



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:26 AM UTC

PDB ID : 4Z17 / pdb_00004z17
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

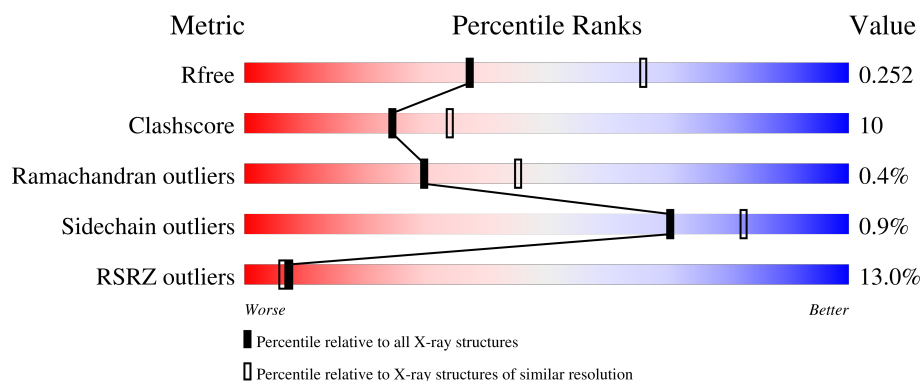
1 Overall quality at a glance

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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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 of 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 $\leq 5\%$. 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	9% 81% 16% .
1	B	426	17% 82% 16% .

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.

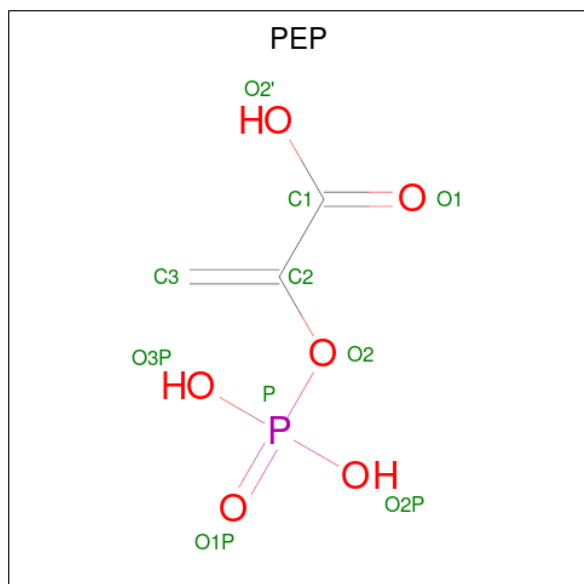
- Molecule 1 is a protein called Enolase.

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 (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is PHOSPHOENOLPYRUVATE (CCD ID: 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		

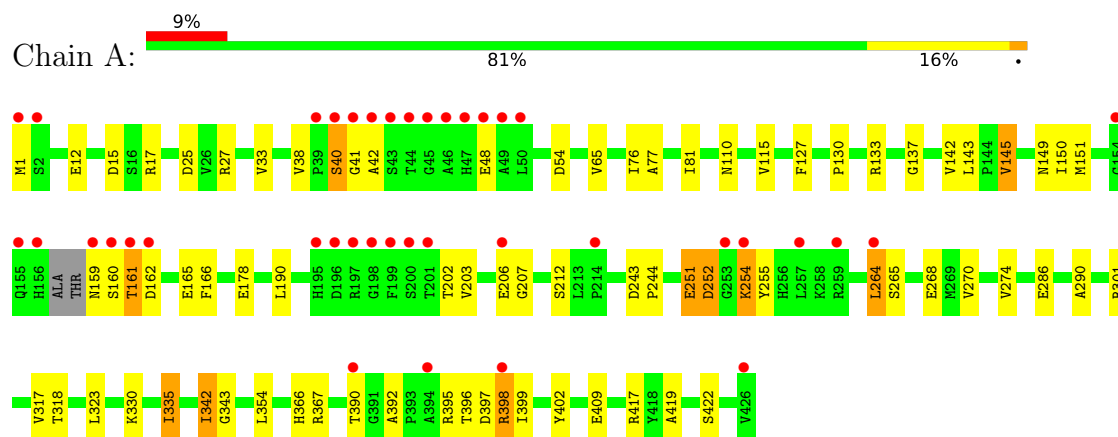
- Molecule 4 is water.

