Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:47 pm BST

PDB ID	:	2DUU
Title	:	Crystal Structure of apo-form of NADP-Dependent Glyceraldehyde-3-Phosphate Dehydrogenase from Synechococcus Sp.
Authors	:	Kitatani, T.; Nakamura, Y.; Wada, K.; Kinoshita, T.; Tamoi, M.; Shigeoka, S.; Tada, T.
Deposited on	:	2006-07-27
Resolution	:	2.90 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

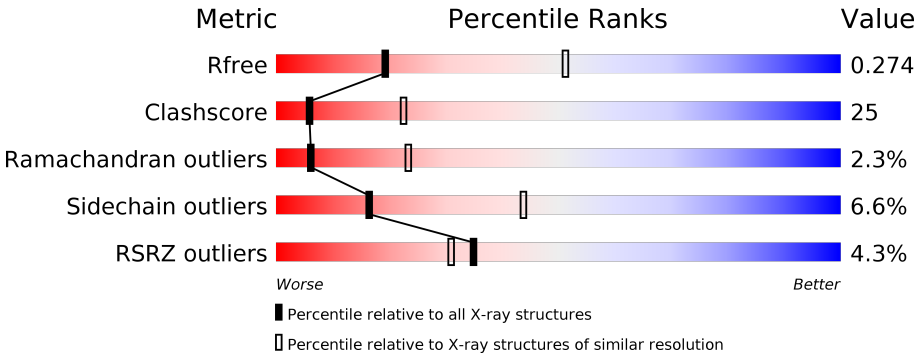
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 respectively. 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	380	% 47% 32% 5% 15%
1	B	380	% 46% 34% 5% 15%
1	O	380	% 48% 33% • 15%
1	P	380	3% 45% 37% • 15%
1	Q	380	7% 45% 37% • 15%
1	R	380	9% 44% 38% • 15%

2 Entry composition

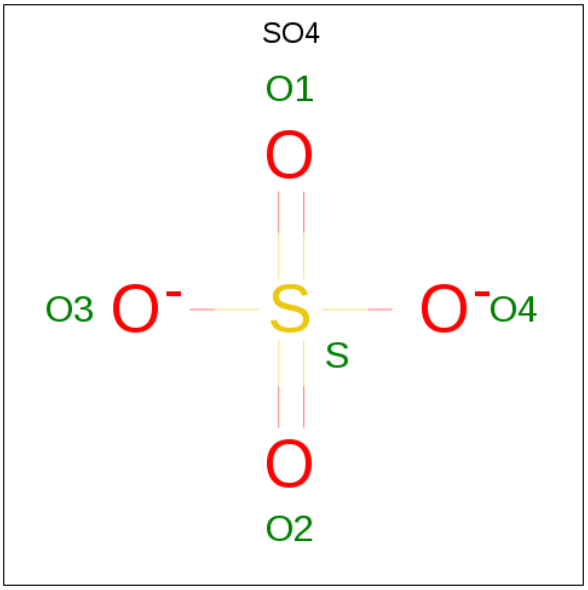
There are 3 unique types of molecules in this entry. The entry contains 15053 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glyceraldehyde 3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2451	1544	423	475	9			
1	B	322	Total	C	N	O	S	0	0	0
			2451	1544	423	475	9			
1	O	322	Total	C	N	O	S	0	0	0
			2451	1544	423	475	9			
1	P	322	Total	C	N	O	S	0	0	0
			2451	1544	423	475	9			
1	Q	322	Total	C	N	O	S	0	0	0
			2451	1544	423	475	9			
1	R	322	Total	C	N	O	S	0	0	0
			2451	1544	423	475	9			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	O	1	Total O S 5 4 1	0	0
2	P	1	Total O S 5 4 1	0	0
2	Q	1	Total O S 5 4 1	0	0
2	R	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

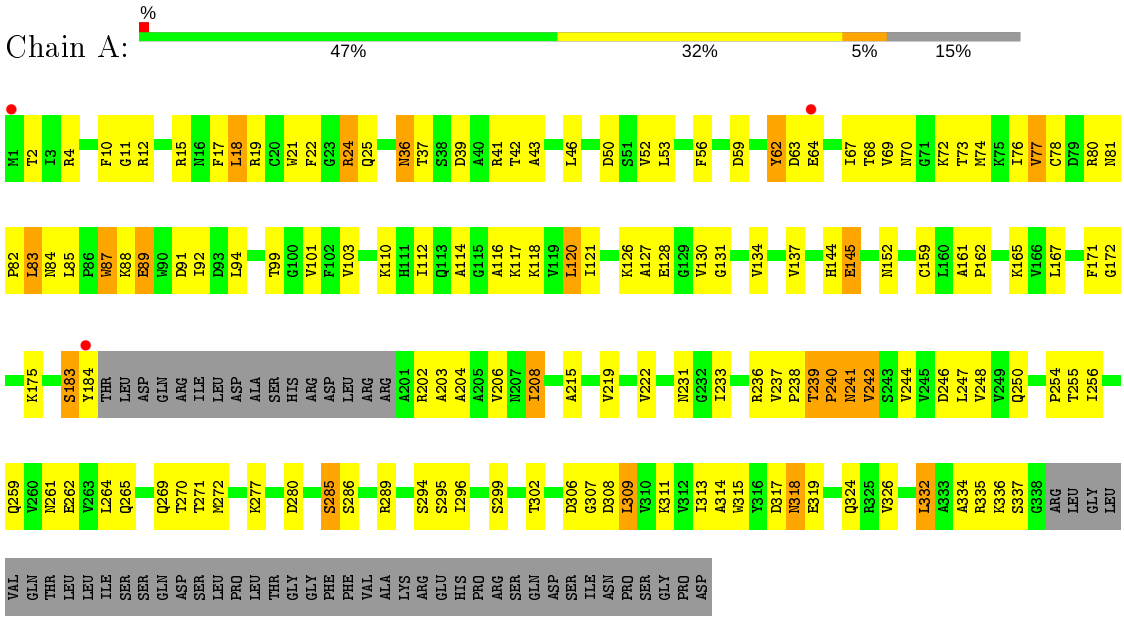
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	68	Total O 68 68	0	0
3	B	87	Total O 87 87	0	0
3	O	61	Total O 61 61	0	0
3	P	57	Total O 57 57	0	0
3	Q	19	Total O 19 19	0	0
3	R	25	Total O 25 25	0	0

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.

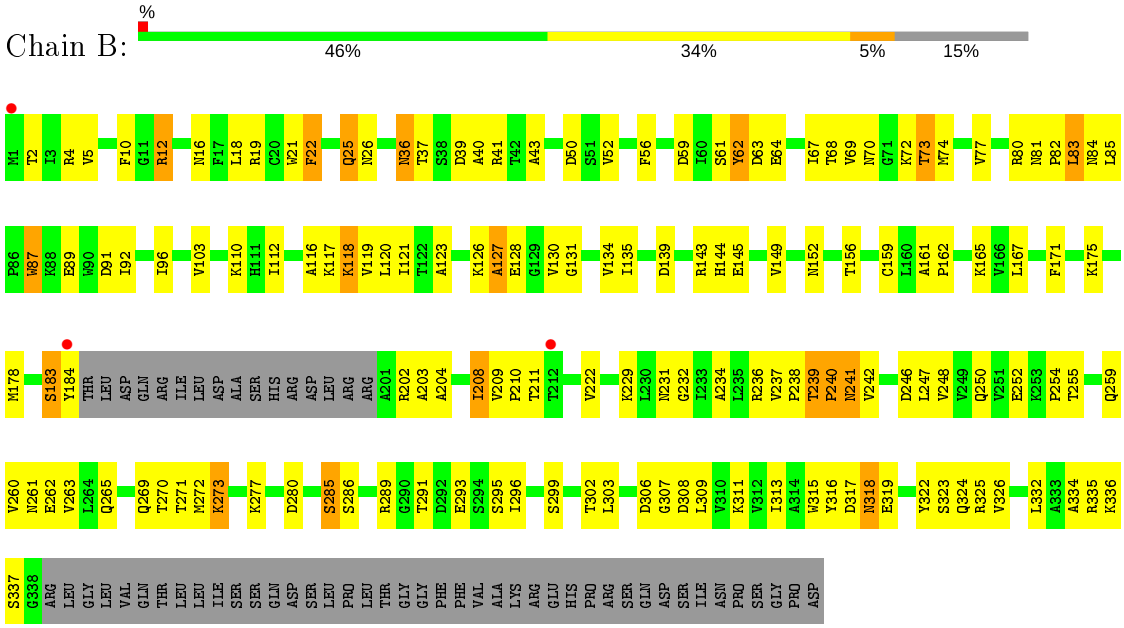
- Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase

Chain A:



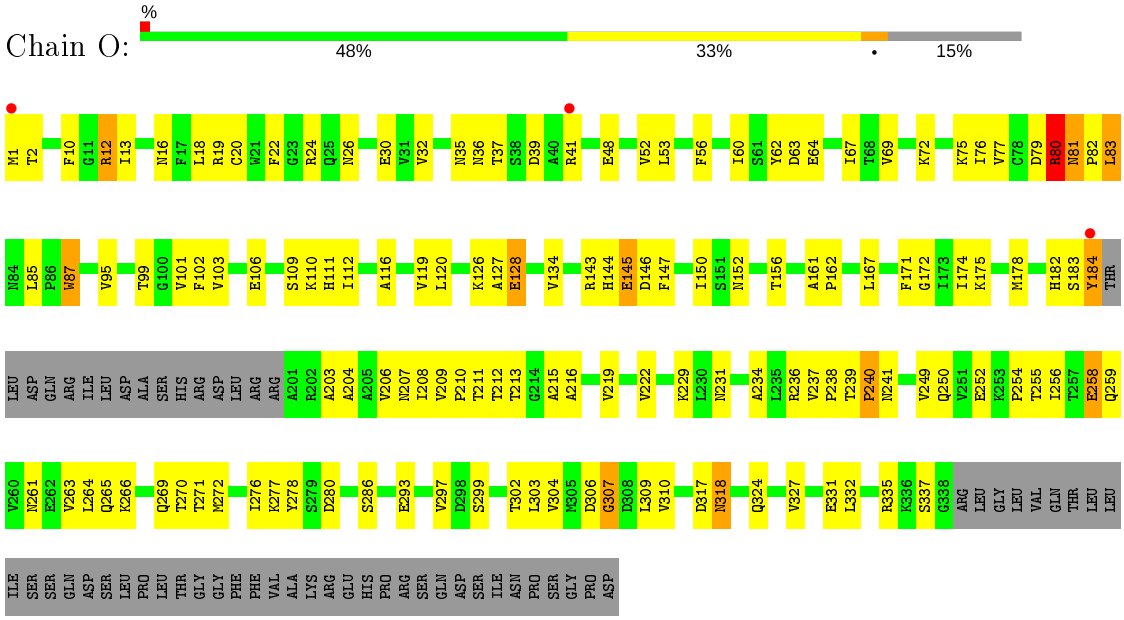
- Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase

Chain B:



