



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 05:37 am GMT

PDB ID : 4Z17
Title : Thermostable enolase from *Chloroflexus aurantiacus*
Authors : Zadvornyy, O.A.; Peters, J.W.
Deposited on : 2015-03-26
Resolution : 2.65 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 : trunk28620
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) : recalc28949

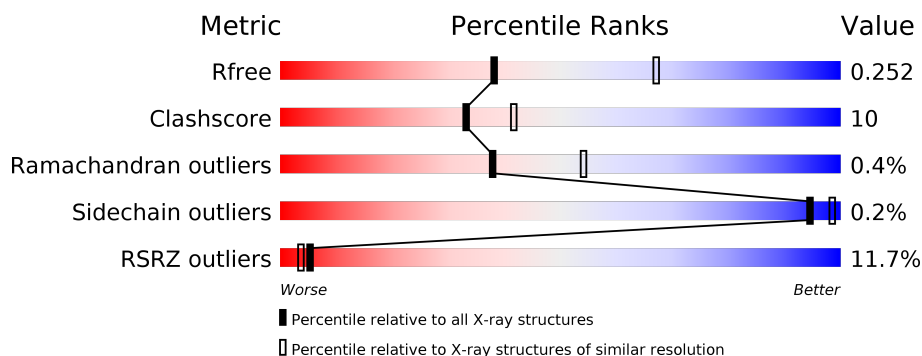
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	3491 (2.70-2.62)
Clashscore	112137	1026 (2.68-2.64)
Ramachandran outliers	110173	1010 (2.68-2.64)
Sidechain outliers	110143	1010 (2.68-2.64)
RSRZ outliers	101464	3511 (2.70-2.62)

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	426	<div> <div>8%</div> <div>83%</div> <div>14%</div> <div>.</div> </div>
1	B	426	<div> <div>15%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6421 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.

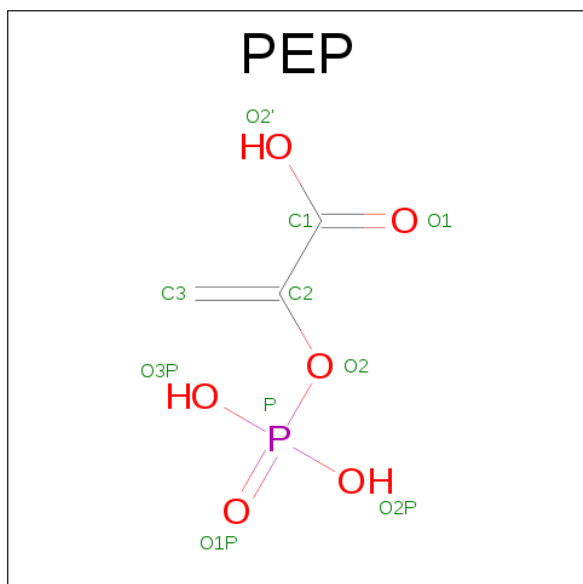
- Molecule 1 is a protein called Enolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3207	2016	564	618	9			
1	B	420	Total	C	N	O	S	0	0	0
			3161	1984	557	612	8			

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

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

- Molecule 3 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula: C₃H₅O₆P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			10	3	6	1		
3	B	1	Total	C	O	P	0	0
			10	3	6	1		

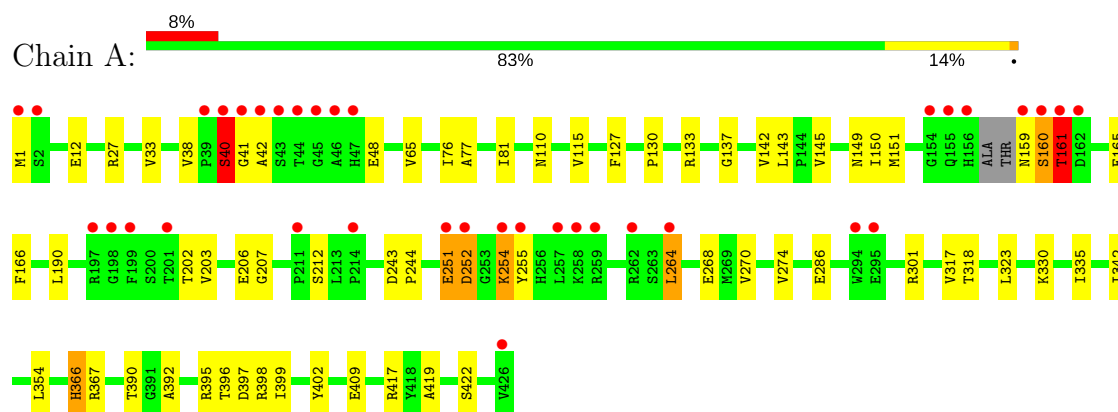
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	O	0	0
			13	13		
4	B	16	Total	O	0	0
			16	16		

