Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 07:20 am BST

PDB ID	:	4Z1Y
Title	:	Thermostable enolase from Chloroflexus aurantiacus with substrate 2-phosphoglycerate
Authors	:	Zadvornyy, O.A.; Peters, J.W.
Deposited on	:	2015-03-27
Resolution	:	2.53 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 ⓘ) were used in the production of this report:

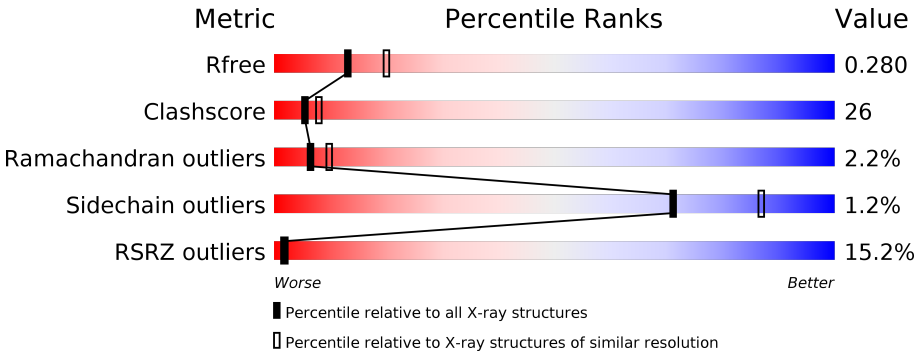
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.53 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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	426	10% 80% 16% .
1	B	426	20% 75% 20% . . .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	2PG	A	502[B]	-	-	-	X
3	2PG	B	502[B]	-	-	X	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6466 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.

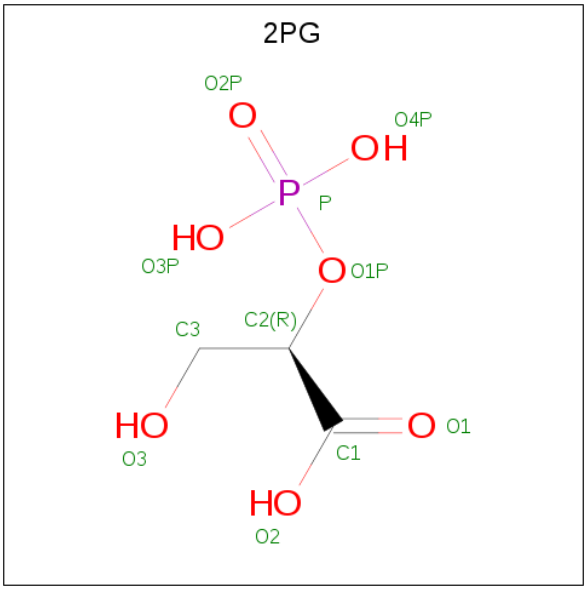
- Molecule 1 is a protein called Enolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	2	7	0
			3250	2037	572	633	8			
1	B	419	Total	C	N	O	S	0	0	0
			3169	1987	559	615	8			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 2-PHOSPHOGLYCERIC ACID (three-letter code: 2PG) (formula: $C_3H_7O_7P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	1
			11	3	7	1		
3	B	1	Total	C	O	P	0	1
			11	3	7	1		

- Molecule 4 is water.

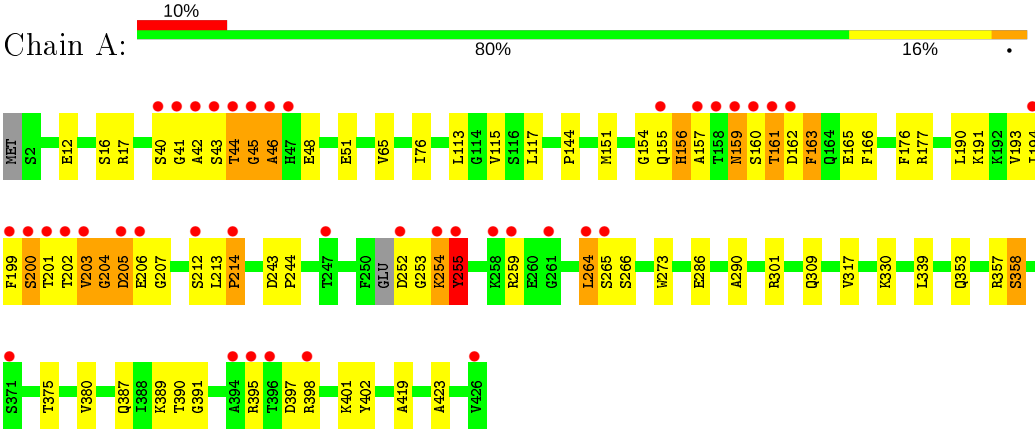
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total	O	0	0
			11	11		
4	B	12	Total	O	0	0
			12	12		

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.