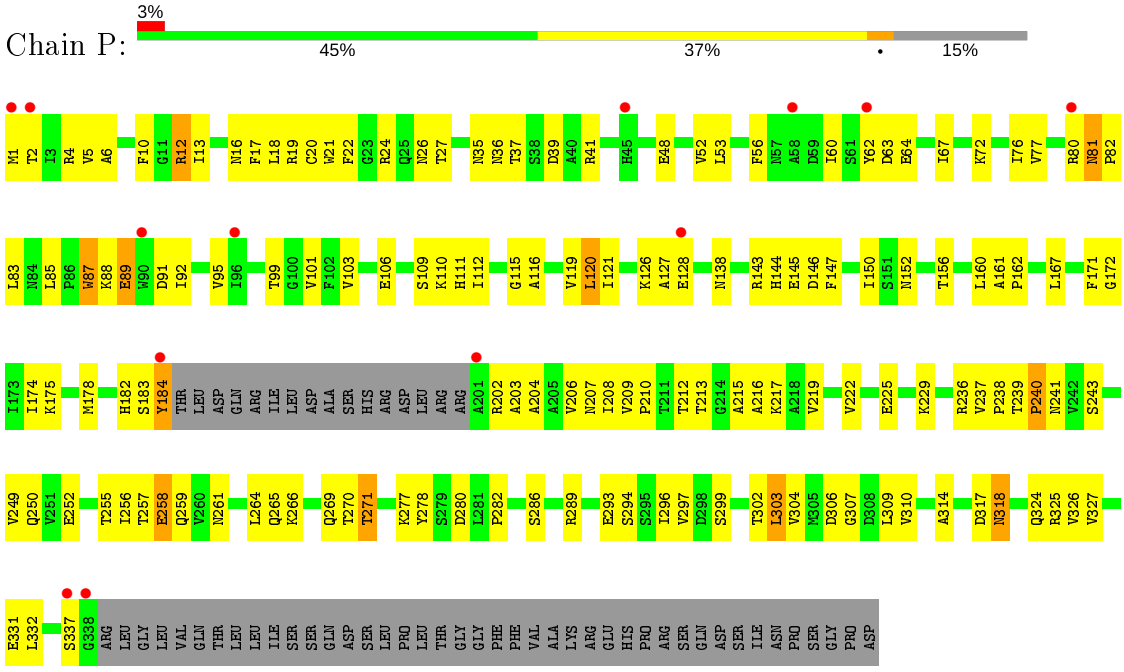
• Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase

Chain O:



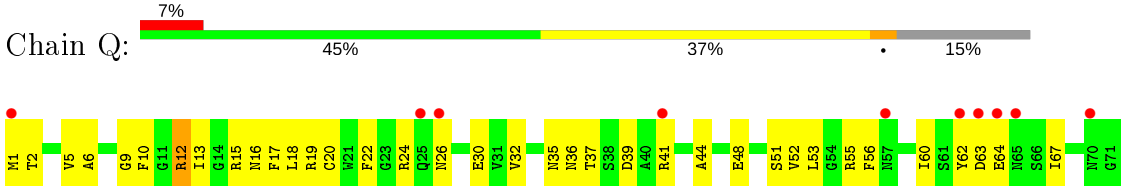
• Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase

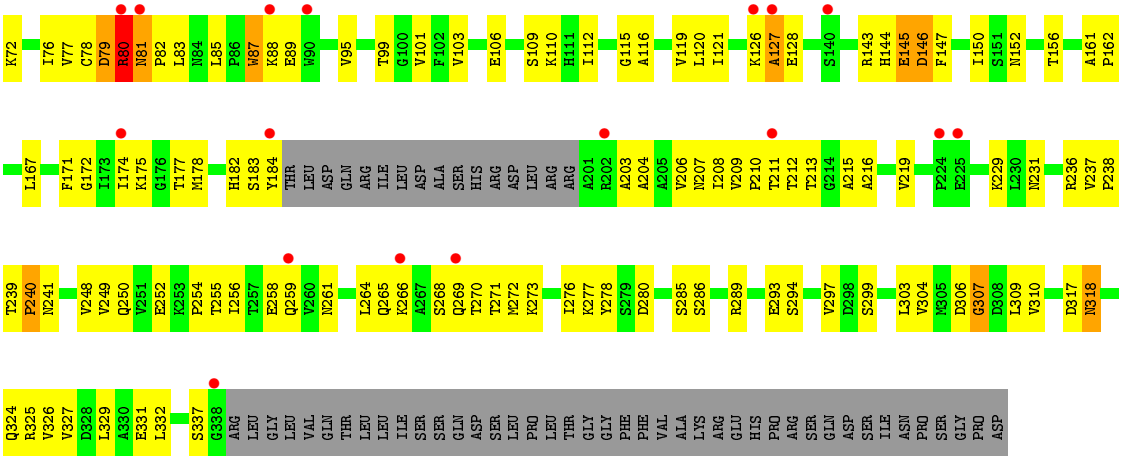
Chain P:



• Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase

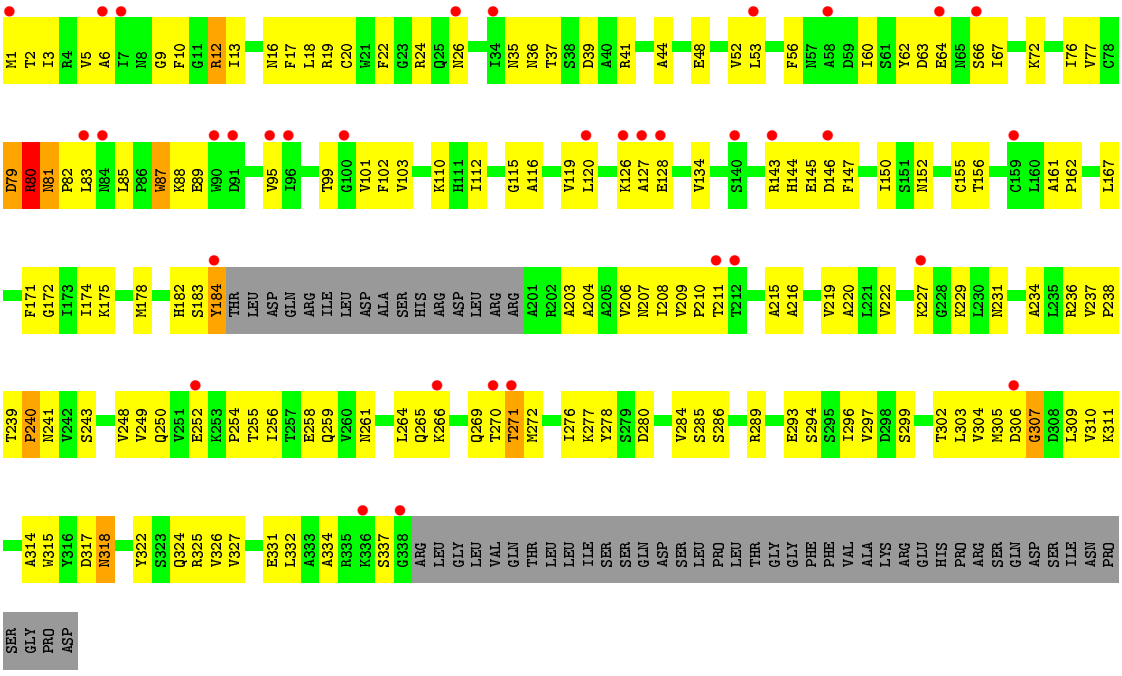
Chain Q:





• Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	151.40Å 79.80Å 207.20Å 90.00° 102.10° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 24.62 – 2.89	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.90) 93.9 (24.62-2.89)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.77 (at 2.89Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.217 , 0.275 0.218 , 0.274	Depositor DCC
R_{free} test set	5442 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å^2)	52.0	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 74.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	15053	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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: SO4

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	0.41	0/2490	0.71	1/3387 (0.0%)
1	B	0.43	0/2490	0.71	2/3387 (0.1%)
1	O	0.56	4/2490 (0.2%)	0.67	1/3387 (0.0%)
1	P	0.54	4/2490 (0.2%)	0.74	4/3387 (0.1%)
1	Q	0.64	9/2490 (0.4%)	0.80	9/3387 (0.3%)
1	R	0.59	6/2490 (0.2%)	0.70	5/3387 (0.1%)
All	All	0.54	23/14940 (0.2%)	0.72	22/20322 (0.1%)

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

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

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	79	ASP	C-O	15.90	1.53	1.23
1	P	80	ARG	CZ-NH2	-12.53	1.16	1.33
1	O	80	ARG	CZ-NH2	-11.42	1.18	1.33
1	R	80	ARG	CG-CD	-11.38	1.23	1.51
1	R	80	ARG	CB-CG	-10.83	1.23	1.52
1	O	80	ARG	CZ-NH1	-10.24	1.19	1.33
1	Q	80	ARG	CZ-NH2	-9.33	1.21	1.33
1	Q	80	ARG	N-CA	8.93	1.64	1.46
1	P	80	ARG	CD-NE	-8.85	1.31	1.46
1	R	80	ARG	CZ-NH2	-8.36	1.22	1.33
1	Q	80	ARG	CG-CD	-8.09	1.31	1.51
1	R	80	ARG	CD-NE	-7.69	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	78	CYS	C-N	7.57	1.51	1.34
1	O	80	ARG	CD-NE	-6.86	1.34	1.46
1	Q	80	ARG	NE-CZ	-6.64	1.24	1.33
1	Q	80	ARG	CD-NE	-6.46	1.35	1.46
1	P	80	ARG	CG-CD	-5.89	1.37	1.51
1	P	80	ARG	NE-CZ	-5.79	1.25	1.33
1	Q	80	ARG	CZ-NH1	-5.72	1.25	1.33
1	O	80	ARG	NE-CZ	-5.56	1.25	1.33
1	Q	79	ASP	CA-C	5.56	1.67	1.52
1	R	80	ARG	C-O	5.08	1.33	1.23
1	R	79	ASP	C-O	-5.07	1.13	1.23