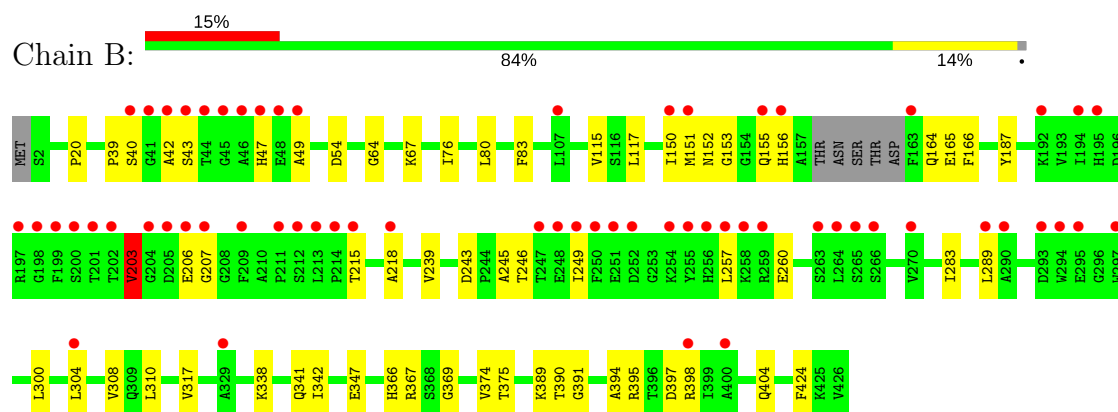
3 Residue-property plots [i](#)

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



• Molecule 1: Enolase



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	146.28Å 146.28Å 101.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.68 – 2.65 37.69 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.6 (37.68-2.65) 99.5 (37.69-2.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.193 , 0.238 0.210 , 0.252	Depositor DCC
R_{free} test set	1556 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.036 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6421	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PEP

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	0.51	0/3257	0.80	11/4411 (0.2%)
1	B	0.51	0/3208	0.76	5/4347 (0.1%)
All	All	0.51	0/6465	0.78	16/8758 (0.2%)

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

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	LYS	CB-CA-C	11.74	133.88	110.40
1	B	42	ALA	N-CA-C	7.87	132.25	111.00
1	B	203	VAL	CB-CA-C	7.58	125.80	111.40
1	A	202	THR	N-CA-CB	-7.29	96.44	110.30
1	A	42	ALA	CB-CA-C	7.21	120.92	110.10
1	B	245	ALA	N-CA-C	7.09	130.15	111.00
1	A	255	TYR	N-CA-CB	6.91	123.04	110.60
1	A	161	THR	CB-CA-C	6.79	129.94	111.60
1	A	251	GLU	N-CA-C	6.21	127.78	111.00
1	B	40	SER	CB-CA-C	-6.01	98.67	110.10
1	A	41	GLY	N-CA-C	5.87	127.77	113.10
1	A	160	SER	C-N-CA	5.77	136.12	121.70
1	A	264	LEU	CB-CA-C	5.64	120.92	110.20
1	B	43	SER	N-CA-C	5.14	124.89	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	SER	CB-CA-C	5.11	119.81	110.10
1	A	255	TYR	N-CA-C	-5.06	97.34	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40	SER	Mainchain

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	3207	0	3193	66	0
1	B	3161	0	3157	59	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	10	0	2	0	0
3	B	10	0	2	0	0
4	A	13	0	0	0	0
4	B	16	0	0	0	0
All	All	6421	0	6354	125	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 10.

