



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:32 PM UTC

PDB ID : 2V27 / pdb_00002v27
Title : Structure of the cold active phenylalanine hydroxylase from Colwellia psychrerythraea 34H
Authors : Leiros, H.-K.S.; Pey, A.L.; Innselset, M.; Moe, E.; Leiros, I.; Steen, I.H.; Martinez, A.
Deposited on : 2007-06-03
Resolution : 1.50 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

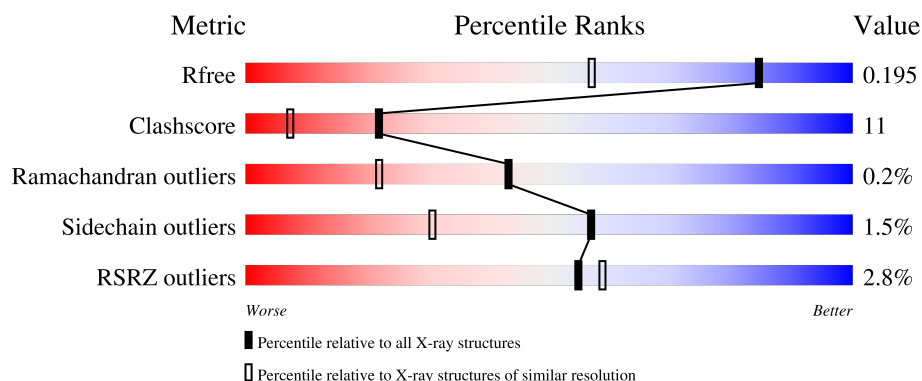
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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 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	275	2% 79% 15% • •
1	B	275	4% 79% 17% • ••

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5346 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 PHENYLALANINE HYDROXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	34	16	0
			2272	1465	369	428	10			
1	B	272	Total	C	N	O	S	36	10	0
			2294	1477	376	430	11			

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

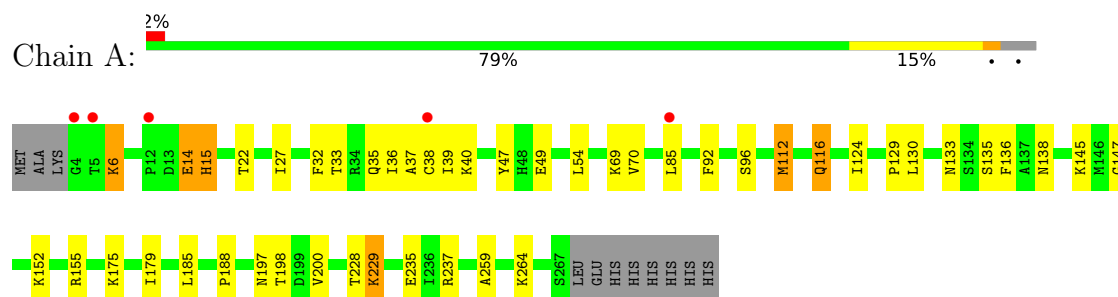
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	409	Total	O	0	0
			409	409		
4	B	359	Total	O	0	0
			359	359		

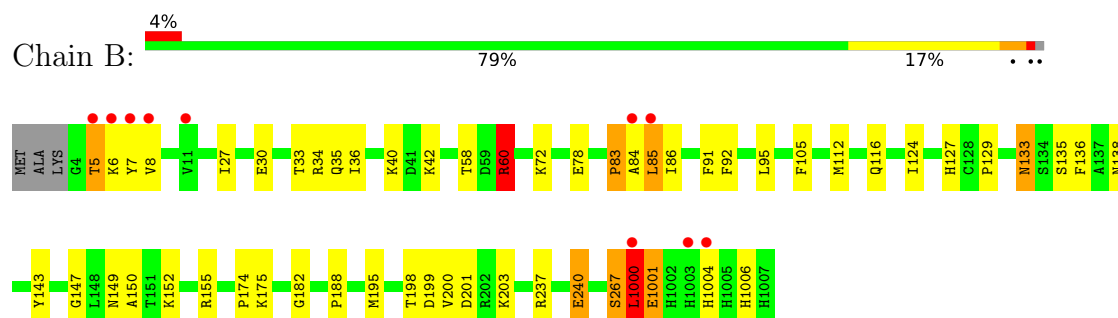
3 Residue-property plots [i](#)