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	79	ASP	O-C-N	16.43	148.98	122.70
1	P	80	ARG	NE-CZ-NH2	-15.03	112.79	120.30
1	Q	79	ASP	CA-C-O	-13.26	92.25	120.10
1	P	80	ARG	NE-CZ-NH1	13.23	126.91	120.30
1	Q	80	ARG	N-CA-C	10.32	138.87	111.00
1	R	80	ARG	NE-CZ-NH2	-10.08	115.26	120.30
1	P	80	ARG	CG-CD-NE	-8.63	93.67	111.80
1	Q	79	ASP	C-N-CA	-8.33	100.89	121.70
1	Q	79	ASP	N-CA-CB	8.16	125.30	110.60
1	Q	78	CYS	C-N-CA	-8.14	101.35	121.70
1	R	80	ARG	CD-NE-CZ	-7.39	113.26	123.60
1	Q	80	ARG	CG-CD-NE	-7.15	96.79	111.80
1	A	208	ILE	N-CA-C	-6.40	93.73	111.00
1	B	208	ILE	N-CA-C	-6.06	94.64	111.00
1	R	80	ARG	CA-CB-CG	5.84	126.24	113.40
1	Q	80	ARG	O-C-N	5.66	131.75	122.70
1	O	80	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	Q	80	ARG	CA-C-N	-5.36	105.41	117.20
1	B	22	PHE	N-CA-C	-5.18	97.02	111.00
1	R	80	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	R	79	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	P	80	ARG	CD-NE-CZ	-5.01	116.59	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Q	80	ARG	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2451	0	2474	123	0
1	B	2451	0	2474	125	0
1	O	2451	0	2474	130	0
1	P	2451	0	2474	131	0
1	Q	2451	0	2474	151	0
1	R	2451	0	2474	141	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
2	O	5	0	0	0	0
2	P	5	0	0	1	0
2	Q	5	0	0	0	0
2	R	5	0	0	0	0
3	A	68	0	0	4	0
3	B	87	0	0	4	0
3	O	61	0	0	5	0
3	P	57	0	0	7	0
3	Q	19	0	0	5	0
3	R	25	0	0	0	0
All	All	15053	0	14844	738	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (738) 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:Q:261:ASN:ND2	1:Q:299:SER:HB2	1.75	1.01
1:P:12:ARG:HD3	1:P:12:ARG:H	1.24	1.00
1:R:12:ARG:H	1:R:12:ARG:HD3	1.30	0.97
1:Q:12:ARG:H	1:Q:12:ARG:HD3	1.31	0.94
1:Q:250:GLN:HE21	1:R:250:GLN:HE21	1.11	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:36:ASN:ND2	1:Q:37:THR:H	1.65	0.92
1:P:36:ASN:ND2	1:P:37:THR:H	1.68	0.91
1:Q:207:ASN:ND2	1:R:286:SER:HB2	1.87	0.89
1:A:206:VAL:HA	3:A:6423:HOH:O	1.71	0.89
1:Q:175:LYS:HE2	1:R:306:ASP:HB3	1.55	0.89
1:Q:261:ASN:HD22	1:Q:299:SER:HB2	1.35	0.87
1:O:36:ASN:ND2	1:O:37:THR:H	1.73	0.86
1:R:80:ARG:HD2	1:R:80:ARG:N	1.88	0.85
1:A:184:TYR:HA	1:A:236:ARG:HH21	1.41	0.84
1:R:144:HIS:CD2	1:R:337:SER:HA	2.12	0.84
1:R:12:ARG:N	1:R:12:ARG:HD3	1.93	0.84
1:B:171:PHE:CE1	1:B:255:THR:HG21	2.13	0.84
1:O:12:ARG:HD3	1:O:12:ARG:H	1.43	0.84
1:R:36:ASN:ND2	1:R:37:THR:H	1.77	0.83
1:R:80:ARG:NE	1:R:80:ARG:H	1.77	0.82
1:P:12:ARG:HD3	1:P:12:ARG:N	1.94	0.82
1:R:171:PHE:CE1	1:R:255:THR:HG21	2.13	0.82
1:Q:171:PHE:CE1	1:Q:255:THR:HG21	2.14	0.81
1:B:252:GLU:HG3	1:O:143:ARG:HH12	1.44	0.81
1:P:99:THR:OG1	1:P:101:VAL:HG12	1.81	0.80
1:Q:250:GLN:NE2	1:R:250:GLN:HE21	1.79	0.80
1:A:171:PHE:CE1	1:A:255:THR:HG21	2.16	0.79
1:O:12:ARG:N	1:O:12:ARG:HD3	1.98	0.79
1:B:19:ARG:NH2	1:B:50:ASP:HB2	1.97	0.78
1:Q:207:ASN:HD21	1:R:286:SER:HB2	1.48	0.78
1:A:21:TRP:HH2	1:A:72:LYS:NZ	1.80	0.78
1:A:184:TYR:HA	1:A:236:ARG:NH2	1.99	0.78
1:Q:12:ARG:HD3	1:Q:12:ARG:N	1.99	0.78
1:O:174:ILE:O	1:O:229:LYS:HE2	1.84	0.77
1:A:82:PRO:HA	1:A:85:LEU:HD12	1.66	0.77
1:B:59:ASP:H	1:B:70:ASN:HD21	1.30	0.77
1:O:1:MET:HG2	1:O:2:THR:HG22	1.66	0.77
1:O:250:GLN:HE21	1:P:250:GLN:HE21	1.34	0.76
1:Q:80:ARG:HA	1:Q:80:ARG:HE	1.50	0.76
1:B:204:ALA:HB2	3:B:6451:HOH:O	1.85	0.76
1:P:171:PHE:CE1	1:P:255:THR:HG21	2.21	0.76
1:P:63:ASP:CG	1:P:64:GLU:H	1.90	0.75
1:B:184:TYR:HA	1:B:236:ARG:HH21	1.50	0.75
1:Q:261:ASN:ND2	1:Q:299:SER:CB	2.49	0.74
1:Q:80:ARG:CA	1:Q:80:ARG:HE	1.96	0.74
1:Q:15:ARG:HD2	3:Q:6466:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ALA:HB3	1:A:67:ILE:HD11	1.68	0.74
1:O:182:HIS:HB2	1:O:236:ARG:HD3	1.70	0.73
1:O:204:ALA:O	1:O:238:PRO:HG3	1.88	0.73
1:R:85:LEU:HD13	1:R:87:TRP:CZ2	2.23	0.73
1:R:174:ILE:O	1:R:229:LYS:HE2	1.89	0.73
1:B:43:ALA:HB3	1:B:67:ILE:HD11	1.70	0.73
1:A:59:ASP:H	1:A:70:ASN:HD21	1.34	0.72
1:P:225:GLU:HG3	3:P:6371:HOH:O	1.88	0.72
1:P:16:ASN:OD1	1:P:53:LEU:HD11	1.88	0.72
1:R:80:ARG:CD	1:R:80:ARG:H	2.02	0.72
1:O:207:ASN:ND2	1:P:286:SER:HB2	2.05	0.71
1:A:285:SER:OG	1:B:208:ILE:HB	1.91	0.71
1:Q:277:LYS:HB2	1:Q:293:GLU:HG2	1.72	0.71
1:R:12:ARG:H	1:R:12:ARG:CD	2.03	0.71
1:B:184:TYR:HA	1:B:236:ARG:NH2	2.04	0.71
1:Q:306:ASP:HB3	1:R:175:LYS:HE2	1.71	0.71
1:R:80:ARG:CD	1:R:80:ARG:N	2.47	0.71
1:A:256:ILE:HB	1:O:106:GLU:OE1	1.89	0.71
1:O:171:PHE:CE1	1:O:255:THR:HG21	2.26	0.70
1:O:144:HIS:CD2	1:O:337:SER:HA	2.26	0.70
1:R:16:ASN:OD1	1:R:53:LEU:HD11	1.91	0.70
1:P:37:THR:HB	3:P:6382:HOH:O	1.91	0.69
1:R:99:THR:OG1	1:R:101:VAL:HG12	1.92	0.69
1:R:277:LYS:HB2	1:R:293:GLU:HG2	1.75	0.69
1:P:182:HIS:HB2	1:P:236:ARG:HD3	1.75	0.69
1:P:144:HIS:CD2	1:P:337:SER:HA	2.28	0.69
1:Q:182:HIS:HB2	1:Q:236:ARG:HD3	1.74	0.69
1:A:309:LEU:HB2	1:B:175:LYS:HE2	1.74	0.68
1:P:63:ASP:CG	1:P:64:GLU:N	2.45	0.68
1:A:103:VAL:HA	1:A:121:ILE:HD13	1.76	0.68
1:Q:144:HIS:CD2	1:Q:337:SER:HA	2.29	0.68
1:O:258:GLU:HB2	3:O:6361:HOH:O	1.92	0.68
1:O:81:ASN:HD21	1:O:83:LEU:CD2	2.07	0.68
1:B:59:ASP:H	1:B:70:ASN:ND2	1.92	0.67
1:P:12:ARG:CD	1:P:12:ARG:H	2.03	0.67
1:Q:63:ASP:CG	1:Q:64:GLU:H	1.97	0.67
1:Q:81:ASN:HD21	1:Q:83:LEU:HD23	1.59	0.67
1:Q:265:GLN:O	1:Q:269:GLN:HG3	1.95	0.67
1:B:286:SER:HB3	1:B:289:ARG:HH11	1.59	0.67
1:A:19:ARG:NH2	1:A:50:ASP:HB2	2.10	0.67
1:R:174:ILE:HD11	1:R:252:GLU:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:VAL:HG23	1:A:222:VAL:HG11	1.77	0.66
1:B:36:ASN:ND2	1:B:37:THR:H	1.93	0.66
1:R:161:ALA:HB3	1:R:162:PRO:HD3	1.77	0.66
1:Q:174:ILE:O	1:Q:229:LYS:HE2	1.95	0.66
1:A:36:ASN:ND2	1:A:37:THR:H	1.91	0.66
1:Q:286:SER:HB2	1:R:207:ASN:HD21	1.61	0.66
1:B:59:ASP:N	1:B:70:ASN:HD21	1.94	0.66
1:O:207:ASN:HD21	1:P:286:SER:HB2	1.60	0.66
1:O:85:LEU:HD13	1:O:87:TRP:CZ2	2.30	0.66
1:Q:12:ARG:CD	1:Q:12:ARG:H	2.09	0.66
1:A:204:ALA:HB2	3:A:6561:HOH:O	1.95	0.66
1:O:128:GLU:HA	3:O:6601:HOH:O	1.94	0.66
1:O:63:ASP:CG	1:O:64:GLU:H	1.99	0.66
1:Q:63:ASP:CG	1:Q:64:GLU:N	2.49	0.66
1:R:80:ARG:HD2	1:R:80:ARG:C	2.03	0.66
1:Q:204:ALA:O	1:Q:238:PRO:HG3	1.96	0.66
1:R:204:ALA:O	1:R:238:PRO:HG3	1.96	0.65
1:Q:174:ILE:HD11	1:Q:252:GLU:HB3	1.76	0.65
1:R:81:ASN:HD21	1:R:83:LEU:HD23	1.62	0.65
1:O:99:THR:OG1	1:O:101:VAL:HG12	1.96	0.65
1:P:174:ILE:O	1:P:229:LYS:HE2	1.97	0.65
1:B:239:THR:HG23	1:B:240:PRO:HD2	1.77	0.64
1:P:174:ILE:HD11	1:P:252:GLU:HB3	1.80	0.64
1:Q:16:ASN:OD1	1:Q:53:LEU:HD11	1.97	0.64
1:O:95:VAL:CG1	1:O:119:VAL:HG22	2.28	0.64
1:B:21:TRP:CH2	1:B:72:LYS:NZ	2.66	0.64
1:Q:250:GLN:HE21	1:R:250:GLN:NE2	1.89	0.64
1:P:95:VAL:CG1	1:P:119:VAL:HG22	2.28	0.64
1:B:103:VAL:HA	1:B:121:ILE:HD13	1.79	0.64
1:B:252:GLU:HG3	1:O:143:ARG:NH1	2.13	0.64
1:A:162:PRO:HB3	1:A:272:MET:CE	2.27	0.64
1:A:59:ASP:N	1:A:70:ASN:HD21	1.96	0.64
1:B:52:VAL:HG13	1:B:241:ASN:ND2	2.13	0.64