All (125) 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:A:390:THR:O	1:A:398:ARG:HD2	1.23	1.37
1:A:301:ARG:NH1	1:A:330:LYS:HA	1.53	1.22
1:A:301:ARG:HD3	1:A:330:LYS:O	1.49	1.13
1:B:304:LEU:HD13	1:B:308:VAL:HB	1.25	1.12
1:A:390:THR:O	1:A:398:ARG:CD	2.12	0.97
1:B:304:LEU:CD1	1:B:308:VAL:HB	1.96	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:HIS:CE1	1:A:398:ARG:NE	2.35	0.94
1:B:304:LEU:HD13	1:B:308:VAL:CB	2.00	0.91
1:B:338:LYS:HD3	1:B:341:GLN:CD	1.92	0.90
1:A:12:GLU:HG3	1:A:65:VAL:HG12	1.56	0.88
1:A:143:LEU:CD2	1:A:409:GLU:HB2	2.04	0.87
1:A:301:ARG:NH1	1:A:330:LYS:CA	2.37	0.86
1:A:366:HIS:ND1	1:A:398:ARG:CZ	2.40	0.85
1:A:301:ARG:CD	1:A:330:LYS:O	2.26	0.84
1:A:301:ARG:HH11	1:A:330:LYS:HA	1.41	0.84
1:B:39:PRO:HG2	1:B:367:ARG:CD	2.08	0.83
1:A:317:VAL:HG12	1:A:317:VAL:O	1.77	0.83
1:A:40:SER:O	1:A:367:ARG:HB3	1.79	0.83
1:B:39:PRO:HG2	1:B:367:ARG:HD2	1.61	0.82
1:B:152:ASN:HD21	1:B:206:GLU:HB3	1.44	0.81
1:A:142:VAL:CG2	1:A:417:ARG:NH2	2.44	0.80
1:B:338:LYS:HD3	1:B:341:GLN:NE2	1.96	0.79
1:B:39:PRO:HB2	1:B:369:GLY:O	1.82	0.79
1:A:12:GLU:HG3	1:A:65:VAL:CG1	2.13	0.78
1:A:366:HIS:CE1	1:A:398:ARG:CZ	2.65	0.78
1:B:338:LYS:HB2	1:B:341:GLN:OE1	1.86	0.76
1:A:48:GLU:HB3	1:A:317:VAL:HG11	1.68	0.75
1:A:143:LEU:HD21	1:A:409:GLU:HB2	1.69	0.73
1:A:254:LYS:HA	1:A:264:LEU:O	1.88	0.73
1:B:366:HIS:ND1	1:B:390:THR:HA	2.03	0.73
1:B:317:VAL:O	1:B:317:VAL:HG12	1.87	0.72
1:B:257:LEU:CD2	1:B:260:GLU:HB3	2.19	0.72
1:A:301:ARG:HH11	1:A:330:LYS:CA	2.01	0.70
1:B:215:THR:OG1	1:B:218:ALA:HB2	1.94	0.68
1:A:366:HIS:ND1	1:A:398:ARG:NE	2.42	0.68
1:A:142:VAL:HG21	1:A:417:ARG:NH2	2.08	0.67
1:A:366:HIS:HE1	1:A:398:ARG:HE	1.43	0.66
1:A:397:ASP:OD1	1:A:398:ARG:HG2	1.94	0.66
1:B:366:HIS:HD1	1:B:390:THR:HA	1.61	0.65
1:A:143:LEU:HD22	1:A:409:GLU:HB2	1.77	0.65
1:A:366:HIS:CE1	1:A:398:ARG:HE	2.15	0.63
1:B:39:PRO:HG2	1:B:367:ARG:NE	2.14	0.63
1:A:366:HIS:HE1	1:A:398:ARG:NE	1.89	0.63