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

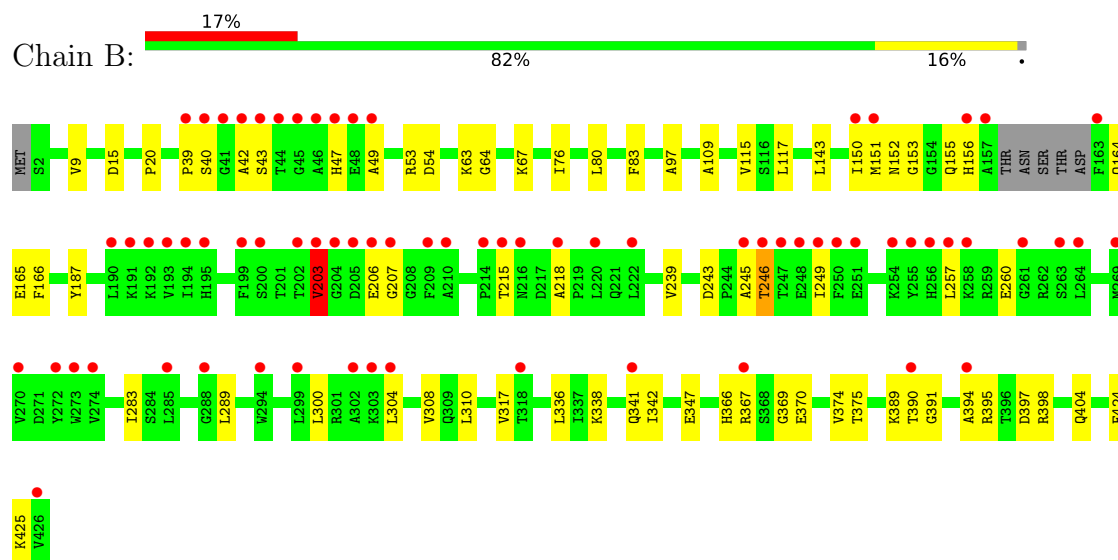
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 37.68 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.6 (37.68-2.65) 99.5 (37.68-2.65)	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, REFMAC	Depositor
R, R_{free}	0.193 , 0.238 0.210 , 0.252	Depositor DCC
R_{free} test set	1556 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.6	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

5.1 Standard geometry

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	0.89	0/3257	1.47	26/4411 (0.6%)
1	B	0.89	0/3208	1.44	19/4347 (0.4%)
All	All	0.89	0/6465	1.46	45/8758 (0.5%)

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 (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	42	ALA	N-CA-C	15.17	132.25	111.92
1	A	254	LYS	CB-CA-C	11.79	133.88	110.42
1	A	162	ASP	N-CA-C	-11.59	97.89	112.72
1	B	43	SER	N-CA-C	11.48	124.89	111.11
1	A	161	THR	CB-CA-C	9.47	129.94	109.10
1	B	245	ALA	N-CA-C	9.09	130.15	110.80
1	B	40	SER	N-CA-C	8.93	124.50	108.69
1	B	203	VAL	CB-CA-C	8.85	125.80	111.29
1	A	202	THR	N-CA-CB	-8.11	96.44	111.53
1	A	160	SER	CA-C-N	8.01	136.12	121.70
1	A	160	SER	C-N-CA	8.01	136.12	121.70
1	A	251	GLU	N-CA-C	7.97	127.78	110.80
1	A	255	TYR	N-CA-CB	7.53	123.04	110.77
1	A	145	VAL	N-CA-C	-7.30	100.39	107.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	ALA	CA-C-N	6.95	129.93	120.54
1	A	290	ALA	C-N-CA	6.95	129.93	120.54
1	A	255	TYR	N-CA-C	-6.58	97.34	108.26
1	B	40	SER	CB-CA-C	-6.27	98.67	109.65
1	A	178	GLU	CB-CG-CD	6.16	123.07	112.60
1	A	41	GLY	N-CA-C	6.16	127.77	113.18
1	A	54	ASP	N-CA-C	6.08	117.58	111.07
1	A	254	LYS	N-CA-C	-5.98	98.07	110.80
1	B	246	THR	N-CA-C	5.94	119.74	111.90
1	A	15	ASP	CA-CB-CG	5.84	118.44	112.60
1	B	15	ASP	CA-CB-CG	5.76	118.36	112.60
1	A	342	ILE	CB-CA-C	5.73	116.80	111.30
1	B	97	ALA	CA-C-N	5.62	128.08	120.38
1	B	97	ALA	C-N-CA	5.62	128.08	120.38
1	A	343	GLY	N-CA-C	5.59	121.34	114.69
1	A	398	ARG	CA-C-N	5.45	128.22	120.53
1	A	398	ARG	C-N-CA	5.45	128.22	120.53
1	A	265	SER	CA-C-N	5.37	127.73	120.38
1	A	265	SER	C-N-CA	5.37	127.73	120.38
1	A	264	LEU	CB-CA-C	5.28	120.92	110.42
1	A	42	ALA	CB-CA-C	5.28	120.92	110.42
1	B	109	ALA	CA-C-N	5.27	127.34	120.28
1	B	109	ALA	C-N-CA	5.27	127.34	120.28
1	B	425	LYS	N-CA-C	-5.20	106.62	113.17
1	B	425	LYS	CA-C-N	5.19	131.04	121.70
1	B	425	LYS	C-N-CA	5.19	131.04	121.70
1	B	53	ARG	CA-C-N	5.16	127.50	120.54
1	B	53	ARG	C-N-CA	5.16	127.50	120.54
1	B	63	LYS	CA-C-N	5.13	125.22	120.34
1	B	63	LYS	C-N-CA	5.13	125.22	120.34
1	A	25	ASP	CA-CB-CG	5.02	117.62	112.60