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: PHENYLALANINE HYDROXYLASE



• Molecule 1: PHENYLALANINE HYDROXYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	40.28Å 86.02Å 87.57Å 90.00° 97.01° 90.00°	Depositor
Resolution (Å)	20.00 – 1.50 20.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-1.50) 99.6 (20.00-1.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.162 , 0.195 0.162 , 0.195	Depositor DCC
R_{free} test set	4712 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	11.6	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 64.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5346	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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: SO4, FE

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	2.37	12/2326 (0.5%)	1.52	16/3150 (0.5%)
1	B	2.26	18/2354 (0.8%)	1.33	16/3189 (0.5%)
All	All	2.31	30/4680 (0.6%)	1.43	32/6339 (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	3
1	B	0	2
All	All	0	5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	GLU	CD-OE1	51.96	2.24	1.25
1	B	6	LYS	CD-CE	50.59	3.04	1.52
1	A	6	LYS	CD-CE	49.45	3.00	1.52
1	A	15	HIS	CG-ND1	41.11	1.83	1.38
1	B	84	ALA	C-N	39.41	1.88	1.33
1	B	60	ARG	NE-CZ	37.96	1.74	1.33
1	B	267	SER	C-N	34.82	1.79	1.33
1	A	14	GLU	CA-C	30.12	1.93	1.52
1	B	1000	LEU	CG-CD1	26.83	2.41	1.52
1	A	152	LYS	CE-NZ	-26.63	0.69	1.49
1	A	235	GLU	CD-OE2	25.29	1.73	1.25
1	B	84	ALA	CA-CB	-24.42	1.11	1.53
1	A	85	LEU	CG-CD1	21.95	2.25	1.52
1	B	40	LYS	CE-NZ	-17.45	0.97	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	HIS	ND1-CE1	-17.35	1.15	1.32
1	B	84	ALA	CA-C	15.35	1.70	1.52
1	A	116	GLN	CD-OE1	15.35	1.52	1.23
1	B	1004	HIS	CB-CG	-13.54	1.31	1.50
1	B	152	LYS	CD-CE	13.51	1.93	1.52
1	B	60	ARG	CD-NE	13.06	1.64	1.46
1	A	235	GLU	CD-OE1	-11.85	1.02	1.25
1	B	83	PRO	CG-CD	10.40	1.86	1.50
1	B	175	LYS	CD-CE	-9.49	1.24	1.52
1	A	6	LYS	CE-NZ	7.91	1.73	1.49
1	B	203	LYS	CD-CE	7.88	1.76	1.52
1	B	1000	LEU	CB-CG	-7.43	1.38	1.53
1	A	229	LYS	CE-NZ	-6.78	1.29	1.49
1	B	85	LEU	CB-CG	-6.46	1.40	1.53
1	B	84	ALA	C-O	6.40	1.31	1.23
1	B	8	VAL	CA-CB	5.01	1.59	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	HIS	ND1-CG-CD2	-31.39	74.71	106.10
1	A	116	GLN	OE1-CD-NE2	-29.73	92.87	122.60
1	B	116	GLN	OE1-CD-NE2	-29.24	93.36	122.60
1	A	15	HIS	ND1-CE1-NE2	-28.05	80.35	108.40
1	B	6	LYS	CD-CE-NZ	-23.61	36.34	111.90
1	A	6	LYS	CD-CE-NZ	-22.41	40.20	111.90
1	B	116	GLN	CG-CD-NE2	15.24	139.26	116.40
1	B	152	LYS	CG-CD-CE	13.03	141.28	111.30
1	A	15	HIS	CB-CG-ND1	11.83	140.45	122.70
1	A	85	LEU	CD1-CG-CD2	-11.41	85.69	110.80
1	A	152	LYS	CD-CE-NZ	-11.00	76.71	111.90
1	A	15	HIS	CG-ND1-CE1	-9.95	92.39	109.30
1	B	175	LYS	CG-CD-CE	9.87	134.00	111.30
1	B	1004	HIS	CA-CB-CG	9.46	123.26	113.80
1	A	116	GLN	CG-CD-OE1	9.26	139.32	120.80
1	B	84	ALA	CB-CA-C	8.26	124.10	109.65
1	A	14	GLU	N-CA-C	8.06	127.96	110.80
1	B	240	GLU	OE1-CD-OE2	-7.73	104.34	122.90
1	B	6	LYS	CB-CG-CD	7.64	128.86	111.30
1	A	14	GLU	CB-CA-C	-7.59	95.32	110.42
1	A	116	GLN	CG-CD-NE2	7.47	127.61	116.40
1	B	203	LYS	CG-CD-CE	-7.17	94.82	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	ALA	N-CA-C	-7.16	96.02	108.69
1	B	267	SER	CA-C-N	-6.72	111.16	120.71
1	B	267	SER	C-N-CA	-6.72	111.16	120.71
1	A	39	ILE	N-CA-C	6.57	119.21	112.90
1	B	1000	LEU	CD1-CG-CD2	5.95	123.89	110.80
1	A	229	LYS	CD-CE-NZ	5.94	130.92	111.90
1	B	152	LYS	CD-CE-NZ	5.94	130.90	111.90
1	A	6	LYS	CG-CD-CE	-5.50	98.65	111.30
1	B	240	GLU	CG-CD-OE2	5.41	130.85	118.40
1	A	152	LYS	CB-CG-CD	5.13	123.11	111.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	GLU	Sidechain,Mainchain
1	A	15	HIS	Sidechain
1	B	240	GLU	Sidechain
1	B	60	ARG	Sidechain