1:A:206:GLU:HG2	1:A:366:HIS:HE1	1.65	0.62
1:B:47:HIS:HA	1:B:317:VAL:HG11	1.81	0.61
1:B:155:GLN:HG2	1:B:156:HIS:N	2.15	0.61
1:B:395:ARG:HB3	1:B:397:ASP:OD1	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:VAL:HB	1:A:207:GLY:HA2	1.84	0.60
1:A:159:ASN:N	1:A:212:SER:HG	1.99	0.60
1:A:390:THR:CG2	1:A:402:TYR:CZ	2.85	0.60
1:B:155:GLN:HG2	1:B:156:HIS:H	1.66	0.59
1:B:239:VAL:HG11	1:B:283:ILE:HB	1.83	0.59
1:B:76:ILE:HG21	1:B:115:VAL:HG21	1.85	0.59
1:B:338:LYS:HD3	1:B:341:GLN:OE1	2.04	0.58
1:A:142:VAL:HG22	1:A:417:ARG:NH2	2.17	0.58
1:A:390:THR:HG23	1:A:402:TYR:CZ	2.39	0.57
1:B:257:LEU:CD2	1:B:260:GLU:CB	2.82	0.57
1:B:151:MET:HB3	1:B:166:PHE:HB2	1.85	0.57
1:A:317:VAL:O	1:A:317:VAL:CG1	2.50	0.57
1:A:301:ARG:HH12	1:A:330:LYS:HA	1.63	0.57
1:A:301:ARG:HH11	1:A:330:LYS:C	2.07	0.57
1:A:48:GLU:HB3	1:A:317:VAL:CG1	2.35	0.56
1:B:257:LEU:HD22	1:B:260:GLU:HB3	1.88	0.55
1:A:165:GLU:HB2	1:A:243:ASP:HB3	1.89	0.55
1:B:394:ALA:HB3	1:B:398:ARG:HH21	1.74	0.53
1:B:283:ILE:HD11	1:B:424:PHE:CD2	2.43	0.53
1:A:76:ILE:HG21	1:A:115:VAL:HG21	1.90	0.52
1:A:264:LEU:HD13	1:A:268:GLU:CD	2.30	0.52
1:B:366:HIS:ND1	1:B:389:LYS:O	2.36	0.52
1:A:366:HIS:CE1	1:A:398:ARG:NH2	2.79	0.51
1:A:390:THR:CG2	1:A:402:TYR:CE1	2.93	0.51
1:B:155:GLN:CG	1:B:156:HIS:H	2.23	0.51
1:B:207:GLY:H	1:B:398:ARG:NH1	2.09	0.51
1:B:150:ILE:HG22	1:B:187:TYR:HD1	1.77	0.50
1:B:39:PRO:C	1:B:367:ARG:HD2	2.32	0.50
1:B:342:ILE:HG12	1:B:347:GLU:HB3	1.95	0.48
1:A:323:LEU:HD23	1:A:354:LEU:HD23	1.95	0.48
1:A:251:GLU:O	1:A:252:ASP:CG	2.51	0.48
1:B:338:LYS:HB2	1:B:341:GLN:CD	2.34	0.48
1:B:155:GLN:CG	1:B:156:HIS:N	2.77	0.47
1:B:283:ILE:HD13	1:B:424:PHE:CE2	2.49	0.47
1:A:160:SER:HA	1:A:161:THR:CB	2.44	0.47
1:A:38:VAL:HG11	1:A:110:ASN:HA	1.97	0.47
1:B:304:LEU:HD11	1:B:310:LEU:HD21	1.97	0.47
1:B:283:ILE:HD11	1:B:424:PHE:CG	2.50	0.47
1:A:206:GLU:HG2	1:A:398:ARG:HH21	1.81	0.46
1:A:130:PRO:HD2	1:A:133:ARG:HB2	1.99	0.45
