1.36	1.32
2	D	403	NDP	O4B-C4B	3.12	1.52	1.45
2	D	403	NDP	O3B-C3B	3.33	1.50	1.43
2	B	401	NDP	C3B-C4B	3.36	1.61	1.53
2	D	403	NDP	C2A-N3A	3.39	1.37	1.32
2	D	403	NDP	PA-O5B	3.43	1.71	1.60
2	B	401	NDP	O3B-C3B	3.56	1.51	1.43
2	C	402	NDP	O3B-C3B	3.92	1.52	1.43
2	A	400	NDP	O3B-C3B	4.71	1.53	1.43
2	D	403	NDP	O4B-C1B	9.10	1.53	1.41

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	403	NDP	O3-PA-O2A	-9.45	69.50	107.61
2	D	403	NDP	PA-O5B-C5B	-9.25	92.81	118.30
2	B	401	NDP	O3X-P2B-O1X	-7.50	81.14	110.50
2	A	400	NDP	O3X-P2B-O1X	-7.46	81.30	110.50
2	D	403	NDP	O3X-P2B-O1X	-7.01	83.07	110.50
2	D	403	NDP	C4B-O4B-C1B	-6.55	102.79	109.77
2	D	403	NDP	N3A-C2A-N1A	-6.22	123.44	128.86
2	B	401	NDP	O3X-P2B-O2X	-6.18	82.69	107.61
2	D	403	NDP	O5B-PA-O1A	-6.16	89.20	106.47
2	A	400	NDP	N3A-C2A-N1A	-5.96	123.66	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NDP	PA-O5B-C5B	-5.70	102.59	118.30
2	D	403	NDP	O3X-P2B-O2X	-5.49	85.48	107.61
2	A	400	NDP	O3X-P2B-O2B	-5.02	83.15	106.00
2	A	400	NDP	O3X-P2B-O2X	-5.02	87.35	107.61
2	C	402	NDP	PA-O5B-C5B	-5.01	104.50	118.30
2	C	402	NDP	N3A-C2A-N1A	-4.74	124.73	128.86
2	B	401	NDP	N3A-C2A-N1A	-4.35	125.07	128.86
2	B	401	NDP	O3X-P2B-O2B	-4.28	86.54	106.00
2	A	400	NDP	PA-O5B-C5B	-4.23	106.65	118.30
2	D	403	NDP	O3X-P2B-O2B	-4.16	87.07	106.00
2	C	402	NDP	O4B-C4B-C5B	-3.93	96.13	109.40
2	A	400	NDP	O4B-C4B-C5B	-3.87	96.34	109.40
2	B	401	NDP	O4B-C4B-C5B	-3.56	97.38	109.40
2	B	401	NDP	O5B-C5B-C4B	-3.55	96.42	109.00
2	C	402	NDP	O5B-C5B-C4B	-3.27	97.40	109.00
2	A	400	NDP	O5B-C5B-C4B	-2.72	99.37	109.00
2	D	403	NDP	O3B-C3B-C4B	-2.60	103.49	111.09
2	B	401	NDP	O2A-PA-O5B	-2.52	100.01	106.73
2	A	400	NDP	O2A-PA-O5B	-2.40	100.34	106.73
2	D	403	NDP	C3B-C2B-C1B	-2.31	98.23	102.75
2	C	402	NDP	O2A-PA-O5B	-2.22	100.83	106.73
2	A	400	NDP	C3B-C2B-C1B	-2.07	98.70	102.75
2	C	402	NDP	C3B-C2B-C1B	-2.01	98.82	102.75
2	B	401	NDP	O2B-P2B-O1X	2.01	117.14	109.26
2	C	402	NDP	O2B-C2B-C3B	2.11	119.44	111.63
2	D	403	NDP	C2B-C3B-C4B	2.12	106.76	101.95
2	A	400	NDP	O2X-P2B-O2B	2.15	115.79	106.00
2	A	400	NDP	O2B-C2B-C3B	2.20	119.76	111.63
2	C	402	NDP	O2B-C2B-C1B	2.31	118.68	110.06
2	B	401	NDP	O2B-C2B-C1B	2.33	118.75	110.06
2	A	400	NDP	O2B-C2B-C1B	2.35	118.83	110.06
2	B	401	NDP	C1B-N9A-C4A	2.40	130.78	126.64
2	A	400	NDP	C1B-N9A-C4A	2.41	130.80	126.64
2	B	401	NDP	O2B-C2B-C3B	2.51	120.92	111.63
2	D	403	NDP	O2X-P2B-O2B	2.60	117.83	106.00
2	C	402	NDP	O2A-PA-O1A	3.15	122.84	110.50