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	2272	0	2235	44	0
1	B	2294	0	2231	54	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	409	0	0	23	0
4	B	359	0	0	11	0
All	All	5346	0	4466	95	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 11.

All (95) 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:6:LYS:NZ	1:A:6:LYS:CE	1.73	1.50
1:B:267:SER:C	1:B:1000:LEU:N	1.79	1.39
1:A:155:ARG:HD3	4:A:2253:HOH:O	1.40	1.19
1:A:38:CYS:HA	4:A:2095:HOH:O	1.46	1.15
1:B:5:THR:HG23	1:B:105:PHE:HB2	1.24	1.09
1:B:5:THR:CG2	1:B:105:PHE:HB2	1.87	1.05
1:A:35:GLN:CD	4:A:2087:HOH:O	2.12	0.92
1:A:33[A]:THR:CG2	4:A:2137:HOH:O	2.17	0.90
1:A:38:CYS:CA	4:A:2095:HOH:O	2.10	0.89
1:A:198[B]:THR:HG21	1:B:198:THR:OG1	1.73	0.89
1:A:33[A]:THR:HG23	4:A:2137:HOH:O	1.73	0.88
1:A:198[B]:THR:HG22	1:B:199:ASP:OD2	1.79	0.82
1:A:40:LYS:HB3	4:A:2091:HOH:O	1.80	0.81
1:A:22[A]:THR:HG22	4:A:2046:HOH:O	1.81	0.80
1:B:5:THR:HA	4:B:2002:HOH:O	1.80	0.79
1:A:49:GLU:HG2	4:A:2115:HOH:O	1.81	0.79
1:B:133:ASN:HD22	1:B:136:PHE:H	1.33	0.76
1:B:33[A]:THR:HG23	4:B:2061:HOH:O	1.87	0.75
1:A:69:LYS:HE2	4:A:2152:HOH:O	1.86	0.74
1:B:143:TYR:OH	1:B:1006:HIS:HE1	1.70	0.74
1:B:5:THR:HG21	1:B:105:PHE:HD2	1.54	0.73
1:A:133:ASN:HD22	1:A:136:PHE:H	1.37	0.69
1:A:69:LYS:HE3	4:A:2161:HOH:O	1.93	0.68
1:B:91:PHE:CE2	1:B:95[B]:LEU:HD11	2.30	0.66
1:A:38:CYS:HB2	4:A:2087:HOH:O	1.95	0.66
1:A:27:ILE:HG23	1:A:112:MET:HE1	1.79	0.64
1:B:5:THR:HG21	1:B:105:PHE:CD2	2.32	0.64
1:B:138:ASN:HB3	1:B:237:ARG:HD2	1.80	0.64
1:B:42:LYS:HD3	1:B:195:MET:HG3	1.80	0.63
1:B:267:SER:C	1:B:1000:LEU:CA	2.69	0.63
1:A:35:GLN:OE1	4:A:2087:HOH:O	2.12	0.62
1:B:237:ARG:HD3	4:B:2301:HOH:O	2.01	0.61
1:A:197:ASN:OD1	1:A:200[B]:VAL:HG23	2.01	0.60
1:B:149:ASN:ND2	4:B:2227:HOH:O	2.34	0.60
1:B:30:GLU:HB3	1:B:112[B]:MET:HE1	1.82	0.59
1:A:38:CYS:CB	4:A:2087:HOH:O	2.52	0.58
1:B:27:ILE:HG23	1:B:112[A]:MET:HE1	1.86	0.57
1:B:30:GLU:CB	1:B:112[B]:MET:HE1	2.33	0.57
1:B:5:THR:HG21	1:B:105:PHE:HB2	1.83	0.56
1:B:112[A]:MET:HA	1:B:112[A]:MET:HE2	1.88	0.56
1:A:96:SER:HB2	1:A:145[B]:LYS:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:THR:CG2	1:B:105:PHE:CD2	2.89	0.55
1:B:5:THR:HG22	4:B:2180:HOH:O	2.05	0.55
1:A:112:MET:HA	1:A:112:MET:HE2	1.90	0.54
1:A:35:GLN:NE2	4:A:2087:HOH:O	2.30	0.54
1:A:237[A]:ARG:HD3	4:A:2357:HOH:O	2.09	0.53
1:B:143:TYR:OH	1:B:1006:HIS:CE1	2.58	0.52