1:O:264:LEU:HD13	1:O:297:VAL:HG11	1.80	0.64
1:O:12:ARG:CD	1:O:12:ARG:H	2.12	0.63
1:O:16:ASN:OD1	1:O:53:LEU:HD11	1.99	0.63
1:P:36:ASN:ND2	1:P:37:THR:N	2.44	0.63
1:Q:95:VAL:CG1	1:Q:119:VAL:HG22	2.29	0.63
1:A:261:ASN:HD21	1:A:302:THR:CB	2.11	0.63
1:A:250:GLN:NE2	1:B:250:GLN:NE2	2.46	0.63
1:R:237:VAL:HG23	1:R:239:THR:HG23	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:75:LYS:HG3	3:O:6628:HOH:O	1.97	0.63
1:Q:286:SER:HB2	1:R:207:ASN:ND2	2.14	0.63
1:R:264:LEU:HD13	1:R:297:VAL:HG11	1.81	0.63
1:Q:22:PHE:HE1	1:Q:72:LYS:HD2	1.64	0.63
1:P:143:ARG:HB2	1:P:146:ASP:OD1	1.98	0.63
1:Q:231:ASN:HB3	1:R:303:LEU:HD11	1.79	0.63
1:Q:81:ASN:HD21	1:Q:83:LEU:CD2	2.10	0.63
1:O:239:THR:HB	1:O:240:PRO:HD2	1.81	0.63
1:B:171:PHE:CD1	1:B:255:THR:HG21	2.34	0.62
1:R:265:GLN:O	1:R:269:GLN:HG3	1.99	0.62
1:O:63:ASP:CG	1:O:64:GLU:N	2.52	0.62
1:B:126:LYS:O	1:B:127:ALA:HB3	1.99	0.62
1:B:144:HIS:CD2	1:B:337:SER:HA	2.34	0.62
1:R:144:HIS:HD2	1:R:337:SER:HA	1.61	0.62
1:O:215:ALA:O	1:O:219:VAL:HG23	1.98	0.62
1:B:2:THR:O	1:B:2:THR:HG23	2.00	0.62
1:B:81:ASN:HB3	1:B:84:ASN:HD22	1.65	0.62
1:O:182:HIS:HB2	1:O:236:ARG:CD	2.29	0.62
1:Q:99:THR:OG1	1:Q:101:VAL:HG12	1.99	0.62
1:O:272:MET:HG3	1:O:276:ILE:HD12	1.81	0.61
1:R:239:THR:HB	1:R:240:PRO:HD2	1.81	0.61
1:O:81:ASN:HD21	1:O:83:LEU:HD22	1.64	0.61
1:Q:80:ARG:NE	1:Q:80:ARG:CA	2.54	0.61
1:O:145:GLU:H	1:O:145:GLU:CD	2.03	0.61
1:P:215:ALA:O	1:P:219:VAL:HG23	1.99	0.61
3:A:6433:HOH:O	1:O:106:GLU:HG3	2.00	0.61
1:O:250:GLN:NE2	1:P:250:GLN:HE21	1.98	0.61
1:R:182:HIS:HB2	1:R:236:ARG:HD3	1.82	0.61
1:A:59:ASP:H	1:A:70:ASN:ND2	1.98	0.61
1:O:39:ASP:OD1	1:O:41:ARG:HG2	2.01	0.61
1:Q:215:ALA:O	1:Q:219:VAL:HG23	2.01	0.61
1:A:144:HIS:CD2	1:A:337:SER:HA	2.36	0.61
1:O:306:ASP:HB3	1:P:175:LYS:HE2	1.83	0.61
1:R:215:ALA:O	1:R:219:VAL:HG23	2.00	0.61
1:R:80:ARG:HD2	1:R:81:ASN:N	2.15	0.61
1:Q:36:ASN:ND2	1:Q:37:THR:N	2.43	0.60
1:A:19:ARG:CZ	1:A:56:PHE:HB2	2.31	0.60
1:O:36:ASN:ND2	1:O:37:THR:N	2.48	0.60
1:A:81:ASN:HB3	1:A:84:ASN:ND2	2.15	0.60
1:A:239:THR:HG23	1:A:240:PRO:HD2	1.81	0.60
1:Q:85:LEU:HD13	1:Q:87:TRP:CZ2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:THR:O	1:B:273:LYS:HB2	2.01	0.60
1:R:81:ASN:HD21	1:R:83:LEU:CD2	2.14	0.60
1:R:95:VAL:CG1	1:R:119:VAL:HG22	2.32	0.60
1:O:22:PHE:HE1	1:O:72:LYS:HD2	1.65	0.60
1:R:63:ASP:CG	1:R:64:GLU:H	2.04	0.60
1:O:19:ARG:NH2	1:O:56:PHE:HB2	2.17	0.60
1:O:286:SER:HB2	1:P:207:ASN:ND2	2.17	0.59
1:Q:52:VAL:HG13	1:Q:241:ASN:ND2	2.16	0.59
1:R:35:ASN:HA	1:R:77:VAL:O	2.02	0.59
1:Q:145:GLU:CD	1:Q:145:GLU:H	2.04	0.59
1:Q:210:PRO:HG3	1:R:315:TRP:HZ2	1.67	0.59
1:O:80:ARG:HG3	1:O:80:ARG:HH11	1.67	0.59
1:P:81:ASN:HD21	1:P:83:LEU:HD23	1.66	0.59
1:A:68:THR:HG23	1:A:73:THR:HG22	1.83	0.59
1:A:81:ASN:HB3	1:A:84:ASN:HD22	1.68	0.59
1:P:282:PRO:HA	3:P:6587:HOH:O	2.01	0.59
1:Q:182:HIS:HB2	1:Q:236:ARG:CD	2.32	0.59
1:O:12:ARG:HG2	1:O:13:ILE:H	1.68	0.59
1:P:241:ASN:HA	1:P:318:ASN:ND2	2.18	0.59
1:Q:80:ARG:NE	1:Q:80:ARG:HA	2.18	0.59
1:R:19:ARG:NH2	1:R:56:PHE:HB2	2.17	0.59
1:Q:41:ARG:HB3	1:Q:62:TYR:CE1	2.38	0.59
1:Q:35:ASN:HA	1:Q:77:VAL:O	2.02	0.59
1:B:183:SER:OG	1:B:239:THR:HG22	2.03	0.59
1:P:204:ALA:O	1:P:238:PRO:HG3	2.02	0.59
1:Q:264:LEU:HD13	1:Q:297:VAL:HG11	1.84	0.59
1:Q:210:PRO:HG3	1:R:315:TRP:CZ2	2.38	0.58
1:R:63:ASP:CG	1:R:64:GLU:N	2.57	0.58
1:A:18:LEU:HD22	1:A:22:PHE:CE2	2.38	0.58
1:Q:161:ALA:HB3	1:Q:162:PRO:HD3	1.84	0.58
1:P:85:LEU:HD13	1:P:87:TRP:CZ2	2.38	0.58
1:Q:261:ASN:HD22	1:Q:299:SER:CB	2.13	0.58
1:Q:67:ILE:HG23	1:Q:76:ILE:CD1	2.34	0.58
1:P:182:HIS:HB2	1:P:236:ARG:CD	2.34	0.58
1:P:81:ASN:HD21	1:P:83:LEU:CD2	2.17	0.57
1:A:255:THR:HG22	1:A:259:GLN:OE1	2.03	0.57
1:O:12:ARG:HG2	1:O:13:ILE:N	2.20	0.57
1:O:250:GLN:HE21	1:P:250:GLN:NE2	2.01	0.57
1:R:266:LYS:NZ	1:R:270:THR:HG21	2.19	0.57
1:Q:209:VAL:HG13	1:R:284:VAL:CG1	2.35	0.57
1:O:41:ARG:HB3	1:O:62:TYR:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:22:PHE:HE1	1:P:72:LYS:HD2	1.69	0.57
1:Q:208:ILE:HB	1:R:285:SER:HB3	1.87	0.57
1:R:48:GLU:HB2	1:R:60:ILE:HD12	1.86	0.57
1:A:21:TRP:CH2	1:A:72:LYS:NZ	2.64	0.57
1:P:62:TYR:HA	1:P:67:ILE:HA	1.86	0.57
1:Q:239:THR:HB	1:Q:240:PRO:HD2	1.84	0.57
1:A:126:LYS:O	1:A:127:ALA:HB3	2.04	0.57
1:O:67:ILE:HG23	1:O:76:ILE:CD1	2.34	0.57
1:P:255:THR:HG22	1:P:259:GLN:NE2	2.20	0.57
1:R:241:ASN:HA	1:R:318:ASN:ND2	2.20	0.56
1:Q:175:LYS:CE	1:R:306:ASP:HB3	2.32	0.56
1:B:89:GLU:OE1	1:B:89:GLU:N	2.36	0.56
1:Q:280:ASP:HA	1:Q:299:SER:OG	2.05	0.56
1:O:265:GLN:O	1:O:269:GLN:HG3	2.06	0.56
1:A:246:ASP:HA	1:A:313:ILE:HD13	1.87	0.56
1:R:143:ARG:HB2	1:R:146:ASP:OD1	2.06	0.56
1:P:81:ASN:HD22	1:P:82:PRO:CD	2.19	0.56
1:B:18:LEU:HD22	1:B:22:PHE:CE2	2.41	0.56
1:O:146:ASP:HB3	1:O:147:PHE:CE1	2.40	0.56
1:O:161:ALA:HB3	1:O:162:PRO:HD3	1.88	0.56
1:P:81:ASN:HD22	1:P:82:PRO:N	2.03	0.56
1:A:87:TRP:HA	1:A:87:TRP:HE3	1.71	0.56
1:Q:120:LEU:HD13	1:Q:150:ILE:HG13	1.88	0.56
1:A:87:TRP:HA	1:A:87:TRP:CE3	2.41	0.55
1:P:239:THR:HB	1:P:240:PRO:HD2	1.88	0.55
1:R:62:TYR:HA	1:R:67:ILE:HA	1.88	0.55
1:A:2:THR:HG23	1:A:2:THR:O	2.05	0.55
1:B:239:THR:HG23	1:B:240:PRO:CD	2.35	0.55
1:P:35:ASN:HA	1:P:77:VAL:O	2.06	0.55
1:A:159:CYS:HA	1:A:295:SER:HB2	1.89	0.55
1:A:4:ARG:HD3	1:A:91:ASP:O	2.05	0.55
1:R:145:GLU:CD	1:R:145:GLU:H	2.09	0.55
1:Q:261:ASN:HD21	1:Q:299:SER:CA	2.19	0.55
1:A:171:PHE:CD1	1:A:255:THR:HG21	2.42	0.55
1:P:161:ALA:HB3	1:P:162:PRO:HD3	1.89	0.55
1:R:183:SER:O	1:R:184:TYR:C	2.45	0.55
1:A:162:PRO:HB3	1:A:272:MET:HE2	1.87	0.55
1:B:18:LEU:HD22	1:B:22:PHE:HE2	1.71	0.55
1:B:19:ARG:CZ	1:B:56:PHE:HB2	2.37	0.55
1:O:82:PRO:HB2	1:O:110:LYS:HB3	1.89	0.55
1:R:278:TYR:CE1	1:R:299:SER:HB3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ASP:HA	1:B:313:ILE:HD13	1.88	0.55
1:A:324:GLN:OE1	1:A:324:GLN:HA	2.07	0.55
1:P:156:THR:OG1	1:P:182:HIS:HE1	1.90	0.55
1:A:99:THR:OG1	1:A:101:VAL:HG22	2.06	0.54
1:B:237:VAL:HG23	1:B:239:THR:HB	1.89	0.54
1:B:81:ASN:HB3	1:B:84:ASN:ND2	2.22	0.54
1:Q:87:TRP:HA	1:Q:87:TRP:CE3	2.42	0.54
1:Q:143:ARG:HB2	1:Q:146:ASP:OD1	2.07	0.54
1:B:162:PRO:HB3	1:B:272:MET:HE2	1.89	0.54
1:B:87:TRP:HA	1:B:87:TRP:CE3	2.42	0.54
1:Q:241:ASN:HA	1:Q:318:ASN:ND2	2.23	0.54
1:Q:87:TRP:HA	1:Q:87:TRP:HE3	1.73	0.54
1:Q:19:ARG:NH2	1:Q:56:PHE:HB2	2.22	0.54
1:A:265:GLN:O	1:A:269:GLN:HG3	2.07	0.54
1:B:202:ARG:O	1:B:204:ALA:N	2.40	0.54
1:A:183:SER:OG	1:A:239:THR:HG22	2.08	0.54
1:B:87:TRP:HE3	1:B:87:TRP:HA	1.73	0.54
1:O:81:ASN:HD22	1:O:82:PRO:N	2.05	0.54
1:P:87:TRP:HA	1:P:87:TRP:HE3	1.73	0.54
1:R:82:PRO:HB2	1:R:110:LYS:HB3	1.90	0.54
1:A:63:ASP:OD1	1:A:64:GLU:N	2.40	0.54
1:P:10:PHE:CZ	1:P:18:LEU:HD12	2.43	0.54
1:P:216:ALA:HB3	3:P:6367:HOH:O	2.07	0.54
1:Q:9:GLY:HA3	1:Q:99:THR:HG22	1.90	0.54
1:R:324:GLN:HA	1:R:324:GLN:OE1	2.07	0.54
1:P:289:ARG:HH12	1:R:289:ARG:HH22	1.55	0.54