2	B	401	NDP	O2A-PA-O1A	3.25	123.21	110.50
2	A	400	NDP	O2A-PA-O1A	3.31	123.45	110.50
2	D	403	NDP	O2X-P2B-O1X	3.39	123.75	110.50
2	D	403	NDP	O5B-C5B-C4B	3.39	121.03	109.00
2	A	400	NDP	O2X-P2B-O1X	3.47	124.07	110.50
2	B	401	NDP	O2X-P2B-O1X	3.73	125.11	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	403	NDP	C1B-N9A-C4A	4.55	134.50	126.64
2	D	403	NDP	O2A-PA-O1A	4.67	128.77	110.50
2	D	403	NDP	O2A-PA-O5B	4.96	119.94	106.73
2	D	403	NDP	O3-PA-O5B	5.12	120.35	106.73
2	D	403	NDP	O3-PA-O1A	5.83	133.33	110.50

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 [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, 95th 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%)	1.71	123 (32%) 0 0	16, 43, 87, 104	0
1	B	379/388 (97%)	1.07	55 (14%) 3 2	17, 35, 63, 88	0
1	C	378/388 (97%)	1.86	136 (35%) 0 0	22, 44, 69, 94	0
1	D	378/388 (97%)	1.44	84 (22%) 1 1	22, 45, 74, 107	0
All	All	1513/1552 (97%)	1.52	398 (26%) 1 0	16, 41, 75, 107	0

All (398) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	10.5
1	C	2	SER	10.4
1	C	68	LEU	9.6
1	C	71	ALA	8.6
1	C	365	LEU	7.8
1	A	68	LEU	7.4
1	A	365	LEU	7.4
1	D	4	PRO	6.6
1	C	65	TYR	6.4
1	C	362	PRO	6.3
1	B	200	PRO	6.0
1	C	356	HIS	6.0
1	A	362	PRO	5.9
1	D	356	HIS	5.9
1	A	356	HIS	5.8
1	B	199	HIS	5.6
1	C	44	ASP	5.5
1	C	45	LEU	5.5
1	C	209	SER	5.4
1	C	386	LEU	5.4
1	A	375	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	76	SER	5.1
1	C	385	SER	4.8
1	A	209	SER	4.7
1	C	161	PRO	4.7
1	B	293	ARG	4.6
1	C	368	VAL	4.5
1	C	52	THR	4.5
1	C	143	GLY	4.5
1	D	303	GLU	4.5
1	A	205	GLY	4.4
1	A	140	ARG	4.4
1	D	126	GLU	4.2
1	A	379	ALA	4.2
1	A	64	LEU	4.2
1	A	185	LEU	4.2
1	D	355	ASP	4.2
1	A	385	SER	4.2
1	A	71	ALA	4.2
1	A	73	ALA	4.2
1	C	375	ALA	4.1
1	C	357	TYR	4.1
1	C	76	SER	4.0
1	C	64	LEU	4.0
1	D	64	LEU	4.0
1	C	374	GLU	4.0
1	D	233	LEU	4.0
1	C	78	GLU	4.0
1	D	74	GLY	3.9
1	D	373	ASN	3.9
1	C	312	MET	3.9
1	B	383	MET	3.9
1	C	315	ILE	3.9
1	C	41	ASN	3.9
1	A	364	SER	3.9
1	C	326	ASN	3.9
1	A	368	VAL	3.8
1	C	62	PRO	3.8
1	C	27	ASN	3.8
1	A	333	VAL	3.8
1	C	34	ILE	3.8
1	A	349	ILE	3.8
1	C	18	HIS	3.8

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

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Mol	Chain	Res	Type	RSRZ
1	C	358	THR	3.3
1	A	371	ILE	3.3
1	D	18	HIS	3.3
1	D	63	SER	3.3
1	C	341	ILE	3.3
1	A	189	ALA	3.3
1	B	386	LEU	3.3
1	B	163	HIS	3.3
1	D	293	ARG	3.3
1	B	4	PRO	3.3
1	D	359	PRO	3.3
1	B	40	ARG	3.3
1	C	355	ASP	3.2
1	A	18	HIS	3.2
1	D	199	HIS	3.2