1:B:5:THR:CG2	1:B:105:PHE:HD2	2.22	0.52
1:A:37:ALA:O	4:A:2091:HOH:O	2.19	0.50
1:A:32:PHE:CE2	1:A:36[A]:ILE:HG13	2.47	0.50
1:B:5:THR:CG2	1:B:105:PHE:CB	2.77	0.50
1:A:138:ASN:HB3	1:A:237[A]:ARG:HD2	1.93	0.49
1:A:35:GLN:HE22	1:A:188:PRO:CD	2.26	0.49
1:A:198[B]:THR:HG21	1:B:198:THR:HG1	1.71	0.49
1:B:5:THR:HG23	1:B:105:PHE:CB	2.17	0.49
1:B:267:SER:CA	1:B:1000:LEU:N	2.69	0.48
1:B:58:THR:HB	4:B:2061:HOH:O	2.13	0.48
1:A:228[B]:THR:HG21	4:A:2347:HOH:O	2.13	0.47
1:A:38:CYS:CB	4:A:2095:HOH:O	2.54	0.47
1:A:130:LEU:HD12	4:A:2287:HOH:O	2.15	0.47
1:B:124:ILE:O	1:B:129:PRO:HD3	2.15	0.47
1:A:33[A]:THR:HG22	4:A:2137:HOH:O	2.02	0.46
1:A:229:LYS:HE3	4:A:2351:HOH:O	2.16	0.46
1:B:133:ASN:ND2	1:B:136:PHE:H	2.07	0.45
1:B:60:ARG:CZ	1:B:60:ARG:CD	2.94	0.45
1:A:92:PHE:CD2	1:A:147:GLY:HA3	2.50	0.45
1:A:179:ILE:CG2	1:A:185[B]:LEU:HG	2.46	0.45
1:B:7:TYR:HA	4:B:2003:HOH:O	2.17	0.45
1:B:33[A]:THR:CG2	4:B:2061:HOH:O	2.57	0.45
1:B:83:PRO:HB3	4:B:2149:HOH:O	2.15	0.45
1:A:54:LEU:HD23	1:A:70[B]:VAL:CG2	2.47	0.45
1:B:36:ILE:HD13	1:B:36:ILE:HA	1.91	0.44
1:B:92:PHE:CD2	1:B:147:GLY:HA3	2.52	0.44
1:B:5:THR:CG2	1:B:5:THR:O	2.65	0.44
1:B:112[A]:MET:HE2	1:B:112[A]:MET:CA	2.46	0.44
1:B:1001:GLU:O	1:B:1001:GLU:HG2	2.17	0.44
1:B:35:GLN:HE22	1:B:188:PRO:CD	2.31	0.43
1:A:259:ALA:O	1:A:264:LYS:HE3	2.18	0.43
1:B:150:ALA:HB3	1:B:155:ARG:HG3	2.00	0.43
1:B:127:HIS:CE1	1:B:182:GLY:HA3	2.53	0.43
1:A:133:ASN:HD21	1:A:135:SER:HB2	1.84	0.43
1:B:86:ILE:O	4:B:2152:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:PHE:CE2	1:B:1006:HIS:CD2	3.07	0.43
1:A:112:MET:HE3	1:A:112:MET:HB2	1.80	0.42
1:B:133:ASN:HD21	1:B:135:SER:HB2	1.85	0.42
1:B:200[A]:VAL:HG22	1:B:201[A]:ASP:N	2.34	0.42
1:A:124:ILE:O	1:A:129:PRO:HD3	2.19	0.42
1:B:34:ARG:NH2	1:B:112[B]:MET:O	2.53	0.42
1:A:38:CYS:C	4:A:2095:HOH:O	2.54	0.42
1:A:47:TYR:CD1	1:A:185[A]:LEU:HD13	2.55	0.42
1:B:174:PRO:HD3	4:B:2296:HOH:O	2.19	0.42
1:B:72:LYS:HE3	1:B:78:GLU:HB3	2.01	0.41
1:B:91:PHE:CE2	1:B:95[B]:LEU:CD1	3.01	0.41
1:A:35:GLN:HE22	1:A:188:PRO:HD3	1.85	0.40
1:B:195:MET:HA	1:B:195:MET:HE2	2.04	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	278/275 (101%)	273 (98%)	5 (2%)	0	100	100
1	B	280/275 (102%)	272 (97%)	7 (2%)	1 (0%)	30	12
All	All	558/550 (102%)	545 (98%)	12 (2%)	1 (0%)	43	22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	85	LEU