1:A:87:TRP:CE3	1:A:92:ILE:HG13	2.43	0.54
1:Q:277:LYS:HB2	1:Q:293:GLU:CG	2.38	0.53
1:B:59:ASP:N	1:B:70:ASN:ND2	2.55	0.53
1:A:12:ARG:HH22	1:A:50:ASP:CG	2.11	0.53
1:O:95:VAL:HG13	1:O:119:VAL:HG22	1.91	0.53
1:O:286:SER:HB2	1:P:207:ASN:HD21	1.72	0.53
1:P:87:TRP:HA	1:P:87:TRP:CE3	2.43	0.53
1:Q:62:TYR:HA	1:Q:67:ILE:HA	1.89	0.53
1:A:145:GLU:CD	1:A:145:GLU:H	2.11	0.53
1:B:156:THR:HB	2:B:2339:SO4:O3	2.07	0.53
1:O:81:ASN:C	1:O:81:ASN:HD22	2.11	0.53
1:R:270:THR:OG1	1:R:271:THR:N	2.42	0.53
1:B:87:TRP:CE3	1:B:92:ILE:HG13	2.43	0.53
1:A:239:THR:HG23	1:A:240:PRO:CD	2.38	0.53
1:B:261:ASN:HD21	1:B:302:THR:CB	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:120:LEU:HD12	1:P:120:LEU:C	2.28	0.53
1:A:237:VAL:HG23	1:A:239:THR:HB	1.91	0.53
1:B:254:PRO:HA	1:B:307:GLY:O	2.08	0.53
1:P:112:ILE:HA	1:P:116:ALA:O	2.08	0.53
1:Q:272:MET:HG3	1:Q:276:ILE:HD12	1.90	0.53
1:R:249:VAL:O	1:R:309:LEU:HD12	2.08	0.53
1:R:1:MET:HG2	1:R:2:THR:HG22	1.91	0.53
1:P:264:LEU:HD13	1:P:297:VAL:HG11	1.91	0.53
1:B:145:GLU:H	1:B:145:GLU:CD	2.11	0.53
1:B:64:GLU:HA	1:B:64:GLU:OE2	2.09	0.53
1:O:209:VAL:HG21	3:O:6496:HOH:O	2.08	0.53
1:P:237:VAL:HG23	1:P:239:THR:HG23	1.91	0.53
1:A:120:LEU:C	1:A:120:LEU:HD12	2.29	0.53
1:O:183:SER:O	1:O:184:TYR:C	2.47	0.53
1:O:80:ARG:CG	1:O:80:ARG:HH11	2.20	0.53
1:A:67:ILE:HD12	1:A:76:ILE:HD11	1.91	0.52
1:B:4:ARG:HD3	1:B:91:ASP:O	2.09	0.52
1:O:277:LYS:HB2	1:O:293:GLU:HG2	1.91	0.52
1:P:88:LYS:HB3	1:P:115:GLY:HA3	1.91	0.52
1:B:19:ARG:HH22	1:B:50:ASP:HB2	1.73	0.52
1:Q:112:ILE:HA	1:Q:116:ALA:O	2.10	0.52
1:R:22:PHE:HE1	1:R:72:LYS:HD2	1.74	0.52
1:P:19:ARG:NH2	1:P:56:PHE:HB2	2.23	0.52
1:Q:183:SER:O	1:Q:184:TYR:C	2.48	0.52
1:Q:39:ASP:OD1	1:Q:41:ARG:HG2	2.09	0.52
1:O:241:ASN:HA	1:O:318:ASN:ND2	2.25	0.52
1:Q:208:ILE:CG1	1:R:239:THR:HG21	2.39	0.52
1:O:79:ASP:HB2	1:O:85:LEU:CD2	2.40	0.52
1:R:41:ARG:HB3	1:R:62:TYR:CE1	2.45	0.52
1:O:48:GLU:HB2	1:O:60:ILE:HD12	1.91	0.52
1:O:35:ASN:HA	1:O:77:VAL:O	2.09	0.52
1:P:183:SER:O	1:P:184:TYR:C	2.48	0.52
1:A:94:LEU:HA	1:A:118:LYS:O	2.10	0.51
1:B:82:PRO:HA	1:B:85:LEU:HD12	1.92	0.51
1:P:103:VAL:HA	1:P:121:ILE:HD13	1.92	0.51
1:R:182:HIS:HB2	1:R:236:ARG:CD	2.39	0.51
1:R:289:ARG:HA	1:R:317:ASP:OD2	2.10	0.51
1:A:52:VAL:HG13	1:A:241:ASN:ND2	2.25	0.51
1:A:255:THR:CG2	1:A:259:GLN:OE1	2.58	0.51
1:B:211:THR:HG23	1:B:234:ALA:HB3	1.91	0.51
1:O:206:VAL:C	1:O:207:ASN:HD22	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:261:ASN:ND2	1:P:302:THR:OG1	2.36	0.51
1:P:213:THR:HA	2:P:4339:SO4:O2	2.10	0.51
1:R:266:LYS:HZ2	1:R:270:THR:HG21	1.74	0.51
1:O:24:ARG:HG3	1:O:24:ARG:HH11	1.76	0.51
1:Q:41:ARG:HB3	1:Q:62:TYR:CZ	2.45	0.51
1:A:202:ARG:O	1:A:204:ALA:N	2.43	0.51
1:P:81:ASN:HD22	1:P:82:PRO:HD2	1.76	0.51
1:A:11:GLY:HA2	1:A:15:ARG:HH21	1.74	0.51
1:A:59:ASP:N	1:A:70:ASN:ND2	2.57	0.51
1:O:254:PRO:HA	1:O:307:GLY:O	2.11	0.51
1:Q:12:ARG:HG2	1:Q:13:ILE:N	2.26	0.51
1:Q:81:ASN:HD22	1:Q:82:PRO:N	2.08	0.51
1:B:134:VAL:HG23	1:B:222:VAL:HG11	1.91	0.51
1:A:175:LYS:CE	1:B:306:ASP:HB3	2.40	0.51
1:P:41:ARG:HB3	1:P:62:TYR:CE1	2.46	0.51
1:P:39:ASP:OD1	1:P:41:ARG:HG2	2.10	0.51
1:R:112:ILE:HA	1:R:116:ALA:O	2.11	0.51
1:A:89:GLU:OE1	1:A:89:GLU:N	2.40	0.51
1:P:182:HIS:HA	1:P:243:SER:OG	2.10	0.51
1:P:303:LEU:HD23	1:P:303:LEU:C	2.32	0.51
1:Q:248:VAL:HG11	1:R:248:VAL:HG11	1.93	0.51
1:Q:324:GLN:OE1	1:Q:324:GLN:HA	2.10	0.51
1:A:256:ILE:HB	1:O:106:GLU:CD	2.32	0.50
1:P:106:GLU:O	1:P:109:SER:HB2	2.11	0.50
1:Q:88:LYS:HB3	1:Q:115:GLY:HA3	1.93	0.50
1:Q:67:ILE:HG23	1:Q:76:ILE:HD11	1.93	0.50
1:A:39:ASP:OD1	1:A:41:ARG:HB3	2.10	0.50
1:Q:212:THR:HG22	1:Q:213:THR:N	2.25	0.50
1:Q:1:MET:HG2	1:Q:2:THR:HG22	1.94	0.50
1:R:67:ILE:HG23	1:R:76:ILE:CD1	2.41	0.50
1:O:182:HIS:HD2	1:O:236:ARG:HE	1.60	0.50
1:Q:10:PHE:CZ	1:Q:18:LEU:HD12	2.46	0.50
1:B:270:THR:OG1	1:B:271:THR:N	2.45	0.50
1:B:162:PRO:HB3	1:B:272:MET:CE	2.41	0.50
1:A:18:LEU:HD22	1:A:22:PHE:HE2	1.77	0.50
1:B:41:ARG:HA	1:B:62:TYR:HD1	1.76	0.50
1:P:277:LYS:HB2	1:P:293:GLU:HG2	1.94	0.50
1:P:62:TYR:HB2	1:P:67:ILE:HG22	1.93	0.50
1:R:12:ARG:HG2	1:R:13:ILE:N	2.27	0.50
1:A:117:LYS:NZ	3:A:6346:HOH:O	2.44	0.50
1:O:80:ARG:NH1	1:O:80:ARG:CG	2.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:249:VAL:O	1:Q:309:LEU:HD12	2.12	0.50
1:P:278:TYR:CE1	1:P:299:SER:HB3	2.47	0.50
1:B:286:SER:HA	1:B:289:ARG:HD3	1.93	0.49
1:O:237:VAL:HG23	1:O:239:THR:HG23	1.94	0.49
1:O:87:TRP:HE3	1:O:87:TRP:HA	1.77	0.49
1:Q:48:GLU:HB2	1:Q:60:ILE:HD12	1.93	0.49
1:R:120:LEU:HD13	1:R:150:ILE:HG13	1.94	0.49
1:Q:261:ASN:HD21	1:Q:299:SER:HB2	1.70	0.49
1:R:134:VAL:HG23	1:R:222:VAL:HG11	1.93	0.49
1:R:39:ASP:OD1	1:R:41:ARG:HG2	2.11	0.49
1:A:175:LYS:NZ	1:A:250:GLN:OE1	2.45	0.49
1:O:52:VAL:HG13	1:O:241:ASN:ND2	2.26	0.49
1:P:24:ARG:HG3	1:P:24:ARG:HH11	1.78	0.49
1:A:120:LEU:HD12	1:A:121:ILE:N	2.28	0.49
1:A:41:ARG:HA	1:A:62:TYR:HD1	1.78	0.49
1:A:59:ASP:O	1:A:69:VAL:HA	2.12	0.49
1:B:59:ASP:O	1:B:69:VAL:HA	2.12	0.49
1:O:41:ARG:HB3	1:O:62:TYR:CZ	2.48	0.49
1:O:87:TRP:CE3	1:O:87:TRP:HA	2.47	0.49
1:A:162:PRO:HB3	1:A:272:MET:HE1	1.92	0.49
1:B:277:LYS:HB3	1:B:296:ILE:HG23	1.93	0.49
1:O:146:ASP:HB3	1:O:147:PHE:CD1	2.48	0.49
1:O:62:TYR:HA	1:O:67:ILE:HA	1.95	0.49
1:P:294:SER:HG	1:P:325:ARG:HH11	1.59	0.49
1:R:171:PHE:CD1	1:R:255:THR:HG21	2.47	0.49
1:A:68:THR:CG2	1:A:73:THR:HG22	2.43	0.49
1:O:249:VAL:O	1:O:309:LEU:HD12	2.12	0.49
1:P:1:MET:HG2	1:P:2:THR:HG22	1.93	0.49
1:R:277:LYS:HB2	1:R:293:GLU:CG	2.42	0.49
1:O:335:ARG:NH2	3:O:6627:HOH:O	2.45	0.49
1:O:67:ILE:HG23	1:O:76:ILE:HD11	1.93	0.49
1:Q:81:ASN:HD22	1:Q:82:PRO:CD	2.26	0.49
1:R:10:PHE:CZ	1:R:18:LEU:HD12	2.48	0.49
1:P:265:GLN:O	1:P:269:GLN:HG3	2.12	0.48
1:R:41:ARG:HB3	1:R:62:TYR:CZ	2.48	0.48
1:B:255:THR:HG22	1:B:259:GLN:OE1	2.13	0.48
1:Q:24:ARG:HD3	3:Q:6401:HOH:O	2.12	0.48
1:R:52:VAL:HG13	1:R:241:ASN:ND2	2.28	0.48
1:A:280:ASP:HA	1:A:299:SER:OG	2.14	0.48
1:Q:250:GLN:NE2	1:R:250:GLN:NE2	2.55	0.48
1:R:82:PRO:HB2	1:R:110:LYS:CB	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:VAL:HG11	1:B:248:VAL:HG11	1.96	0.48
1:O:261:ASN:ND2	1:O:302:THR:OG1	2.44	0.48
1:A:308:ASP:OD2	1:B:175:LYS:HE3	2.13	0.48
1:P:48:GLU:HB2	1:P:60:ILE:HD12	1.95	0.48
1:P:81:ASN:HD22	1:P:81:ASN:C	2.17	0.48
1:R:62:TYR:HB2	1:R:67:ILE:HG22	1.95	0.48
1:P:12:ARG:HG2	1:P:13:ILE:N	2.28	0.48
1:R:216:ALA:HB1	1:R:231:ASN:HA	1.95	0.48
1:A:42:THR:O	1:A:46:LEU:HG	2.13	0.48
1:O:82:PRO:HB2	1:O:110:LYS:CB	2.44	0.48
1:O:10:PHE:CZ	1:O:18:LEU:HD12	2.49	0.48
1:Q:77:VAL:HG23	3:Q:6376:HOH:O	2.13	0.48
1:Q:266:LYS:NZ	1:Q:270:THR:HG21	2.29	0.48
1:Q:36:ASN:HD22	1:Q:37:THR:H	1.54	0.48
1:R:272:MET:HG3	1:R:276:ILE:HD12	1.94	0.48
1:A:315:TRP:HZ2	1:B:210:PRO:CG	2.27	0.48
1:Q:206:VAL:C	1:Q:207:ASN:HD22	2.16	0.48
1:Q:81:ASN:C	1:Q:81:ASN:HD22	2.17	0.47
1:A:250:GLN:HE21	1:B:250:GLN:HE22	1.61	0.47