1	C	30	ARG	3.2
1	C	383	MET	3.2
1	D	377	ILE	3.2
1	B	68	LEU	3.2
1	C	67	ASP	3.2
1	D	341	ILE	3.2
1	B	356	HIS	3.2
1	D	135	MET	3.1
1	A	13	THR	3.1
1	C	378	GLN	3.1
1	C	98	MET	3.1
1	C	325	MET	3.1
1	C	297	PHE	3.1
1	A	208	ILE	3.1
1	D	363	SER	3.1
1	C	11	GLY	3.1
1	C	115	ARG	3.1
1	A	125	LYS	3.1
1	C	316	LYS	3.1
1	D	186	ALA	3.1
1	A	12	ALA	3.1
1	A	376	ARG	3.1
1	A	290	THR	3.0
1	B	385	SER	3.0
1	C	57	ALA	3.0
1	C	196	ALA	3.0
1	D	112	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	19	SER	3.0
1	A	380	ALA	3.0
1	D	111	LEU	3.0
1	D	327	ALA	3.0
1	D	332	ALA	3.0
1	A	341	ILE	3.0
1	B	219	GLY	3.0
1	A	8	THR	3.0
1	B	15	SER	3.0
1	C	96	TRP	3.0
1	A	126	GLU	3.0
1	C	49	ALA	3.0
1	A	383	MET	3.0
1	C	29	ASP	3.0
1	C	77	VAL	3.0
1	B	3	GLN	3.0
1	D	73	ALA	3.0
1	D	76	SER	3.0
1	A	350	VAL	3.0
1	C	51	ARG	3.0
1	D	57	ALA	2.9
1	C	372	ASP	2.9
1	C	15	SER	2.9
1	C	290	THR	2.9
1	C	159	CYS	2.9
1	A	54	ALA	2.9
1	D	124	ASN	2.9
1	A	143	GLY	2.9
1	D	160	PHE	2.9
1	B	233	LEU	2.9
1	C	20	THR	2.9
1	A	357	TYR	2.9
1	C	87	VAL	2.9
1	D	381	ALA	2.9
1	B	70	GLU	2.9
1	A	325	MET	2.9
1	C	150	ASP	2.9
1	B	162	HIS	2.9
1	B	30	ARG	2.9
1	D	130	SER	2.8
1	C	54	ALA	2.8
1	D	334	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	75	SER	2.8
1	C	195	ARG	2.8
1	C	311	ALA	2.8
1	A	337	LEU	2.8
1	B	42	VAL	2.8
1	C	191	VAL	2.8
1	A	127	SER	2.8
1	A	331	ILE	2.8
1	C	48	ALA	2.8
1	C	80	ALA	2.8
1	C	330	GLU	2.8
1	A	326	ASN	2.8
1	A	322	PRO	2.8
1	B	148	PRO	2.8
1	C	118	LYS	2.7
1	B	102	ILE	2.7
1	A	75	SER	2.7
1	C	151	SER	2.7
1	C	101	ILE	2.7
1	C	97	THR	2.7
1	A	28	LEU	2.7
1	C	37	THR	2.7
1	C	322	PRO	2.7
1	C	240	VAL	2.7
1	A	321	ARG	2.7
1	D	307	ALA	2.7
1	A	318	GLY	2.7
1	D	291	LYS	2.7
1	D	385	SER	2.7
1	A	198	GLN	2.6
1	A	30	ARG	2.6
1	C	119	THR	2.6
1	A	23	LEU	2.6
1	B	291	LYS	2.6
1	D	319	GLY	2.6
1	D	353	THR	2.6
1	B	111	LEU	2.6
1	C	364	SER	2.6
1	A	276	TRP	2.6
1	C	167	TYR	2.6
1	A	373	ASN	2.6
1	B	64	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	23	LEU	2.6
1	C	162	HIS	2.6
1	B	135	MET	2.6
1	A	37	THR	2.6
1	C	270	ILE	2.6
1	C	333	VAL	2.6
1	C	61	ASP	2.6
1	C	84	ASP	2.6
1	A	215	MET	2.6
1	A	31	TYR	2.6
1	B	377	ILE	2.5
1	D	357	TYR	2.5
1	A	369	PHE	2.5
1	A	159	CYS	2.5
1	A	55	LYS	2.5
1	C	184	SER	2.5
1	A	187	GLU	2.5
1	B	44	ASP	2.5
1	B	60	ALA	2.5
1	B	186	ALA	2.5
1	D	40	ARG	2.5
1	B	363	SER	2.5
1	A	63	SER	2.5
1	D	234	GLU	2.5
1	A	206	ALA	2.5
1	C	12	ALA	2.5
1	C	122	LEU	2.5
1	C	26	ARG	2.5
1	C	294	GLN	2.5
1	A	184	SER	2.5
1	B	256	SER	2.5
1	A	53	ASN	2.5
1	D	69	LYS	2.5