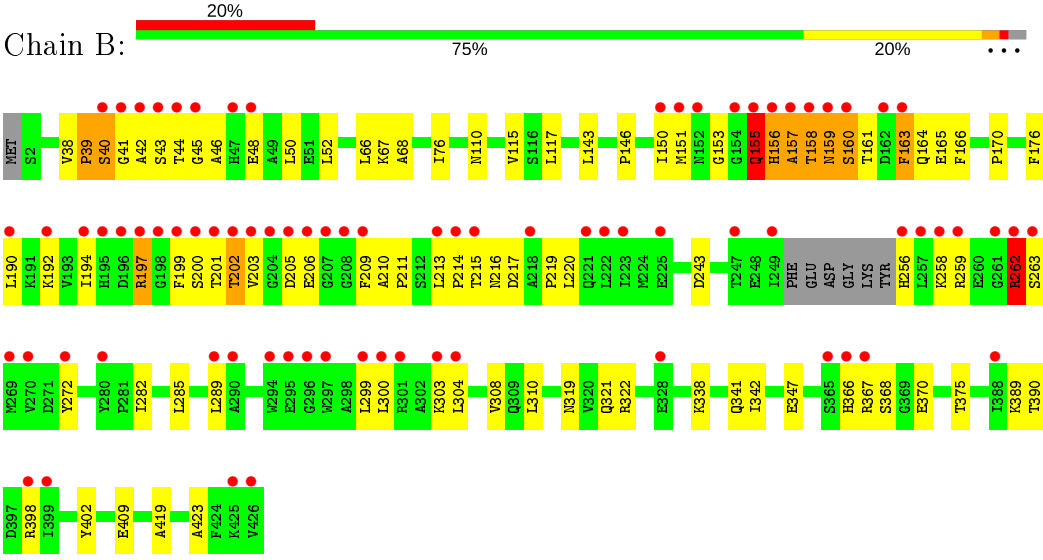
- Molecule 1: Enolase

Chain A:



- Molecule 1: Enolase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	146.32Å 146.32Å 101.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.70 – 2.53 37.70 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.9 (37.70-2.53) 99.8 (37.70-2.53)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.08 (at 2.54Å)	Xtriage
Refinement program	BUSTER 2.10.1, REFMAC	Depositor
R, R_{free}	0.214 , 0.252 0.246 , 0.280	Depositor DCC
R_{free} test set	1794 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	48.6	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.024 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6466	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: MG, 2PG

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	0.48	0/3300	0.74	4/4471 (0.1%)
1	B	0.60	4/3217 (0.1%)	1.02	20/4360 (0.5%)
All	All	0.55	4/6517 (0.1%)	0.89	24/8831 (0.3%)

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	A	0	1
1	B	0	4
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	158	THR	C-N	-12.79	1.04	1.34
1	B	155	GLN	C-N	-10.25	1.10	1.34
1	B	264	LEU	C-N	9.82	1.56	1.34
1	B	262	ARG	C-N	-9.19	1.12	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	265	SER	N-CA-CB	20.31	140.97	110.50
1	B	158	THR	O-C-N	-17.01	95.48	122.70
1	B	159	ASN	N-CA-CB	-14.99	83.61	110.60
1	B	262	ARG	O-C-N	-13.45	101.17	122.70
1	B	155	GLN	O-C-N	-13.12	101.70	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	156	HIS	N-CA-CB	-12.48	88.14	110.60
1	B	155	GLN	CB-CA-C	-11.33	87.74	110.40
1	B	262	ARG	CB-CA-C	-11.13	88.14	110.40
1	B	264	LEU	CB-CA-C	10.87	130.85	110.20
1	B	158	THR	CA-C-N	10.81	140.98	117.20
1	B	263	SER	N-CA-CB	-10.07	95.39	110.50
1	B	262	ARG	CA-C-N	9.95	139.09	117.20
1	A	264	LEU	CB-CA-C	9.61	128.45	110.20
1	B	155	GLN	N-CA-C	9.32	136.17	111.00
1	B	155	GLN	CA-C-N	7.78	134.32	117.20
1	B	159	ASN	N-CA-C	6.72	129.15	111.00
1	B	264	LEU	N-CA-C	-6.65	93.03	111.00
1	B	265	SER	N-CA-C	-6.62	93.12	111.00
1	A	205	ASP	N-CA-C	6.38	128.23	111.00
1	A	204	GLY	O-C-N	-6.03	113.05	122.70
1	A	255	TYR	CB-CA-C	5.95	122.30	110.40
1	B	158	THR	CB-CA-C	-5.76	96.04	111.60
1	B	262	ARG	C-N-CA	5.74	136.04	121.70
1	B	158	THR	N-CA-C	-5.67	95.69	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	204	GLY	Mainchain
1	B	155	GLN	Mainchain
1	B	158	THR	Mainchain
1	B	262	ARG	Mainchain
1	B	264	LEU	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	3250	0	3244	130	0
1	B	3169	0	3171	229	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
3	A	11	0	4	0	0
3	B	11	0	4	4	0
4	A	11	0	0	0	0
4	B	12	0	0	0	0
All	All	6466	0	6423	334	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 26.