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	249/243 (102%)	246 (99%)	3 (1%)	63	38
1	B	251/243 (103%)	247 (98%)	4 (2%)	55	28
All	All	500/486 (103%)	493 (99%)	7 (1%)	57	33

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	MET
1	A	116	GLN
1	A	175	LYS
1	B	5	THR
1	B	133	ASN
1	B	1000	LEU
1	B	1001	GLU

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

Mol	Chain	Res	Type
1	A	35	GLN
1	A	133	ASN
1	A	250	GLN
1	B	35	GLN
1	B	133	ASN
1	B	257	HIS
1	B	1006	HIS

5.3.3 RNA ⓘ

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 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	SO4	B	3009	-	4,4,4	0.57	0	6,6,6	0.44	0
3	SO4	A	1269	-	4,4,4	0.78	0	6,6,6	0.75	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.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	84:ALA	C	85:LEU	N	1.88
1	B	267:SER	C	1000:LEU	N	1.79

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	264/275 (96%)	-0.50	5 (1%) 66 70	4, 11, 21, 45	36 (13%)
1	B	272/275 (98%)	-0.22	10 (3%) 45 49	5, 13, 28, 59	32 (11%)
All	All	536/550 (97%)	-0.36	15 (2%) 55 59	4, 12, 26, 59	68 (12%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	THR	4.9
1	B	6	LYS	3.6
1	B	1000	LEU	3.5
1	A	85	LEU	3.5
1	A	38	CYS	3.3
1	B	1004	HIS	3.3
1	B	8	VAL	3.2
1	A	5	THR	3.0
1	B	7	TYR	3.0
1	B	84	ALA	2.7
1	B	11	VAL	2.6
1	B	1003	HIS	2.4
1	A	4	GLY	2.3
1	B	85	LEU	2.3
1	A	12	PRO	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 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($\text{\AA}^2$)	Q<0.9
3	SO4	A	1269	5/5	0.91	0.10	16,18,20,25	5
2	FE	A	1268	1/1	0.99	0.02	12,12,12,12	0
3	SO4	B	3009	5/5	0.99	0.06	12,13,13,13	0
2	FE	B	3008	1/1	1.00	0.01	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.