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	67	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	126	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 (126) 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:338:LYS:HD3	1:B:341:GLN:CD	1.92	0.95
1:B:304:LEU:CD1	1:B:308:VAL:HB	1.96	0.94
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: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:40:SER:O	1:A:367:ARG:HB3	1.79	0.83
1:A:317:VAL:HG12	1:A:317:VAL:O	1.77	0.82
1:B:39:PRO:HG2	1:B:367:ARG:HD2	1.61	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG12	1:B:317:VAL:O	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:A:301:ARG:HH11	1:A:330:LYS:C	2.07	0.61
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
1:A:203:VAL:HB	1:A:207:GLY:HA2	1.84	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:264:LEU:HD13	1:A:268:GLU:CD	2.30	0.57
1:A:301:ARG:HH12	1:A:330:LYS:HA	1.63	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:VAL:O	1:A:317:VAL:CG1	2.50	0.57
1:A:48:GLU:HB3	1:A:317:VAL:CG1	2.35	0.56
1:A:159:ASN:N	1:A:212:SER:HG	2.04	0.55
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:39:PRO:C	1:B:367:ARG:HD2	2.32	0.54
1:A:251:GLU:O	1:A:252:ASP:CG	2.51	0.53
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:B:338:LYS:HB2	1:B:341:GLN:CD	2.34	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: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:301:ARG:HD3	1:A:330:LYS:C	2.29	0.48
1:A:1:MET:HE2	1:A:127:PHE:HA	1.95	0.47
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:38:VAL:HG11	1:A:110:ASN:HA	1.97	0.47
1:B:283:ILE:HD11	1:B:424:PHE:CG	2.50	0.47
1:B:304:LEU:HD11	1:B:310:LEU:HD21	1.97	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:20:PRO:HG2	1:B:64:GLY:HA2	1.99	0.45
1:B:165:GLU:HB2	1:B:243:ASP:HB3	1.97	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:54:ASP:HA	1:B:67:LYS:HD2	1.98	0.45
1:B:317:VAL:O	1:B:317:VAL:CG1	2.60	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:301:ARG:CD	1:A:330:LYS:C	2.90	0.43
1:A:151:MET:HB3	1:A:166:PHE:HB2	1.99	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%)	24	39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	416/426 (98%)	375 (90%)	40 (10%)	1 (0%)	43	60
All	All	836/852 (98%)	763 (91%)	70 (8%)	3 (0%)	30	45

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 [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	325/332 (98%)	323 (99%)	2 (1%)	78	88
1	B	321/332 (97%)	317 (99%)	4 (1%)	63	79
All	All	646/664 (97%)	640 (99%)	6 (1%)	70	82

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	335	ILE
1	B	9	VAL
1	B	143	LEU
1	B	336	LEU
1	B	370	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	221	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	256	HIS
1	A	324	GLN
1	A	341	GLN
1	A	366	HIS
1	B	47	HIS
1	B	88	GLN
1	B	152	ASN
1	B	195	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	502	2	9,9,9	1.52	2 (22%)	11,13,13	1.77	3 (27%)
3	PEP	A	502	2	9,9,9	1.64	2 (22%)	11,13,13	1.62	3 (27%)

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	B	502	2	-	4/9/9/9	-
3	PEP	A	502	2	-	5/9/9/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	PEP	O2-C2	2.89	1.47	1.39
3	B	502	PEP	O2-C2	2.66	1.46	1.39
3	B	502	PEP	C2-C1	-2.40	1.47	1.49
3	A	502	PEP	C2-C1	-2.37	1.47	1.49

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	PEP	O2'-C1-C2	3.53	119.93	113.91
3	A	502	PEP	O2'-C1-C2	2.97	118.98	113.91
3	B	502	PEP	O2-C2-C3	-2.69	119.71	124.85
3	A	502	PEP	O2-C2-C3	-2.55	119.98	124.85
3	B	502	PEP	O1-C1-C2	-2.31	118.30	121.79
3	A	502	PEP	C3-C2-C1	-2.05	118.93	122.73

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	PEP	O1-C1-C2-C3
3	A	502	PEP	O1-C1-C2-O2
3	A	502	PEP	O2'-C1-C2-C3
3	A	502	PEP	O2'-C1-C2-O2
3	B	502	PEP	O1-C1-C2-C3
3	B	502	PEP	O1-C1-C2-O2
3	B	502	PEP	O2'-C1-C2-C3
3	B	502	PEP	O2'-C1-C2-O2
3	A	502	PEP	C2-O2-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