All (334) 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:B:209:PHE:CD2	1:B:211:PRO:HD3	1.46	1.46
1:B:156:HIS:N	1:B:157:ALA:CB	1.77	1.45
1:B:161:THR:CG2	1:B:216:ASN:OD1	1.73	1.36
1:B:156:HIS:N	1:B:157:ALA:HB2	1.01	1.31
1:A:42[A]:ALA:O	1:A:51:GLU:CG	1.78	1.29
1:B:156:HIS:CB	1:B:157:ALA:HB2	1.62	1.27
1:B:41:GLY:CA	1:B:367:ARG:HD3	1.64	1.26
1:A:395:ARG:NH1	1:B:395:ARG:CG	2.02	1.23
1:B:366:HIS:CD2	1:B:390:THR:HA	1.75	1.22
1:A:254:LYS:CB	1:A:264:LEU:O	1.88	1.20
1:A:254:LYS:HB3	1:A:264:LEU:O	1.06	1.18
1:A:160:SER:O	1:A:161:THR:CG2	1.92	1.17
1:A:160:SER:O	1:A:161:THR:HG22	1.02	1.17
1:B:262:ARG:NH1	1:B:272:TYR:CD2	2.12	1.17
1:A:17:ARG:NH1	1:A:205:ASP:OD2	1.80	1.15
1:B:156:HIS:CA	1:B:157:ALA:HB2	1.76	1.15
1:B:161:THR:HG23	1:B:216:ASN:OD1	1.32	1.14
1:B:390:THR:O	1:B:398:ARG:HD2	1.49	1.13
1:B:156:HIS:HB3	1:B:157:ALA:HA	1.23	1.12
1:B:41:GLY:HA3	1:B:367:ARG:HD3	1.16	1.12
1:A:395:ARG:NH1	1:B:395:ARG:HG2	1.60	1.12
1:B:44:THR:HB	1:B:45:GLY:CA	1.78	1.12
1:A:17:ARG:CZ	1:A:205:ASP:OD2	1.96	1.11
1:A:42[A]:ALA:O	1:A:51:GLU:HG2	0.93	1.11
1:B:209:PHE:CD2	1:B:211:PRO:CD	2.33	1.10
1:A:254:LYS:HG3	1:A:265:SER:HA	1.25	1.10
1:B:156:HIS:HB3	1:B:157:ALA:CA	1.79	1.10
1:B:209:PHE:HE2	1:B:211:PRO:CB	1.63	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:HIS:HB2	1:B:157:ALA:HB2	1.28	1.08
1:B:156:HIS:CB	1:B:157:ALA:CB	2.30	1.08
1:A:395:ARG:HH11	1:B:395:ARG:CG	1.63	1.06
1:A:395:ARG:HH22	1:B:203:VAL:HG21	1.18	1.06
1:A:395:ARG:NH2	1:B:203:VAL:HG21	1.71	1.04
1:B:304:LEU:HD13	1:B:308:VAL:CG2	1.86	1.04
1:B:366:HIS:HD2	1:B:390:THR:CA	1.70	1.04
1:B:213:LEU:HD13	1:B:219:PRO:HG3	1.38	1.03
1:A:395:ARG:HH11	1:B:395:ARG:HG2	0.90	1.03
1:B:262:ARG:NH1	1:B:272:TYR:HD2	1.48	1.03
1:A:395:ARG:NH2	1:B:203:VAL:CG2	2.22	1.03
1:B:370:GLU:CG	1:B:398:ARG:HH12	1.72	1.02
1:B:44:THR:HB	1:B:45:GLY:HA2	1.35	1.02
1:B:258:LYS:HA	1:B:259:ARG:HD2	1.40	1.01
1:B:366:HIS:HD2	1:B:390:THR:HA	0.90	1.01
1:B:41:GLY:N	1:B:367:ARG:HD3	1.76	1.00
1:B:41:GLY:HA3	1:B:367:ARG:CD	1.91	0.99
1:A:395:ARG:HH22	1:B:203:VAL:CG2	1.74	0.97
1:B:370:GLU:CB	1:B:398:ARG:HH12	1.77	0.96
1:B:209:PHE:CE2	1:B:211:PRO:CD	2.48	0.96
1:B:304:LEU:HD13	1:B:308:VAL:CB	1.93	0.96
1:B:304:LEU:CD1	1:B:308:VAL:HB	1.95	0.96
1:B:341:GLN:NE2	1:B:367:ARG:HH22	1.64	0.95
1:B:209:PHE:CE2	1:B:211:PRO:HB3	2.02	0.94
1:B:367:ARG:HG3	3:B:502[B]:2PG:O2P	1.67	0.94
1:B:44:THR:HB	1:B:45:GLY:C	1.86	0.94
1:A:252:ASP:HB2	1:A:253:GLY:HA2	1.48	0.94
1:A:395:ARG:NH1	1:B:395:ARG:HG3	1.80	0.93
1:B:213:LEU:CD1	1:B:219:PRO:HG3	1.98	0.93
1:B:209:PHE:HE2	1:B:211:PRO:HB3	1.32	0.92
1:B:209:PHE:CE2	1:B:211:PRO:CB	2.53	0.92
1:B:341:GLN:HE21	1:B:367:ARG:HH22	1.01	0.92
1:B:209:PHE:CE2	1:B:211:PRO:HD3	2.05	0.91
1:B:41:GLY:N	1:B:367:ARG:CD	2.32	0.91
1:B:338:LYS:HD3	1:B:341:GLN:NE2	1.85	0.90
1:B:304:LEU:HD13	1:B:308:VAL:HB	1.50	0.90
1:B:209:PHE:HD2	1:B:211:PRO:CD	1.75	0.90
1:B:161:THR:HG21	1:B:216:ASN:OD1	1.71	0.89
1:A:160:SER:HB2	1:A:212:SER:HA	1.54	0.89