1:O:255:THR:O	1:O:307:GLY:HA2	2.14	0.47
1:P:120:LEU:HD13	1:P:150:ILE:HG13	1.96	0.47
1:R:12:ARG:HG2	1:R:13:ILE:H	1.78	0.47
1:R:24:ARG:HG3	1:R:24:ARG:HH11	1.80	0.47
1:P:138:ASN:CG	1:P:222:VAL:HG12	2.35	0.47
1:R:81:ASN:HD22	1:R:82:PRO:N	2.12	0.47
1:B:247:LEU:O	1:B:311:LYS:HA	2.14	0.47
1:O:278:TYR:CE1	1:O:299:SER:HB3	2.49	0.47
1:O:303:LEU:HD23	1:O:303:LEU:C	2.35	0.47
1:Q:56:PHE:HD2	1:Q:60:ILE:HD11	1.79	0.47
1:R:303:LEU:C	1:R:303:LEU:HD23	2.34	0.47
1:P:10:PHE:CE1	1:P:18:LEU:HD12	2.49	0.47
1:Q:55:ARG:HB3	3:Q:6444:HOH:O	2.15	0.47
1:A:83:LEU:HD13	1:A:110:LYS:HB3	1.97	0.47
1:A:10:PHE:CZ	1:A:18:LEU:HD12	2.50	0.47
1:B:240:PRO:HG2	1:B:241:ASN:H	1.79	0.47
1:P:12:ARG:HG2	1:P:13:ILE:H	1.80	0.47
1:Q:44:ALA:HB2	1:Q:62:TYR:HB3	1.96	0.47
1:R:88:LYS:HB3	1:R:115:GLY:HA3	1.96	0.47
1:R:17:PHE:CE2	1:R:326:VAL:HG12	2.50	0.47
1:B:130:VAL:HG23	1:B:131:GLY:N	2.29	0.47
1:B:296:ILE:HD12	1:B:315:TRP:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:81:ASN:HD21	1:O:83:LEU:HD23	1.77	0.47
1:P:327:VAL:O	1:P:331:GLU:HB2	2.15	0.47
1:Q:209:VAL:HG13	1:R:284:VAL:HG12	1.94	0.47
1:B:145:GLU:N	1:B:145:GLU:OE2	2.47	0.47
1:A:315:TRP:HZ2	1:B:210:PRO:HG3	1.79	0.47
1:Q:67:ILE:HG23	1:Q:76:ILE:HD12	1.97	0.47
1:R:20:CYS:HB3	1:R:324:GLN:OE1	2.15	0.47
1:A:254:PRO:HA	1:A:307:GLY:O	2.15	0.46
1:O:212:THR:HG22	1:O:213:THR:N	2.30	0.46
1:Q:303:LEU:HD23	1:Q:303:LEU:C	2.34	0.46
1:R:56:PHE:HD2	1:R:60:ILE:HD11	1.80	0.46
1:B:322:TYR:O	1:B:326:VAL:HG23	2.14	0.46
1:O:19:ARG:CZ	1:O:56:PHE:HB2	2.45	0.46
1:P:289:ARG:HA	1:P:317:ASP:OD2	2.15	0.46
1:Q:82:PRO:HB2	1:Q:110:LYS:HB3	1.97	0.46
1:P:138:ASN:ND2	1:P:222:VAL:HG12	2.31	0.46
1:Q:82:PRO:HB2	1:Q:110:LYS:CB	2.45	0.46
1:R:3:ILE:HD13	1:R:334:ALA:HA	1.97	0.46
1:R:36:ASN:ND2	1:R:37:THR:N	2.55	0.46
1:Q:62:TYR:HB2	1:Q:67:ILE:HG22	1.98	0.46
1:R:184:TYR:C	1:R:184:TYR:CD1	2.89	0.46
1:R:67:ILE:HG23	1:R:76:ILE:HD11	1.98	0.46
1:B:85:LEU:HD13	1:B:87:TRP:CZ2	2.50	0.46
1:Q:103:VAL:HG23	1:Q:126:LYS:HB2	1.97	0.46
1:R:261:ASN:ND2	1:R:302:THR:OG1	2.40	0.46
1:B:119:VAL:CG1	1:B:149:VAL:HG22	2.46	0.46
1:A:208:ILE:HB	1:B:285:SER:OG	2.15	0.46
1:P:160:LEU:HD12	1:P:160:LEU:O	2.16	0.46
1:A:296:ILE:HD12	1:A:315:TRP:O	2.15	0.46
1:P:21:TRP:HE1	1:P:27:THR:HG21	1.81	0.46
1:B:117:LYS:NZ	3:B:6553:HOH:O	2.46	0.46
1:O:112:ILE:HA	1:O:116:ALA:O	2.16	0.46
1:O:209:VAL:HA	1:O:210:PRO:HD3	1.76	0.46
1:P:5:VAL:HG12	1:P:6:ALA:N	2.30	0.46
1:R:255:THR:O	1:R:307:GLY:HA2	2.16	0.46
1:Q:177:THR:OG1	1:R:311:LYS:HD2	2.16	0.46
1:R:81:ASN:HD22	1:R:82:PRO:CD	2.29	0.46
1:B:159:CYS:SG	1:B:316:TYR:HB3	2.56	0.46
1:A:332:LEU:HD22	1:A:336:LYS:HG3	1.97	0.45
1:B:139:ASP:OD1	1:B:139:ASP:N	2.49	0.45
1:O:156:THR:OG1	1:O:182:HIS:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:212:THR:HG22	1:P:213:THR:N	2.31	0.45
1:Q:229:LYS:C	1:R:305:MET:HE1	2.37	0.45
1:O:303:LEU:HD23	1:O:304:VAL:N	2.31	0.45
1:B:280:ASP:HA	1:B:299:SER:OG	2.16	0.45
1:O:324:GLN:OE1	1:O:324:GLN:HA	2.16	0.45
1:O:56:PHE:HD2	1:O:60:ILE:HD11	1.81	0.45
1:P:95:VAL:HG13	1:P:119:VAL:HG22	1.98	0.45
1:P:249:VAL:O	1:P:309:LEU:HD12	2.15	0.45
1:Q:327:VAL:O	1:Q:331:GLU:HB2	2.17	0.45
1:A:17:PHE:CE2	1:A:326:VAL:HG12	2.51	0.45
1:P:255:THR:O	1:P:307:GLY:HA2	2.16	0.45
1:P:257:THR:HA	1:P:304:VAL:HG23	1.98	0.45
1:P:256:ILE:HG13	1:P:259:GLN:H	1.81	0.45
1:Q:126:LYS:O	1:Q:127:ALA:HB3	2.16	0.45
1:B:255:THR:HB	1:B:259:GLN:OE1	2.16	0.45
1:R:254:PRO:HA	1:R:307:GLY:O	2.16	0.45
1:B:159:CYS:HA	1:B:295:SER:HB2	1.99	0.45
1:B:161:ALA:O	1:B:165:LYS:HB2	2.17	0.45
1:B:39:ASP:OD1	1:B:41:ARG:HB3	2.16	0.45
1:Q:156:THR:OG1	1:Q:182:HIS:HE1	1.99	0.45
1:R:280:ASP:HA	1:R:299:SER:OG	2.17	0.45
1:R:87:TRP:HE3	1:R:87:TRP:HA	1.82	0.45
1:O:20:CYS:HB3	1:O:324:GLN:OE1	2.17	0.45
1:O:67:ILE:HG23	1:O:76:ILE:HD12	1.98	0.45
1:O:208:ILE:CG1	1:P:239:THR:HG21	2.47	0.45
1:Q:171:PHE:CD1	1:Q:255:THR:HG21	2.52	0.45
1:Q:20:CYS:HB3	1:Q:324:GLN:OE1	2.16	0.45
1:R:146:ASP:HB3	1:R:147:PHE:CD1	2.52	0.45
1:B:229:LYS:HZ1	1:O:143:ARG:HH21	1.65	0.45
1:R:44:ALA:HB2	1:R:62:TYR:HB3	1.98	0.45
1:R:63:ASP:HB3	1:R:66:SER:O	2.17	0.45
1:B:324:GLN:HA	1:B:324:GLN:OE1	2.17	0.45
1:O:280:ASP:HA	1:O:299:SER:OG	2.17	0.45
1:P:184:TYR:CD1	1:P:184:TYR:C	2.89	0.45
1:R:303:LEU:HD23	1:R:304:VAL:N	2.31	0.45
1:A:317:ASP:O	1:A:318:ASN:C	2.56	0.44
1:Q:317:ASP:O	1:Q:318:ASN:C	2.55	0.44
1:A:88:LYS:HB3	1:A:89:GLU:OE1	2.18	0.44
1:O:106:GLU:O	1:O:109:SER:HB2	2.16	0.44
1:O:250:GLN:NE2	1:P:250:GLN:NE2	2.64	0.44
1:P:20:CYS:HB3	1:P:324:GLN:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:265:GLN:HG3	1:P:278:TYR:CD2	2.52	0.44
1:Q:212:THR:CG2	1:Q:213:THR:N	2.80	0.44
1:Q:81:ASN:HD22	1:Q:82:PRO:HD2	1.82	0.44
1:R:317:ASP:O	1:R:318:ASN:C	2.56	0.44
1:R:81:ASN:HD22	1:R:82:PRO:HD2	1.82	0.44
1:A:77:VAL:CG2	1:A:78:CYS:N	2.81	0.44
1:B:255:THR:CG2	1:B:259:GLN:OE1	2.65	0.44
1:Q:256:ILE:HG13	1:Q:259:GLN:H	1.83	0.44
1:Q:41:ARG:HD3	3:Q:6624:HOH:O	2.15	0.44
1:A:286:SER:HB3	1:A:289:ARG:HH11	1.82	0.44
1:R:9:GLY:HA3	1:R:99:THR:HG22	1.98	0.44
1:A:24:ARG:NH1	1:A:324:GLN:OE1	2.50	0.44
1:B:334:ALA:C	1:B:336:LYS:H	2.21	0.44
1:O:182:HIS:CD2	1:O:236:ARG:HE	2.36	0.44
1:O:256:ILE:HG13	1:O:259:GLN:H	1.82	0.44
1:O:79:ASP:HB2	1:O:85:LEU:HD21	2.00	0.44
1:P:52:VAL:HG13	1:P:241:ASN:ND2	2.33	0.44
1:R:79:ASP:HB2	1:R:85:LEU:HD23	2.00	0.44
1:A:175:LYS:HE2	1:B:306:ASP:HB3	1.99	0.44
1:A:59:ASP:HB2	1:A:70:ASN:HD22	1.82	0.44
1:B:10:PHE:CZ	1:B:18:LEU:HD12	2.53	0.44
1:B:211:THR:CG2	1:B:234:ALA:HB3	2.48	0.44
1:B:265:GLN:O	1:B:269:GLN:HG3	2.18	0.44
1:P:324:GLN:HA	1:P:324:GLN:OE1	2.17	0.44
1:A:87:TRP:HB2	1:A:114:ALA:O	2.17	0.44
1:A:315:TRP:CZ2	1:B:210:PRO:HG3	2.53	0.44
1:B:334:ALA:O	1:B:336:LYS:N	2.51	0.44
1:P:17:PHE:CE2	1:P:326:VAL:HG12	2.52	0.44
1:P:4:ARG:HD3	1:P:91:ASP:O	2.18	0.44
1:Q:261:ASN:HB3	1:Q:278:TYR:OH	2.18	0.44
1:P:145:GLU:CD	1:P:145:GLU:H	2.20	0.44
1:A:277:LYS:HB3	1:A:296:ILE:HG23	1.99	0.43
1:B:21:TRP:HH2	1:B:72:LYS:NZ	2.13	0.43
1:O:175:LYS:HE2	1:P:306:ASP:HB3	1.99	0.43
1:Q:12:ARG:HG2	1:Q:13:ILE:H	1.81	0.43
1:R:87:TRP:CE3	1:R:87:TRP:HA	2.52	0.43
1:O:317:ASP:O	1:O:318:ASN:C	2.55	0.43
1:O:62:TYR:HB2	1:O:67:ILE:HG22	1.99	0.43
1:O:134:VAL:HG23	1:O:222:VAL:HG11	2.01	0.43
1:P:182:HIS:HD2	1:P:236:ARG:HE	1.65	0.43
1:P:56:PHE:HD2	1:P:60:ILE:HD11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:37:THR:O	1:Q:37:THR:HG22	2.18	0.43
1:R:296:ILE:O	1:R:314:ALA:HA	2.17	0.43
1:A:50:ASP:OD1	1:A:53:LEU:HB2	2.17	0.43
1:B:317:ASP:O	1:B:318:ASN:C	2.56	0.43
1:B:135:ILE:HB	1:B:325:ARG:HD3	1.99	0.43
1:B:68:THR:HG23	1:B:73:THR:HG22	2.00	0.43
1:P:103:VAL:HG23	1:P:126:LYS:HB2	1.99	0.43
1:P:146:ASP:HB3	1:P:147:PHE:CD1	2.54	0.43
1:P:217:LYS:HE3	3:P:6492:HOH:O	2.16	0.43
1:Q:255:THR:O	1:Q:307:GLY:HA2	2.17	0.43
1:A:204:ALA:O	1:A:238:PRO:HG3	2.18	0.43