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, 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%)	0.57	39 (9%) 14 11	20, 49, 99, 138	25 (5%)
1	B	420/426 (98%)	0.77	71 (16%) 4 3	32, 64, 139, 151	4 (0%)
All	All	844/852 (99%)	0.67	110 (13%) 7 6	20, 54, 127, 151	29 (3%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	46	ALA	19.1
1	B	47	HIS	11.1
1	A	200	SER	10.5
1	A	199	PHE	10.4
1	A	161	THR	9.8
1	A	44	THR	9.6
1	B	48	GLU	9.5
1	A	46	ALA	8.9
1	A	154	GLY	8.9
1	A	159	ASN	8.7
1	B	42	ALA	8.2
1	A	160	SER	8.0
1	B	45	GLY	8.0
1	A	39	PRO	7.8
1	A	195	HIS	7.6
1	A	40	SER	7.5
1	A	197	ARG	7.4
1	A	196	ASP	6.8
1	A	45	GLY	6.6
1	A	42	ALA	6.5
1	A	162	ASP	6.4
1	A	156	HIS	6.4
1	A	198	GLY	6.1
1	A	426	VAL	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	43	SER	6.0
1	A	48	GLU	5.7
1	A	41	GLY	5.6
1	A	50	LEU	5.4
1	A	155	GLN	4.9
1	A	264	LEU	4.8
1	B	258	LYS	4.7
1	A	49	ALA	4.6
1	B	157	ALA	4.6
1	B	255	TYR	4.4
1	B	249	ILE	4.4
1	B	264	LEU	4.2
1	B	394	ALA	4.1
1	B	156	HIS	4.1
1	B	426	VAL	4.0
1	B	41	GLY	3.9
1	B	218	ALA	3.8
1	B	209	PHE	3.7
1	B	39	PRO	3.7
1	B	270	VAL	3.7
1	B	192	LYS	3.7
1	A	47	HIS	3.6
1	B	247	THR	3.6
1	B	40	SER	3.6
1	B	261	GLY	3.5
1	B	304	LEU	3.5
1	B	250	PHE	3.5
1	B	202	THR	3.4
1	B	251	GLU	3.3
1	B	257	LEU	3.3
1	B	44	THR	3.3
1	B	207	GLY	3.3
1	B	263	SER	3.2
1	B	193	VAL	3.2
1	B	215	THR	3.2
1	B	199	PHE	3.1
1	B	195	HIS	3.1
1	B	214	PRO	3.1
1	A	390	THR	3.1
1	B	256	HIS	3.1
1	B	203	VAL	3.1
1	B	150	ILE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	254	LYS	2.8
1	B	151	MET	2.8
1	B	269	MET	2.7
1	A	253	GLY	2.7
1	B	246	THR	2.7
1	A	398	ARG	2.7
1	B	341	GLN	2.7
1	B	190	LEU	2.7
1	A	201	THR	2.7
1	A	2	SER	2.6
1	B	294	TRP	2.6
1	B	254	LYS	2.6
1	B	288	GLY	2.6
1	B	273	TRP	2.6
1	A	1	MET	2.6
1	B	220	LEU	2.6
1	B	191	LYS	2.6
1	B	245	ALA	2.5
1	A	206	GLU	2.5
1	B	216	ASN	2.5
1	A	394	ALA	2.5
1	B	210	ALA	2.4
1	B	163	PHE	2.4
1	B	194	ILE	2.4
1	B	205	ASP	2.4
1	A	259	ARG	2.4
1	B	299	LEU	2.4
1	B	318	THR	2.3
1	B	367	ARG	2.3
1	B	43	SER	2.3
1	B	222	LEU	2.3
1	B	274	VAL	2.2
1	B	302	ALA	2.2
1	A	214	PRO	2.2
1	A	257	LEU	2.2
1	B	303	LYS	2.2
1	B	49	ALA	2.2
1	B	248	GLU	2.2
1	B	285	LEU	2.2
1	B	200	SER	2.2
1	B	206	GLU	2.1
1	B	390	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	204	GLY	2.1
1	B	272	TYR	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 oligosaccharides 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, 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	B-factors(Å ²)	Q<0.9
3	PEP	B	502	10/10	0.71	0.18	137,141,144,144	0
2	MG	B	501	1/1	0.76	0.14	75,75,75,75	0
3	PEP	A	502	10/10	0.82	0.17	126,126,127,127	0
2	MG	B	503	1/1	0.87	0.07	73,73,73,73	0
2	MG	A	501	1/1	0.88	0.09	64,64,64,64	0
2	MG	A	503	1/1	0.91	0.12	78,78,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.