1:B:156:HIS:CB	1:B:157:ALA:CA	2.46	0.89
1:B:44:THR:CG2	1:B:48:GLU:CG	2.51	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:GLU:HG3	1:B:398:ARG:NH1	1.88	0.89
1:B:370:GLU:CG	1:B:398:ARG:NH1	2.37	0.88
1:B:41:GLY:CA	1:B:367:ARG:CD	2.50	0.88
1:B:197:ARG:CG	1:B:199:PHE:HE2	1.87	0.88
1:B:156:HIS:HB2	1:B:157:ALA:CB	1.98	0.88
1:B:209:PHE:HE2	1:B:211:PRO:CA	1.87	0.88
1:A:252:ASP:HB2	1:A:253:GLY:CA	2.05	0.87
1:A:395:ARG:HH12	1:B:395:ARG:HG3	1.35	0.86
1:B:342:ILE:HD11	1:B:347:GLU:HB3	1.57	0.86
1:B:44:THR:CB	1:B:45:GLY:C	2.43	0.86
1:B:197:ARG:CG	1:B:199:PHE:CE2	2.59	0.86
1:A:254:LYS:CG	1:A:265:SER:HA	2.03	0.86
1:B:338:LYS:CD	1:B:341:GLN:NE2	2.39	0.86
1:B:44:THR:HG22	1:B:45:GLY:O	1.75	0.85
1:B:156:HIS:N	1:B:157:ALA:HB3	1.90	0.85
1:A:390:THR:HG22	1:A:390:THR:O	1.77	0.85
1:B:262:ARG:HH12	1:B:272:TYR:HD2	1.06	0.85
1:B:304:LEU:HD13	1:B:308:VAL:HG21	1.57	0.85
1:B:42:ALA:HB1	1:B:43:SER:HA	1.57	0.84
1:A:202:THR:O	1:A:203:VAL:HG13	1.77	0.84
1:B:44:THR:CG2	1:B:45:GLY:O	2.26	0.84
1:B:205:ASP:O	1:B:395:ARG:NH1	2.10	0.84
1:B:197:ARG:HG3	1:B:199:PHE:CE2	2.12	0.83
1:A:309:GLN:HE22	1:A:387:GLN:HE22	1.26	0.83
1:B:44:THR:CB	1:B:45:GLY:O	2.26	0.83
1:A:366:HIS:ND1	1:A:390:THR:HA	1.95	0.82
1:B:370:GLU:HB2	1:B:398:ARG:HH12	1.41	0.82
1:A:206:GLU:HA	1:A:398:ARG:HE	1.43	0.82
1:B:44:THR:HG23	1:B:48:GLU:CD	2.00	0.82
1:B:44:THR:HB	1:B:45:GLY:O	1.79	0.82
1:B:209:PHE:CE2	1:B:211:PRO:N	2.48	0.81
1:B:390:THR:O	1:B:398:ARG:CD	2.28	0.81
1:B:44:THR:CA	1:B:45:GLY:C	2.48	0.81
1:A:12:GLU:HG3	1:A:65:VAL:HG12	1.62	0.81
1:A:366:HIS:ND1	1:A:389:LYS:O	2.12	0.81
1:B:342:ILE:CD1	1:B:347:GLU:HB3	2.10	0.81
1:B:48:GLU:O	1:B:50:LEU:HD22	1.82	0.79
1:B:197:ARG:HG3	1:B:199:PHE:CD2	2.18	0.79
1:A:206:GLU:HA	1:A:398:ARG:NE	1.95	0.79
1:A:202:THR:O	1:A:203:VAL:CG1	2.30	0.79
1:A:160:SER:HB2	1:A:212:SER:CA	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ARG:NH1	1:B:272:TYR:CE2	2.50	0.79
1:A:202:THR:HB	1:B:202:THR:OG1	1.84	0.78
1:A:395:ARG:NH2	1:B:203:VAL:HG22	1.97	0.77
1:B:338:LYS:HB2	1:B:341:GLN:OE1	1.85	0.77
1:B:44:THR:HA	1:B:45:GLY:C	2.04	0.77
1:B:366:HIS:CD2	1:B:390:THR:CA	2.54	0.77
1:A:254:LYS:O	1:A:255:TYR:HB2	1.85	0.76
1:A:45[B]:GLY:O	1:A:46[B]:ALA:HB3	1.86	0.76
1:B:197:ARG:NH2	1:B:199:PHE:CZ	2.54	0.76
1:A:154:GLY:H	1:A:161:THR:HG23	1.51	0.75
1:A:160:SER:HB3	1:A:213:LEU:O	1.86	0.75
1:B:44:THR:CB	1:B:45:GLY:CA	2.56	0.74
1:A:202:THR:CB	1:B:202:THR:HG21	2.19	0.72
1:B:44:THR:HG22	1:B:48:GLU:HG2	1.71	0.72
1:B:338:LYS:HD3	1:B:367:ARG:NH2	2.03	0.72
1:B:42:ALA:H	1:B:367:ARG:NH1	1.88	0.72
1:B:209:PHE:CE2	1:B:211:PRO:CA	2.71	0.72
1:A:203:VAL:HG23	1:A:203:VAL:O	1.90	0.72
1:B:40:SER:C	1:B:367:ARG:HD2	2.09	0.72
1:A:252:ASP:CB	1:A:253:GLY:CA	2.68	0.71
1:A:390:THR:O	1:A:398:ARG:HD2	1.90	0.71
1:B:197:ARG:CD	1:B:199:PHE:HE2	2.02	0.71
1:B:197:ARG:NH2	1:B:199:PHE:CE2	2.58	0.71
1:B:258:LYS:HG2	1:B:259:ARG:CD	2.21	0.71
1:B:341:GLN:NE2	1:B:367:ARG:NH2	2.37	0.71