1:A:43:ALA:CB	1:A:67:ILE:HD11	2.43	0.43
1:Q:106:GLU:O	1:Q:109:SER:HB2	2.19	0.43
1:R:327:VAL:O	1:R:331:GLU:HB2	2.19	0.43
1:P:270:THR:OG1	1:P:271:THR:N	2.49	0.43
1:P:296:ILE:O	1:P:314:ALA:HA	2.18	0.43
1:Q:254:PRO:HA	1:Q:307:GLY:O	2.18	0.43
1:P:202:ARG:NH2	1:Q:51:SER:OG	2.52	0.43
1:R:209:VAL:HA	1:R:210:PRO:HD3	1.73	0.43
1:A:306:ASP:HB3	1:B:175:LYS:HE3	2.00	0.43
1:A:308:ASP:OD2	1:B:175:LYS:CE	2.67	0.43
1:A:250:GLN:NE2	1:B:250:GLN:HE22	2.14	0.43
1:Q:146:ASP:HB3	1:Q:147:PHE:CD1	2.54	0.43
1:Q:22:PHE:CE1	1:Q:72:LYS:HD2	2.49	0.43
1:R:211:THR:HG21	1:R:236:ARG:NE	2.33	0.43
1:A:334:ALA:C	1:A:336:LYS:H	2.21	0.43
1:B:291:THR:HG22	1:B:293:GLU:H	1.83	0.43
1:O:22:PHE:CE1	1:O:72:LYS:HD2	2.51	0.43
1:Q:294:SER:HG	1:Q:325:ARG:HH11	1.66	0.43
1:R:101:VAL:HG13	1:R:102:PHE:CD1	2.53	0.43
1:A:233:ILE:HD11	1:B:303:LEU:HD13	2.01	0.43
1:B:260:VAL:O	1:B:263:VAL:HG22	2.19	0.43
1:P:317:ASP:O	1:P:318:ASN:C	2.57	0.43
1:O:184:TYR:C	1:O:184:TYR:CD1	2.92	0.42
1:O:22:PHE:CZ	1:O:69:VAL:HB	2.54	0.42
1:A:112:ILE:HA	1:A:116:ALA:O	2.18	0.42
1:A:334:ALA:O	1:A:336:LYS:N	2.52	0.42
1:B:118:LYS:HG3	1:B:119:VAL:N	2.34	0.42
1:O:259:GLN:O	1:O:263:VAL:HG13	2.19	0.42
1:P:212:THR:CG2	1:P:213:THR:N	2.82	0.42
1:Q:184:TYR:CD1	1:Q:184:TYR:C	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:10:PHE:CE1	1:R:18:LEU:HD12	2.54	0.42
1:Q:209:VAL:HG13	1:R:284:VAL:HG11	2.01	0.42
1:Q:48:GLU:O	1:Q:55:ARG:HA	2.20	0.42
1:R:79:ASP:HB2	1:R:85:LEU:CD2	2.49	0.42
1:B:121:ILE:HG22	1:B:123:ALA:H	1.83	0.42
1:O:211:THR:HG23	1:O:234:ALA:HB3	2.02	0.42
1:O:79:ASP:HB2	1:O:85:LEU:HD23	2.02	0.42
1:P:67:ILE:HG23	1:P:76:ILE:CD1	2.49	0.42
1:Q:24:ARG:HG3	1:Q:24:ARG:HH11	1.84	0.42
1:Q:268:SER:O	1:Q:273:LYS:HA	2.18	0.42
1:P:206:VAL:C	1:P:207:ASN:HD22	2.23	0.42
1:R:156:THR:OG1	1:R:182:HIS:HE1	2.02	0.42
1:Q:120:LEU:HD11	1:Q:329:LEU:HD23	2.01	0.42
1:Q:211:THR:HG21	1:Q:236:ARG:NE	2.35	0.42
1:Q:303:LEU:HD23	1:Q:304:VAL:N	2.34	0.42
1:A:137:VAL:HG13	1:A:165:LYS:HG3	2.01	0.42
1:A:175:LYS:HE2	1:B:308:ASP:OD2	2.20	0.42
1:B:209:VAL:HA	1:B:210:PRO:HD3	1.78	0.42
1:B:204:ALA:O	1:B:238:PRO:HG3	2.20	0.42
1:O:182:HIS:O	1:O:237:VAL:HG22	2.19	0.42
1:O:265:GLN:HG3	1:O:278:TYR:CD2	2.55	0.42
1:R:220:ALA:CB	1:R:227:LYS:HA	2.50	0.42
1:A:50:ASP:OD1	1:A:53:LEU:HD12	2.19	0.42
1:B:63:ASP:OD1	1:B:64:GLU:N	2.53	0.42
1:O:327:VAL:O	1:O:331:GLU:HB2	2.20	0.42
1:Q:10:PHE:CE1	1:Q:18:LEU:HD12	2.54	0.42
1:P:144:HIS:HD2	3:P:6357:HOH:O	2.03	0.42
1:P:5:VAL:CG1	1:P:6:ALA:N	2.83	0.42
1:Q:289:ARG:HA	1:Q:317:ASP:OD2	2.19	0.42
1:Q:30:GLU:O	1:Q:32:VAL:HG13	2.19	0.42
1:B:121:ILE:HG22	1:B:123:ALA:N	2.35	0.42
1:B:61:SER:OG	1:B:68:THR:HB	2.20	0.42
1:B:5:VAL:HG11	1:B:96:ILE:HD13	2.02	0.42
1:Q:18:LEU:HA	1:Q:18:LEU:HD23	1.90	0.42
1:Q:261:ASN:HD21	1:Q:299:SER:HA	1.85	0.42
1:R:37:THR:HG22	1:R:37:THR:O	2.19	0.42
1:A:130:VAL:HG23	1:A:131:GLY:N	2.35	0.41
1:B:178:MET:O	1:B:232:GLY:HA2	2.20	0.41
1:P:171:PHE:CD1	1:P:255:THR:HG21	2.55	0.41
1:P:280:ASP:HA	1:P:299:SER:OG	2.19	0.41
1:R:103:VAL:HG23	1:R:126:LYS:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ALA:C	1:A:336:LYS:N	2.73	0.41
1:B:161:ALA:HB3	1:B:162:PRO:HD3	2.02	0.41
1:O:143:ARG:HB2	1:O:146:ASP:OD1	2.21	0.41
1:P:241:ASN:HA	1:P:318:ASN:HD22	1.85	0.41
1:Q:17:PHE:CE2	1:Q:326:VAL:HG12	2.55	0.41
1:R:211:THR:HG23	1:R:234:ALA:HB3	2.02	0.41
1:Q:208:ILE:HD11	1:R:239:THR:HG21	2.00	0.41
1:R:294:SER:HG	1:R:325:ARG:HH11	1.64	0.41
1:A:184:TYR:CA	1:A:236:ARG:NH2	2.77	0.41
1:A:241:ASN:HB2	1:A:242:VAL:H	1.52	0.41
1:A:264:LEU:HA	1:A:264:LEU:HD23	1.88	0.41
1:O:101:VAL:HG13	1:O:102:PHE:CD1	2.55	0.41
1:P:209:VAL:HA	1:P:210:PRO:HD3	1.69	0.41
3:B:6634:HOH:O	1:P:258:GLU:HB2	2.19	0.41
1:Q:241:ASN:HA	1:Q:318:ASN:HD22	1.83	0.41
1:R:182:HIS:HA	1:R:243:SER:OG	2.19	0.41
1:O:266:LYS:NZ	1:O:270:THR:HG21	2.35	0.41
1:P:88:LYS:HG3	1:P:89:GLU:N	2.36	0.41
1:B:126:LYS:O	1:B:127:ALA:CB	2.63	0.41
1:B:143:ARG:NH2	1:O:252:GLU:OE1	2.53	0.41
1:O:103:VAL:HG23	1:O:126:LYS:HB2	2.02	0.41
1:O:95:VAL:HG11	1:O:111:HIS:HB3	2.01	0.41
1:P:22:PHE:CE1	1:P:72:LYS:HD2	2.53	0.41
1:A:89:GLU:CD	1:A:89:GLU:H	2.22	0.41
1:B:334:ALA:C	1:B:336:LYS:N	2.72	0.41
1:B:40:ALA:HB3	1:B:63:ASP:O	2.20	0.41
1:P:36:ASN:HD22	1:P:37:THR:H	1.60	0.41
1:R:206:VAL:C	1:R:207:ASN:HD22	2.24	0.41
1:R:19:ARG:CZ	1:R:56:PHE:HB2	2.50	0.41
1:A:161:ALA:O	1:A:165:LYS:HB2	2.21	0.41
1:B:83:LEU:HD13	1:B:110:LYS:HG2	2.01	0.41
1:B:5:VAL:CG1	1:B:96:ILE:HD13	2.50	0.41
1:B:229:LYS:NZ	1:O:143:ARG:HH21	2.19	0.41
1:P:182:HIS:CD2	1:P:236:ARG:HE	2.39	0.41
1:Q:83:LEU:H	1:Q:83:LEU:HD22	1.86	0.41
1:R:256:ILE:HG13	1:R:259:GLN:H	1.85	0.41
1:R:5:VAL:HG12	1:R:6:ALA:N	2.35	0.41
1:A:247:LEU:O	1:A:311:LYS:HA	2.21	0.41
1:Q:182:HIS:O	1:Q:237:VAL:HG22	2.20	0.41
1:Q:182:HIS:HD2	1:Q:236:ARG:HE	1.68	0.41
1:Q:261:ASN:HD21	1:Q:299:SER:CB	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:239:THR:HG21	1:P:208:ILE:CG1	2.51	0.41
1:Q:95:VAL:HG13	1:Q:119:VAL:HG22	2.02	0.41
1:A:255:THR:HB	1:A:259:GLN:OE1	2.20	0.41
1:A:270:THR:OG1	1:A:271:THR:N	2.54	0.41
1:A:82:PRO:HA	1:A:85:LEU:CD1	2.44	0.41
1:B:25:GLN:NE2	1:B:26:ASN:H	2.18	0.41
1:B:16:ASN:HB3	1:B:323:SER:OG	2.20	0.41
1:O:10:PHE:CE1	1:O:18:LEU:HD12	2.56	0.41
1:O:30:GLU:O	1:O:32:VAL:HG13	2.21	0.41
1:Q:175:LYS:HE2	1:R:306:ASP:CB	2.39	0.41
1:A:36:ASN:ND2	1:A:37:THR:N	2.65	0.41
1:P:82:PRO:HB2	1:P:110:LYS:CB	2.51	0.41
1:Q:103:VAL:HA	1:Q:121:ILE:HD13	2.02	0.41
1:A:241:ASN:HA	1:A:318:ASN:ND2	2.36	0.40
1:O:120:LEU:HD13	1:O:150:ILE:HG13	2.02	0.40
1:R:171:PHE:HE1	1:R:255:THR:HG21	1.78	0.40
1:R:325:ARG:HA	1:R:325:ARG:NE	2.36	0.40
1:B:112:ILE:HA	1:B:116:ALA:O	2.21	0.40
1:P:95:VAL:HG11	1:P:111:HIS:HB3	2.04	0.40
1:R:155:CYS:HB3	1:R:322:TYR:HB2	2.03	0.40
1:B:12:ARG:HH22	1:B:50:ASP:CG	2.19	0.40
1:B:25:GLN:HG3	3:B:6584:HOH:O	2.21	0.40
1:P:92:ILE:O	1:P:116:ALA:HA	2.21	0.40
1:P:266:LYS:NZ	1:P:270:THR:HG21	2.37	0.40
1:Q:285:SER:HB3	1:R:208:ILE:HB	2.03	0.40
1:A:244:VAL:HG23	1:A:314:ALA:O	2.21	0.40
1:A:4:ARG:CD	1:A:91:ASP:O	2.69	0.40
1:B:277:LYS:HB2	1:B:293:GLU:CG	2.51	0.40
1:O:18:LEU:HA	1:O:18:LEU:HD23	1.91	0.40
1:O:216:ALA:HB1	1:O:231:ASN:HA	2.04	0.40
1:P:19:ARG:CZ	1:P:56:PHE:HB2	2.51	0.40
1:P:41:ARG:NH2	3:P:6476:HOH:O	2.53	0.40
1:Q:216:ALA:HB1	1:Q:231:ASN:HA	2.02	0.40
1:Q:5:VAL:HG12	1:Q:6:ALA:N	2.35	0.40
1:A:215:ALA:O	1:A:219:VAL:HG23	2.22	0.40
1:A:236:ARG:HE	1:A:236:ARG:HB3	1.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	318/380 (84%)	282 (89%)	28 (9%)	8 (2%)	5	21
1	B	318/380 (84%)	282 (89%)	28 (9%)	8 (2%)	5	21
1	O	318/380 (84%)	286 (90%)	25 (8%)	7 (2%)	6	24
1	P	318/380 (84%)	291 (92%)	21 (7%)	6 (2%)	8	28
1	Q	318/380 (84%)	284 (89%)	26 (8%)	8 (2%)	5	21
1	R	318/380 (84%)	287 (90%)	24 (8%)	7 (2%)	6	24
All	All	1908/2280 (84%)	1712 (90%)	152 (8%)	44 (2%)	6	23