1:B:165:GLU:HB2	1:B:243:ASP:HB3	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:PRO:HG2	1:B:64:GLY:HA2	1.99	0.45
1:A:77:ALA:O	1:A:81:ILE:HG13	2.15	0.45
1:A:27:ARG:HG3	1:A:33:VAL:HG22	1.99	0.45
1:A:206:GLU:HG2	1:A:398:ARG:HE	1.81	0.45
1:B:317:VAL:CG1	1:B:317:VAL:O	2.60	0.45
1:B:54:ASP:HA	1:B:67:LYS:HD2	1.98	0.45
1:A:270:VAL:O	1:A:274:VAL:HG23	2.17	0.45
1:A:323:LEU:HD13	1:A:335:ILE:HD12	1.98	0.45
1:B:338:LYS:CD	1:B:341:GLN:OE1	2.65	0.45
1:A:1:MET:HG3	1:A:127:PHE:CE1	2.53	0.44
1:B:239:VAL:HG12	1:B:283:ILE:HG22	1.99	0.44
1:A:395:ARG:NH1	1:A:397:ASP:OD2	2.51	0.44
1:B:289:LEU:HD12	1:B:300:LEU:HD22	2.00	0.44
1:A:143:LEU:HD22	1:A:409:GLU:CB	2.47	0.43
1:A:151:MET:HB3	1:A:166:PHE:HB2	1.99	0.43
1:A:301:ARG:HD3	1:A:330:LYS:C	2.29	0.43
1:A:150:ILE:HD12	1:A:190:LEU:HD22	2.01	0.43
1:B:80:LEU:O	1:B:83:PHE:HB2	2.18	0.42
1:B:117:LEU:HD22	1:B:375:THR:HG21	2.02	0.42
1:B:397:ASP:OD1	1:B:398:ARG:HG3	2.19	0.42
1:B:395:ARG:H	1:B:398:ARG:HH21	1.68	0.42
1:B:374:VAL:HG21	1:B:404:GLN:HB2	2.01	0.42
1:B:203:VAL:HG13	1:B:207:GLY:HA2	2.01	0.42
1:B:395:ARG:CB	1:B:397:ASP:OD1	2.65	0.42
1:A:318:THR:O	1:A:342:ILE:HD12	2.20	0.42
1:B:391:GLY:HA3	1:B:398:ARG:HD2	2.02	0.42
1:B:246:THR:HA	1:B:249:ILE:HB	2.02	0.41
1:A:149:ASN:O	1:A:392:ALA:HB2	2.19	0.41
1:B:153:GLY:O	1:B:164:GLN:HG3	2.21	0.41
1:A:419:ALA:O	1:A:422:SER:HB3	2.20	0.41
1:A:133:ARG:HD2	1:A:137:GLY:O	2.21	0.41
1:A:145:VAL:HG23	1:A:419:ALA:HB3	2.03	0.40
1:B:304:LEU:CD1	1:B:308:VAL:CB	2.78	0.40
1:A:244:PRO:HD2	1:A:286:GLU:O	2.22	0.40
1:B:49:ALA:HB3	1:B:341:GLN:O	2.21	0.40
1:A:396:THR:HA	1:A:399:ILE:HB	2.02	0.40
1:B:39:PRO:HD2	1:B:367:ARG:CZ	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	420/426 (99%)	388 (92%)	30 (7%)	2 (0%)	32	49
1	B	416/426 (98%)	375 (90%)	40 (10%)	1 (0%)	51	69
All	All	836/852 (98%)	763 (91%)	70 (8%)	3 (0%)	38	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	203	VAL
1	A	161	THR
1	A	252	ASP