1:A:252:ASP:CB	1:A:253:GLY:HA2	2.18	0.71
1:A:357:ARG:O	1:A:358:SER:OG	2.09	0.70
1:B:42:ALA:CB	1:B:43:SER:HA	2.16	0.70
1:B:200:SER:O	1:B:209:PHE:CE1	2.44	0.70
1:B:42:ALA:H	1:B:367:ARG:HH11	1.36	0.70
1:A:202:THR:HB	1:B:202:THR:HG21	1.73	0.70
1:B:341:GLN:HE21	1:B:367:ARG:NH2	1.85	0.70
1:B:256:HIS:NE2	1:B:264:LEU:HD23	2.08	0.69
1:B:42:ALA:HB1	1:B:43:SER:CA	2.23	0.69
1:B:41:GLY:N	1:B:367:ARG:HD2	2.08	0.69
1:A:390:THR:O	1:A:390:THR:CG2	2.41	0.68
1:B:200:SER:O	1:B:209:PHE:HE1	1.77	0.68
1:A:45[B]:GLY:O	1:A:46[B]:ALA:CB	2.42	0.68
1:B:163:PHE:HD2	1:B:166:PHE:CZ	2.13	0.66
1:A:43[B]:SER:C	1:A:44[B]:THR:HG1	1.99	0.66
1:B:338:LYS:HB2	1:B:341:GLN:CD	2.16	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:THR:CB	1:B:45:GLY:HA2	2.20	0.66
1:A:254:LYS:HG3	1:A:265:SER:CA	2.14	0.66
1:A:12:GLU:HG3	1:A:65:VAL:CG1	2.25	0.65
1:B:338:LYS:HD2	1:B:341:GLN:NE2	2.12	0.65
1:A:395:ARG:HH12	1:B:395:ARG:CG	1.89	0.65
1:A:154:GLY:O	1:A:157:ALA:HB3	1.96	0.65
1:A:203:VAL:HG12	1:A:207:GLY:O	1.96	0.65
1:A:160:SER:HB3	1:A:213:LEU:N	2.12	0.64
1:B:41:GLY:HA3	1:B:367:ARG:CG	2.27	0.64
1:B:44:THR:CG2	1:B:48:GLU:HG2	2.24	0.64
1:B:143:LEU:HD13	1:B:409:GLU:HB2	1.79	0.64
1:B:209:PHE:CD2	1:B:210:ALA:N	2.66	0.64
1:B:48:GLU:O	1:B:50:LEU:CD2	2.46	0.64
1:B:338:LYS:CD	1:B:341:GLN:CD	2.66	0.64
1:A:202:THR:HB	1:B:202:THR:CG2	2.29	0.63
1:A:191:LYS:HE3	1:A:201:THR:HG21	1.80	0.63
1:A:202:THR:C	1:A:203:VAL:HG13	2.19	0.63
1:B:213:LEU:HD13	1:B:219:PRO:CG	2.25	0.62
1:B:258:LYS:HG2	1:B:259:ARG:HD3	1.81	0.62
1:B:258:LYS:HG2	1:B:259:ARG:HD2	1.81	0.62
1:B:370:GLU:CB	1:B:398:ARG:NH1	2.59	0.62
1:B:44:THR:CG2	1:B:48:GLU:HG3	2.30	0.62
1:B:153:GLY:HA2	1:B:160:SER:OG	2.00	0.62
1:B:197:ARG:HD2	1:B:199:PHE:CE2	2.35	0.61
1:A:202:THR:HB	1:B:202:THR:CB	2.31	0.61
1:B:367:ARG:NH1	3:B:502[B]:2PG:O4P	2.33	0.61
1:A:43[B]:SER:O	1:A:44[B]:THR:OG1	2.13	0.61
1:B:44:THR:CG2	1:B:48:GLU:CD	2.69	0.60
1:A:177:ARG:HH22	1:B:66:LEU:HD21	1.66	0.60
1:B:202:THR:CG2	1:B:203:VAL:N	2.64	0.60
1:B:76:ILE:HG21	1:B:115:VAL:HG21	1.83	0.60
1:A:202:THR:HA	1:B:202:THR:HG21	1.82	0.60
1:B:52:LEU:HD21	1:B:67:LYS:HB3	1.83	0.59
1:A:165:GLU:HG3	1:A:243:ASP:HB3	1.85	0.59
1:B:44:THR:HG21	1:B:48:GLU:HG3	1.85	0.59
1:B:209:PHE:CE2	1:B:211:PRO:CG	2.85	0.59
1:B:256:HIS:NE2	1:B:264:LEU:CD2	2.66	0.58
1:B:304:LEU:CD1	1:B:308:VAL:CB	2.66	0.58
1:B:39:PRO:O	1:B:40:SER:HB3	2.02	0.58
1:A:202:THR:CA	1:B:202:THR:HG21	2.34	0.58
1:B:197:ARG:HH21	1:B:199:PHE:HZ	1.48	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44[B]:THR:O	1:A:45[B]:GLY:C	2.42	0.58
1:B:151:MET:SD	1:B:219:PRO:HB3	2.44	0.58
1:B:209:PHE:HE2	1:B:211:PRO:CG	2.16	0.57
1:B:44:THR:HA	1:B:46:ALA:CB	2.33	0.57
1:B:338:LYS:HD3	1:B:341:GLN:CD	2.24	0.57
1:A:395:ARG:CZ	1:B:203:VAL:HG21	2.33	0.57
1:B:202:THR:HG23	1:B:203:VAL:N	2.20	0.57
1:B:366:HIS:CD2	1:B:390:THR:C	2.78	0.57
1:A:254:LYS:O	1:A:255:TYR:CB	2.51	0.57
1:B:209:PHE:HD2	1:B:211:PRO:HD3	0.78	0.57