1	C	127	SER	2.5
1	A	343	PHE	2.5
1	B	47	ASP	2.5
1	D	278	LYS	2.4
1	C	120	VAL	2.4
1	C	160	PHE	2.4
1	A	74	GLY	2.4
1	A	119	THR	2.4
1	C	382	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	51	ARG	2.4
1	B	65	TYR	2.4
1	C	359	PRO	2.4
1	A	36	LEU	2.4
1	A	354	LEU	2.4
1	A	9	VAL	2.4
1	A	26	ARG	2.4
1	C	269	PRO	2.4
1	D	134	LEU	2.4
1	A	136	ILE	2.4
1	D	346	ILE	2.4
1	A	33	VAL	2.4
1	A	149	VAL	2.4
1	C	266	MET	2.4
1	A	358	THR	2.4
1	D	147	LEU	2.4
1	C	367	ASP	2.4
1	D	44	ASP	2.4
1	D	323	ALA	2.3
1	D	296	ASP	2.3
1	C	379	ALA	2.3
1	C	380	ALA	2.3
1	A	109	ALA	2.3
1	A	195	ARG	2.3
1	C	83	ALA	2.3
1	C	206	ALA	2.3
1	D	338	ASP	2.3
1	C	5	ARG	2.3
1	A	101	ILE	2.3
1	B	250	VAL	2.3
1	A	110	THR	2.3
1	D	81	ALA	2.3
1	A	78	GLU	2.3
1	A	22	ASP	2.3
1	A	51	ARG	2.3
1	C	10	LEU	2.3
1	C	124	ASN	2.3
1	A	32	GLN	2.3
1	B	303	GLU	2.3
1	A	58	VAL	2.3
1	A	77	VAL	2.3
1	A	193	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	130	SER	2.3
1	C	259	ALA	2.3
1	B	234	GLU	2.3
1	A	3	GLN	2.2
1	B	194	GLU	2.2
1	D	226	PHE	2.2
1	B	74	GLY	2.2
1	A	308	LEU	2.2
1	B	122	LEU	2.2
1	C	146	LEU	2.2
1	D	382	LEU	2.2
1	A	323	ALA	2.2
1	B	302	TYR	2.2
1	A	315	ILE	2.2
1	D	50	LYS	2.2
1	A	335	ALA	2.2
1	C	123	ALA	2.2
1	D	65	TYR	2.2
1	A	384	GLU	2.2
1	C	226	PHE	2.2
1	C	43	LYS	2.2
1	A	219	GLY	2.2
1	A	146	LEU	2.2
1	A	83	ALA	2.2
1	B	358	THR	2.2
1	A	336	PHE	2.2
1	B	369	PHE	2.2
1	C	19	SER	2.2
1	D	208	ILE	2.2
1	B	198	GLN	2.2
1	B	7	VAL	2.2
1	C	156	ILE	2.2
1	D	28	LEU	2.2
1	C	279	ARG	2.2
1	C	33	VAL	2.1
1	D	34	ILE	2.1
1	C	4	PRO	2.1
1	C	166	ASP	2.1
1	C	128	LEU	2.1
1	A	355	ASP	2.1
1	B	367	ASP	2.1
1	D	342	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	362	PRO	2.1
1	D	236	PHE	2.1
1	D	24	ILE	2.1
1	D	331	ILE	2.1
1	D	55	LYS	2.1
1	C	110	THR	2.1
1	A	151	SER	2.1
1	A	316	LYS	2.1
1	D	150	ASP	2.1
1	A	45	LEU	2.1
1	B	324	VAL	2.1
1	C	14	GLY	2.1
1	C	32	GLN	2.1
1	D	175	ALA	2.1
1	C	282	THR	2.1
1	B	292	LEU	2.1
1	A	65	TYR	2.1
1	A	20	THR	2.1
1	D	66	ASN	2.1
1	D	358	THR	2.1
1	B	184	SER	2.1
1	D	258	LEU	2.1
1	D	261	ILE	2.1
1	A	186	ALA	2.1
1	D	193	PRO	2.0
1	A	92	MET	2.0
1	A	97	THR	2.0
1	A	243	GLN	2.0
1	B	284	ALA	2.0
1	D	155	ALA	2.0
1	C	229	PHE	2.0
1	D	336	PHE	2.0
1	C	283	PRO	2.0
1	C	376	ARG	2.0
1	D	7	VAL	2.0
1	D	101	ILE	2.0
1	D	207	LYS	2.0
1	D	259	ALA	2.0
1	A	310	LEU	2.0
1	A	382	LEU	2.0
1	A	62	PRO	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, 95th 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(\AA^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.