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	325/332 (98%)	324 (100%)	1 (0%)	94	97
1	B	321/332 (97%)	321 (100%)	0	100	100
All	All	646/664 (97%)	645 (100%)	1 (0%)	94	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	366	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	149	ASN
1	A	221	GLN
1	A	256	HIS
1	A	366	HIS
1	B	88	GLN
1	B	152	ASN
1	B	319	ASN

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 6 ligands modelled in this entry, 4 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	PEP	A	502	2	6,9,9	1.45	1 (16%)	9,13,13	1.20	1 (11%)
3	PEP	B	502	2	6,9,9	1.29	1 (16%)	9,13,13	1.20	1 (11%)

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	PEP	A	502	2	-	0/5/9/9	0/0/0/0
3	PEP	B	502	2	-	0/5/9/9	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	PEP	O2-C2	2.56	1.46	1.39
3	A	502	PEP	O2-C2	2.78	1.47	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	PEP	O2-C2-C3	-2.68	119.71	124.87
3	A	502	PEP	O2-C2-C3	-2.54	119.98	124.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	424/426 (99%)	0.40	36 (8%)	11 9	31, 53, 99, 138	25 (5%)
1	B	420/426 (98%)	0.88	63 (15%)	3 2	32, 65, 139, 151	4 (0%)
All	All	844/852 (99%)	0.64	99 (11%)	5 4	31, 56, 127, 151	29 (3%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	42	ALA	18.1
1	A	46	ALA	13.0
1	B	46	ALA	12.1
1	B	264	LEU	9.3
1	B	44	THR	9.2
1	A	156	HIS	7.8
1	A	43	SER	7.6
1	B	41	GLY	7.5
1	A	47	HIS	7.5
1	B	47	HIS	7.4
1	B	200	SER	7.4
1	B	251	GLU	6.6
1	A	40	SER	6.4
1	B	209	PHE	6.2
1	B	45	GLY	5.9
1	B	248	GLU	5.9
1	A	39	PRO	5.8
1	B	204	GLY	5.8
1	B	48	GLU	5.7
1	A	197	ARG	5.7
1	A	254	LYS	5.5
1	B	259	ARG	5.5
1	A	44	THR	5.5
1	B	215	THR	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	202	THR	5.1
1	B	156	HIS	5.0
1	B	256	HIS	4.9
1	B	249	ILE	4.9
1	B	263	SER	4.7
1	B	255	TYR	4.7
1	B	205	ASP	4.6
1	A	264	LEU	4.6
1	A	259	ARG	4.6
1	B	252	ASP	4.5
1	B	250	PHE	4.5
1	B	294	TRP	4.4
1	B	218	ALA	4.4
1	B	214	PRO	4.4
1	B	290	ALA	4.4
1	A	41	GLY	4.2
1	A	199	PHE	4.1
1	B	198	GLY	4.1
1	B	206	GLU	4.1
1	A	251	GLU	4.0
1	B	43	SER	4.0
1	B	155	GLN	4.0
1	A	42	ALA	3.9
1	B	212	SER	3.6
1	A	1	MET	3.6
1	A	198	GLY	3.6
1	A	155	GLN	3.5
1	A	257	LEU	3.5
1	B	295	GLU	3.5
1	B	194	ILE	3.5
1	B	213	LEU	3.5
1	B	199	PHE	3.5
1	A	161	THR	3.3
1	B	266	SER	3.3
1	B	247	THR	3.2
1	B	304	LEU	3.2
1	A	252	ASP	3.1
1	B	254	LYS	3.1
1	B	297	TRP	3.1
1	B	40	SER	3.1
1	B	195	HIS	3.0
1	B	207	GLY	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	426	VAL	3.0
1	B	265	SER	3.0
1	B	197	ARG	2.9
1	A	211	PRO	2.9
1	B	49	ALA	2.9
1	A	201	THR	2.9
1	B	163	PHE	2.8
1	B	192	LYS	2.8
1	A	255	TYR	2.8
1	A	159	ASN	2.8
1	B	151	MET	2.7
1	A	162	ASP	2.7
1	A	45	GLY	2.7
1	A	154	GLY	2.7
1	A	295	GLU	2.6
1	B	329	ALA	2.6
1	A	258	LYS	2.5
1	B	211	PRO	2.4
1	A	2	SER	2.4
1	B	201	THR	2.4
1	A	294	TRP	2.4
1	B	257	LEU	2.4
1	A	160	SER	2.3
1	A	214	PRO	2.3
1	B	107	LEU	2.2
1	B	270	VAL	2.2
1	A	262	ARG	2.2
1	B	398	ARG	2.2
1	B	150	ILE	2.1
1	B	289	LEU	2.1
1	B	258	LYS	2.1
1	B	400	ALA	2.1
1	B	293	ASP	2.1

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(Å ²)	Q<0.9
2	MG	B	501	1/1	0.61	0.26	1.23	75,75,75,75	0
2	MG	A	501	1/1	0.72	0.18	0.77	64,64,64,64	0
3	PEP	B	502	10/10	0.76	0.35	-0.02	137,141,144,144	0
3	PEP	A	502	10/10	0.85	0.26	-0.16	126,126,127,127	0
2	MG	B	503	1/1	0.89	0.23	-	73,73,73,73	0
2	MG	A	503	1/1	0.85	0.34	-	78,78,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.