1:B:44:THR:HA	1:B:46:ALA:N	2.21	0.56
1:A:155:GLN:C	1:A:157:ALA:H	2.09	0.56
1:A:17:ARG:NH2	1:A:205:ASP:OD2	2.35	0.56
1:A:206:GLU:HA	1:A:398:ARG:CZ	2.35	0.56
1:B:40:SER:C	1:B:367:ARG:CD	2.73	0.56
1:A:254:LYS:HD2	1:A:266:SER:H	1.70	0.56
1:A:194:ILE:HG23	1:A:199:PHE:HB2	1.87	0.56
1:B:197:ARG:NH2	1:B:199:PHE:HZ	2.04	0.55
1:B:258:LYS:HA	1:B:259:ARG:CD	2.26	0.55
1:B:341:GLN:HG3	1:B:367:ARG:HH21	1.70	0.55
1:B:165:GLU:HB2	1:B:243:ASP:HB3	1.88	0.55
1:B:163:PHE:HD2	1:B:166:PHE:HZ	1.53	0.55
1:B:285:LEU:HD23	1:B:310:LEU:HD22	1.88	0.54
1:A:160:SER:O	1:A:161:THR:CB	2.55	0.54
1:A:205:ASP:O	1:A:398:ARG:NH2	2.40	0.54
1:B:190:LEU:HG	1:B:194:ILE:HD12	1.88	0.54
1:B:143:LEU:HD11	1:B:409:GLU:HA	1.90	0.54
1:A:214:PRO:HA	1:A:259:ARG:HH21	1.73	0.54
1:A:40[A]:SER:O	1:A:367:ARG:HB3	2.08	0.53
1:B:143:LEU:CD1	1:B:409:GLU:HB2	2.38	0.53
1:B:159:ASN:O	1:B:159:ASN:CG	2.46	0.53
1:A:160:SER:CB	1:A:213:LEU:N	2.72	0.53
1:B:43:SER:O	1:B:44:THR:OG1	2.25	0.53
1:A:76:ILE:HG21	1:A:115:VAL:HG21	1.91	0.53
1:B:341:GLN:CG	1:B:367:ARG:NH2	2.72	0.53
1:B:215:THR:HG22	1:B:217:ASP:H	1.73	0.53
1:A:160:SER:C	1:A:161:THR:HG22	2.09	0.52
1:A:390:THR:HG21	1:A:401:LYS:HB2	1.91	0.52
1:B:143:LEU:CD1	1:B:409:GLU:HG3	2.40	0.52
1:B:197:ARG:HH21	1:B:199:PHE:HE2	1.46	0.51
1:B:304:LEU:HD12	1:B:308:VAL:HB	1.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:LEU:CD1	1:B:409:GLU:CB	2.88	0.51
1:B:143:LEU:CD1	1:B:409:GLU:CG	2.89	0.51
1:B:209:PHE:HE2	1:B:211:PRO:N	1.94	0.51
1:B:42:ALA:O	1:B:367:ARG:NH1	2.43	0.51
1:B:155:GLN:C	1:B:157:ALA:CB	2.61	0.51
1:A:254:LYS:CG	1:A:264:LEU:O	2.58	0.50
1:A:395:ARG:NH1	1:B:395:ARG:CD	2.73	0.50
1:B:197:ARG:O	1:B:197:ARG:HD3	2.11	0.50
1:B:44:THR:HA	1:B:46:ALA:HB3	1.93	0.50
1:A:162:ASP:O	1:A:163:PHE:O	2.30	0.50
1:B:338:LYS:HD2	1:B:341:GLN:CD	2.31	0.50
1:B:161:THR:HG23	1:B:216:ASN:CG	2.23	0.50
1:B:38:VAL:HG11	1:B:110:ASN:HA	1.94	0.49
1:B:370:GLU:HB2	1:B:398:ARG:NH1	2.19	0.49
1:B:44:THR:HG23	1:B:48:GLU:OE1	2.12	0.49
1:A:254:LYS:HD2	1:A:266:SER:N	2.27	0.49
1:B:197:ARG:CD	1:B:197:ARG:O	2.60	0.49
1:A:151:MET:HB3	1:A:166:PHE:HB2	1.94	0.49
1:A:395:ARG:HG2	1:B:395:ARG:HE	1.76	0.49
1:A:206:GLU:HA	1:A:398:ARG:NH2	2.28	0.49
1:B:159:ASN:O	1:B:159:ASN:OD1	2.30	0.49
1:B:209:PHE:HE2	1:B:211:PRO:CD	2.07	0.49
1:A:254:LYS:CD	1:A:265:SER:HA	2.43	0.49
1:A:16:SER:O	1:B:394:ALA:O	2.30	0.48
1:A:200:SER:OG	1:A:201:THR:N	2.46	0.48
1:B:197:ARG:CD	1:B:199:PHE:CE2	2.85	0.48
1:B:319:ASN:HD22	1:B:322:ARG:HG2	1.78	0.48
1:A:206:GLU:O	1:A:398:ARG:HG3	2.14	0.48
1:A:144:PRO:HG3	1:A:380:VAL:HG11	1.96	0.47
1:B:366:HIS:CD2	1:B:389:LYS:O	2.67	0.47
1:A:203:VAL:HB	1:A:207:GLY:HA2	1.96	0.47
1:A:203:VAL:CG2	1:A:203:VAL:O	2.61	0.47
1:B:258:LYS:CA	1:B:259:ARG:HD2	2.29	0.47
1:B:419:ALA:HB1	1:B:423:ALA:HB2	1.95	0.47
1:A:390:THR:O	1:A:398:ARG:CD	2.60	0.47
1:A:255:TYR:OH	1:A:290:ALA:N	2.39	0.47
1:A:46[B]:ALA:O	1:A:317:VAL:HG11	2.15	0.47
1:A:253:GLY:O	1:A:254:LYS:HE2	2.14	0.46
1:B:52:LEU:HD23	1:B:68:ALA:N	2.30	0.46