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	ALA
1	A	318	ASN
1	B	203	ALA
1	B	242	VAL
1	B	318	ASN
1	O	128	GLU
1	O	240	PRO
1	O	318	ASN
1	P	128	GLU
1	P	240	PRO
1	P	318	ASN
1	Q	80	ARG
1	Q	240	PRO
1	Q	318	ASN
1	R	240	PRO
1	R	318	ASN
1	A	183	SER
1	A	242	VAL
1	B	183	SER
1	B	285	SER

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Mol	Chain	Res	Type
1	O	203	ALA
1	O	307	GLY
1	P	203	ALA
1	Q	128	GLU
1	Q	203	ALA
1	R	128	GLU
1	R	203	ALA
1	A	240	PRO
1	A	285	SER
1	B	127	ALA
1	B	240	PRO
1	R	127	ALA
1	A	335	ARG
1	O	127	ALA
1	P	127	ALA
1	Q	127	ALA
1	Q	172	GLY
1	B	335	ARG
1	P	172	GLY
1	Q	307	GLY
1	R	172	GLY
1	O	172	GLY
1	R	307	GLY
1	A	172	GLY

5.3.2 Protein sidechains

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	269/321 (84%)	245 (91%)	24 (9%)	9 29
1	B	269/321 (84%)	246 (91%)	23 (9%)	10 30
1	O	269/321 (84%)	254 (94%)	15 (6%)	21 52
1	P	269/321 (84%)	254 (94%)	15 (6%)	21 52
1	Q	269/321 (84%)	254 (94%)	15 (6%)	21 52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	R	269/321 (84%)	255 (95%)	14 (5%)	23 55
All	All	1614/1926 (84%)	1508 (93%)	106 (7%)	16 44

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	24	ARG
1	A	25	GLN
1	A	36	ASN
1	A	62	TYR
1	A	74	MET
1	A	77	VAL
1	A	80	ARG
1	A	83	LEU
1	A	87	TRP
1	A	89	GLU
1	A	120	LEU
1	A	128	GLU
1	A	145	GLU
1	A	152	ASN
1	A	167	LEU
1	A	231	ASN
1	A	239	THR
1	A	241	ASN
1	A	262	GLU
1	A	294	SER
1	A	309	LEU
1	A	319	GLU
1	A	332	LEU
1	B	12	ARG
1	B	25	GLN
1	B	36	ASN
1	B	62	TYR
1	B	73	THR
1	B	74	MET
1	B	77	VAL
1	B	80	ARG
1	B	83	LEU
1	B	87	TRP
1	B	118	LYS
1	B	120	LEU

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Mol	Chain	Res	Type
1	B	128	GLU
1	B	152	ASN
1	B	167	LEU
1	B	231	ASN
1	B	239	THR
1	B	241	ASN
1	B	262	GLU
1	B	273	LYS
1	B	309	LEU
1	B	319	GLU
1	B	332	LEU
1	O	12	ARG
1	O	26	ASN
1	O	80	ARG
1	O	81	ASN
1	O	83	LEU
1	O	87	TRP
1	O	145	GLU
1	O	152	ASN
1	O	167	LEU
1	O	178	MET
1	O	184	TYR
1	O	258	GLU
1	O	271	THR
1	O	310	VAL
1	O	332	LEU
1	P	12	ARG
1	P	26	ASN
1	P	81	ASN
1	P	87	TRP
1	P	89	GLU
1	P	120	LEU
1	P	152	ASN
1	P	167	LEU
1	P	178	MET
1	P	184	TYR
1	P	258	GLU
1	P	271	THR
1	P	303	LEU
1	P	310	VAL
1	P	332	LEU
1	Q	12	ARG

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Mol	Chain	Res	Type
1	Q	26	ASN
1	Q	79	ASP
1	Q	81	ASN
1	Q	87	TRP
1	Q	89	GLU
1	Q	145	GLU
1	Q	146	ASP
1	Q	152	ASN
1	Q	167	LEU
1	Q	178	MET
1	Q	258	GLU
1	Q	271	THR
1	Q	310	VAL
1	Q	332	LEU
1	R	12	ARG
1	R	26	ASN
1	R	80	ARG
1	R	81	ASN
1	R	87	TRP
1	R	89	GLU
1	R	152	ASN
1	R	167	LEU
1	R	178	MET
1	R	184	TYR
1	R	258	GLU
1	R	271	THR
1	R	310	VAL
1	R	332	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	70	ASN
1	A	84	ASN
1	A	182	HIS
1	A	261	ASN
1	A	265	GLN
1	B	25	GLN
1	B	36	ASN
1	B	70	ASN
1	B	84	ASN

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Mol	Chain	Res	Type
1	B	158	ASN
1	B	241	ASN
1	B	261	ASN
1	B	265	GLN
1	O	36	ASN
1	O	81	ASN
1	O	84	ASN
1	O	144	HIS
1	O	158	ASN
1	O	182	HIS
1	O	207	ASN
1	O	259	GLN
1	O	261	ASN
1	O	265	GLN
1	P	36	ASN
1	P	81	ASN
1	P	84	ASN
1	P	144	HIS
1	P	158	ASN
1	P	182	HIS
1	P	207	ASN
1	P	250	GLN
1	P	259	GLN
1	P	261	ASN
1	P	265	GLN
1	P	318	ASN
1	Q	36	ASN
1	Q	81	ASN
1	Q	84	ASN
1	Q	144	HIS
1	Q	158	ASN
1	Q	182	HIS
1	Q	207	ASN
1	Q	250	GLN
1	Q	259	GLN
1	Q	265	GLN
1	Q	318	ASN
1	R	36	ASN
1	R	81	ASN
1	R	158	ASN
1	R	182	HIS
1	R	207	ASN

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Mol	Chain	Res	Type
1	R	259	GLN
1	R	261	ASN
1	R	265	GLN

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

6 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	SO4	R	6339	-	4,4,4	0.11	0	6,6,6	0.11	0
2	SO4	Q	5339	-	4,4,4	0.24	0	6,6,6	0.05	0
2	SO4	B	2339	-	4,4,4	0.27	0	6,6,6	0.21	0
2	SO4	P	4339	-	4,4,4	0.15	0	6,6,6	0.12	0
2	SO4	O	3339	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	A	1339	-	4,4,4	0.26	0	6,6,6	0.07	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2339	SO4	1	0
2	P	4339	SO4	1	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	322/380 (84%)	-0.22	3 (0%) 84 84	20, 43, 80, 92	0
1	B	322/380 (84%)	-0.37	3 (0%) 84 84	17, 40, 73, 91	0
1	O	322/380 (84%)	-0.19	3 (0%) 84 84	19, 48, 80, 92	0
1	P	322/380 (84%)	0.01	13 (4%) 38 33	22, 52, 89, 92	0
1	Q	322/380 (84%)	0.47	27 (8%) 11 8	56, 85, 92, 93	0
1	R	322/380 (84%)	0.61	35 (10%) 5 4	43, 85, 92, 93	0
All	All	1932/2280 (84%)	0.05	84 (4%) 35 31	17, 61, 91, 93	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	1	MET	8.5
1	P	1	MET	6.1
1	Q	1	MET	5.3
1	B	1	MET	4.9
1	A	1	MET	4.8
1	R	1	MET	4.5
1	R	270	THR	4.3
1	Q	25	GLN	4.3
1	Q	90	TRP	4.3
1	R	128	GLU	4.2
1	Q	80	ARG	3.9
1	R	212	THR	3.8
1	R	338	GLY	3.8
1	Q	269	GLN	3.6
1	R	64	GLU	3.4
1	P	184	TYR	3.4
1	R	336	LYS	3.4
1	Q	184	TYR	3.3
1	R	184	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	Q	65	ASN	3.1
1	R	127	ALA	3.0
1	Q	64	GLU	3.0
1	P	62	TYR	2.9
1	P	337	SER	2.9
1	P	338	GLY	2.9
1	R	100	GLY	2.8
1	R	7	ILE	2.8
1	O	184	TYR	2.8
1	Q	26	ASN	2.8
1	R	143	ARG	2.8
1	Q	338	GLY	2.8
1	R	66	SER	2.8
1	R	159	CYS	2.8
1	P	128	GLU	2.7
1	R	90	TRP	2.7
1	R	6	ALA	2.7
1	Q	225	GLU	2.6
1	Q	140	SER	2.6
1	P	58	ALA	2.6
1	R	227	LYS	2.6
1	R	96	ILE	2.6
1	R	252	GLU	2.6
1	Q	202	ARG	2.6
1	R	266	LYS	2.6
1	R	58	ALA	2.5
1	R	26	ASN	2.5
1	R	126	LYS	2.5
1	R	146	ASP	2.5
1	B	184	TYR	2.5
1	R	140	SER	2.5
1	R	211	THR	2.5
1	R	306	ASP	2.4
1	P	2	THR	2.4
1	P	80	ARG	2.4
1	P	96	ILE	2.4
1	R	84	ASN	2.4
1	R	271	THR	2.4
1	Q	70	ASN	2.4
1	R	53	LEU	2.4
1	R	83	LEU	2.4
1	Q	41	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	Q	57	ASN	2.3
1	Q	224	PRO	2.3
1	Q	127	ALA	2.3
1	A	184	TYR	2.3
1	P	45	HIS	2.3
1	P	90	TRP	2.2
1	R	120	LEU	2.2
1	Q	62	TYR	2.2
1	Q	259	GLN	2.2
1	Q	266	LYS	2.2
1	A	64	GLU	2.2
1	B	212	THR	2.2
1	R	91	ASP	2.2
1	R	95	VAL	2.2
1	P	201	ALA	2.2
1	Q	174	ILE	2.2
1	Q	211	THR	2.2
1	Q	126	LYS	2.1
1	R	34	ILE	2.1
1	Q	81	ASN	2.0
1	Q	88	LYS	2.0
1	O	41	ARG	2.0
1	Q	63	ASP	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. 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	R	6339	5/5	0.96	0.11	64,67,68,68	5
2	SO4	B	2339	5/5	0.96	0.13	41,42,43,44	5
2	SO4	O	3339	5/5	0.96	0.12	30,30,32,32	5
2	SO4	P	4339	5/5	0.97	0.14	45,46,48,49	5
2	SO4	Q	5339	5/5	0.97	0.07	87,88,88,89	5
2	SO4	A	1339	5/5	0.97	0.13	29,30,33,34	5

6.5 Other polymers

There are no such residues in this entry.