1:B:338:LYS:CD	1:B:341:GLN:HE22	2.25	0.46
1:B:338:LYS:HD2	1:B:341:GLN:HE22	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:LEU:HD12	1:B:300:LEU:HD22	1.97	0.46
1:B:367:ARG:CG	3:B:502[B]:2PG:O2P	2.51	0.46
1:A:44[B]:THR:O	1:A:45[B]:GLY:O	2.34	0.45
1:A:46[B]:ALA:N	1:A:48:GLU:OE1	2.37	0.45
1:A:397:ASP:HB3	1:B:396:THR:OG1	2.16	0.45
1:B:164:GLN:HB3	1:B:243:ASP:O	2.17	0.45
1:B:319:ASN:HB3	1:B:322:ARG:HG2	1.97	0.45
1:A:113:LEU:HD11	1:A:339:LEU:HG	1.99	0.45
1:B:215:THR:HG22	1:B:216:ASN:N	2.32	0.45
1:A:391:GLY:HA3	1:A:398:ARG:HD2	1.98	0.44
1:A:42[A]:ALA:O	1:A:51:GLU:CD	2.49	0.44
1:B:189:MET:HA	1:B:192:LYS:HD2	1.99	0.44
1:B:341:GLN:CG	1:B:367:ARG:HH21	2.30	0.44
1:A:154:GLY:N	1:A:163:PHE:O	2.51	0.44
1:A:252:ASP:HB2	1:A:253:GLY:HA3	1.93	0.44
1:B:367:ARG:HG2	1:B:368:SER:H	1.83	0.44
1:B:367:ARG:O	1:B:398:ARG:NH2	2.49	0.44
1:B:206:GLU:OE2	3:B:502[B]:2PG:C3	2.65	0.44
1:B:367:ARG:HG2	1:B:368:SER:N	2.32	0.44
1:A:254:LYS:HD2	1:A:265:SER:HA	2.00	0.44
1:A:397:ASP:OD1	1:A:398:ARG:HG2	2.18	0.44
1:B:256:HIS:CD2	1:B:264:LEU:HD23	2.51	0.44
1:B:48:GLU:H	1:B:48:GLU:HG2	1.63	0.43
1:B:209:PHE:CG	1:B:210:ALA:N	2.85	0.43
1:B:143:LEU:HD12	1:B:409:GLU:HG3	2.01	0.43
1:A:117:LEU:HD22	1:A:375:THR:HG21	2.01	0.43
1:B:163:PHE:CD2	1:B:166:PHE:HZ	2.34	0.43
1:A:419:ALA:HB1	1:A:423:ALA:HB2	2.00	0.43
1:A:176:PHE:HZ	1:A:402:TYR:HD1	1.67	0.43
1:B:220:LEU:HD21	1:B:282:ILE:HD11	2.00	0.43
1:A:160:SER:CB	1:A:212:SER:C	2.87	0.43
1:B:176:PHE:HZ	1:B:402:TYR:HD1	1.67	0.42
1:B:319:ASN:HD21	1:B:321:GLN:HB3	1.84	0.42
1:A:160:SER:OG	1:A:212:SER:HB3	2.18	0.42
1:A:202:THR:O	1:A:203:VAL:HG12	2.14	0.42
1:A:44[A]:THR:CG2	1:A:45[A]:GLY:N	2.83	0.42
1:B:163:PHE:CD2	1:B:166:PHE:CZ	3.00	0.42
1:B:299:LEU:HD11	1:B:303:LYS:HE2	2.01	0.42
1:A:40[A]:SER:HA	1:A:41[A]:GLY:HA3	1.64	0.42
1:A:157:ALA:HB1	1:A:160:SER:O	2.18	0.42
1:A:395:ARG:HB2	1:A:397:ASP:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44[A]:THR:HG22	1:A:45[A]:GLY:N	2.34	0.42
1:B:150:ILE:HG22	1:B:187:TYR:HD1	1.84	0.42
1:B:190:LEU:HG	1:B:194:ILE:CD1	2.49	0.42
1:A:206:GLU:CA	1:A:398:ARG:HE	2.22	0.42
1:B:52:LEU:HD23	1:B:68:ALA:HA	2.00	0.42
1:A:353:GLN:O	1:A:357:ARG:HG2	2.20	0.42
1:A:254:LYS:HD3	1:A:254:LYS:HA	1.36	0.41
1:A:357:ARG:O	1:A:358:SER:CB	2.68	0.41
1:B:52:LEU:HD23	1:B:68:ALA:CA	2.49	0.41
1:B:117:LEU:HD22	1:B:375:THR:HG21	2.03	0.41
1:A:190:LEU:HG	1:A:194:ILE:HD12	2.02	0.41
1:B:146:PRO:HD2	1:B:170:PRO:HD2	2.02	0.41
1:B:338:LYS:HD2	1:B:341:GLN:OE1	2.20	0.41
1:A:301:ARG:HD3	1:A:330:LYS:O	2.20	0.41
1:A:193:VAL:O	1:A:197:ARG:HG2	2.22	0.40
1:A:40[B]:SER:O	1:A:367:ARG:HB3	2.21	0.40
1:A:163:PHE:CE1	1:A:273:TRP:HH2	2.39	0.40
1:A:244:PRO:HD2	1:A:286:GLU:O	2.20	0.40
1:A:155:GLN:C	1:A:157:ALA:N	2.75	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	427/426 (100%)	383 (90%)	30 (7%)	14 (3%)	4 4
1	B	415/426 (97%)	379 (91%)	29 (7%)	7 (2%)	9 15
All	All	842/852 (99%)	762 (90%)	59 (7%)	21 (2%)	6 8

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	ASN
1	A	163	PHE
1	B	264	LEU
1	A	45[A]	GLY
1	A	45[B]	GLY
1	A	46[A]	ALA
1	A	46[B]	ALA
1	A	203	VAL
1	A	255	TYR
1	B	40	SER
1	A	44[A]	THR
1	A	44[B]	THR
1	A	156	HIS
1	A	358	SER
1	B	157	ALA
1	B	155	GLN
1	B	163	PHE
1	A	161	THR
1	B	39	PRO
1	A	214	PRO
1	B	214	PRO

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	333/332 (100%)	329 (99%)	4 (1%)	71	87
1	B	326/332 (98%)	322 (99%)	4 (1%)	71	87
All	All	659/664 (99%)	651 (99%)	8 (1%)	71	87

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	HIS
1	A	159	ASN
1	A	200	SER

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Mol	Chain	Res	Type
1	A	254	LYS
1	B	160	SER
1	B	197	ARG
1	B	201	THR
1	B	202	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	256	HIS
1	A	309	GLN
1	B	88	GLN
1	B	319	ASN
1	B	341	GLN
1	B	366	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

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\|>2$
3	2PG	A	502[B]	-	7,10,10	0.95	0	8,14,14	0.91	0
3	2PG	B	502[B]	2	7,10,10	1.00	0	8,14,14	0.83	0

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
3	2PG	A	502[B]	-	-	3/7/11/11	-
3	2PG	B	502[B]	2	-	2/7/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502[B]	2PG	C1-C2-C3-O3
3	B	502[B]	2PG	O1P-C2-C3-O3
3	A	502[B]	2PG	O1P-C2-C3-O3
3	A	502[B]	2PG	C2-O1P-P-O2P
3	A	502[B]	2PG	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502[B]	2PG	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	262:ARG	C	263:SER	N	1.12
1	B	155:GLN	C	156:HIS	N	1.10
1	B	158:THR	C	159:ASN	N	1.04

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	424/426 (99%)	0.67	43 (10%) 7 6	30, 49, 97, 120	0
1	B	419/426 (98%)	1.20	85 (20%) 1 0	27, 58, 128, 144	0
All	All	843/852 (98%)	0.94	128 (15%) 2 2	27, 53, 111, 144	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	44[A]	THR	11.5
1	B	44	THR	11.4
1	B	426	VAL	9.9
1	B	157	ALA	8.7
1	B	42	ALA	8.5
1	B	196	ASP	8.3
1	A	264	LEU	8.3
1	A	202	THR	7.9
1	B	155	GLN	7.9
1	A	43[A]	SER	7.2
1	A	46[A]	ALA	7.1
1	B	218	ALA	7.1
1	A	42[A]	ALA	7.1
1	B	261	GLY	7.1
1	B	43	SER	6.8
1	A	45[A]	GLY	6.7
1	A	159	ASN	6.5
1	A	158	THR	6.5
1	B	262	ARG	6.5
1	A	252	ASP	6.4
1	B	207	GLY	6.3
1	B	209	PHE	6.2
1	B	201	THR	6.1
1	B	203	VAL	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	261	GLY	6.0
1	B	156	HIS	6.0
1	B	264	LEU	5.9
1	B	213	LEU	5.9
1	A	41[A]	GLY	5.9
1	B	159	ASN	5.8
1	B	256	HIS	5.7
1	A	203	VAL	5.6
1	B	160	SER	5.6
1	B	206	GLU	5.5
1	B	47	HIS	5.5
1	B	200	SER	5.3
1	B	195	HIS	5.3
1	B	214	PRO	5.3
1	B	198	GLY	5.2
1	B	199	PHE	5.2
1	B	204	GLY	5.0
1	B	158	THR	5.0
1	A	200	SER	4.9
1	A	47	HIS	4.9
1	B	259	ARG	4.7
1	A	201	THR	4.5
1	B	45	GLY	4.5
1	B	194	ILE	4.4
1	B	154	GLY	4.4
1	B	208	GLY	4.4
1	B	151	MET	4.4
1	B	258	LYS	4.3
1	B	197	ARG	4.3
1	B	202	THR	4.3
1	B	263	SER	4.3
1	A	258	LYS	4.1
1	A	205	ASP	4.1
1	B	249	ILE	4.1
1	A	199	PHE	3.9
1	A	162	ASP	3.9
1	B	290	ALA	3.8
1	A	254	LYS	3.8
1	B	163	PHE	3.8
1	A	395	ARG	3.8
1	A	160	SER	3.7
1	A	426	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	304	LEU	3.6
1	B	215	THR	3.6
1	B	152	ASN	3.5
1	A	161	THR	3.5
1	B	225	GLU	3.5
1	B	205	ASP	3.5
1	B	41	GLY	3.5
1	B	192	LYS	3.5
1	B	222	LEU	3.4
1	A	157	ALA	3.4
1	B	150	ILE	3.3
1	A	194	ILE	3.2
1	A	195	HIS	3.2
1	B	396	THR	3.1
1	A	396	THR	3.1
1	B	266	SER	3.1
1	B	328	GLU	3.1
1	B	247	THR	3.1
1	B	398	ARG	2.9
1	A	255	TYR	2.8
1	B	162	ASP	2.8
1	A	398	ARG	2.8
1	B	280	TYR	2.8
1	A	394	ALA	2.7
1	B	295	GLU	2.7
1	B	300	LEU	2.7
1	B	221	GLN	2.7
1	B	365	SER	2.6
1	B	367	ARG	2.6
1	A	247	THR	2.6
1	A	40[A]	SER	2.6
1	B	269	MET	2.6
1	B	48	GLU	2.5
1	B	190	LEU	2.5
1	B	303	LYS	2.5
1	B	297	TRP	2.5
1	B	265	SER	2.5
1	B	289	LEU	2.5
1	A	206	GLU	2.5
1	B	399	ILE	2.4
1	A	214	PRO	2.4
1	B	270	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	366	HIS	2.4
1	B	301	ARG	2.4
1	B	394	ALA	2.4
1	B	40	SER	2.4
1	B	299	LEU	2.4
1	B	296	GLY	2.3
1	B	388	ILE	2.3
1	B	366	HIS	2.3
1	B	395	ARG	2.2
1	B	272	TYR	2.2
1	A	365	SER	2.2
1	A	259	ARG	2.1
1	B	223	ILE	2.1
1	B	425	LYS	2.1
1	B	294	TRP	2.1
1	A	265	SER	2.1
1	A	371	SER	2.1
1	B	257	LEU	2.1
1	A	212	SER	2.0
1	A	155	GLN	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	2PG	A	502[B]	11/11	0.64	0.72	93,95,100,100	11
3	2PG	B	502[B]	11/11	0.68	0.59	97,99,104,104	11
2	MG	B	501	1/1	0.88	0.36	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	A	501	1/1	0.91	0.38	41,41,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.