



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2017 – 12:56 PM EDT

PDB ID : 2H5G
Title : Crystal structure of human pyrroline-5-carboxylate synthetase
Authors : Papagrigoriou, E.; Shafqat, N.; Turnbull, A.P.; Berridge, G.; Hozjan, V.; Kavanagh, K.; Gileadi, O.; Smee, C.; Bray, J.; Gorrec, F.; Sundstrom, M.; Arrowsmith, C.; Weigelt, J.; Edwards, A.; Oppermann, U.; Structural Genomics Consortium (SGC)
Deposited on : unknown
Resolution : 2.25 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	:	rb-20030345
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)	:	rb-20030345

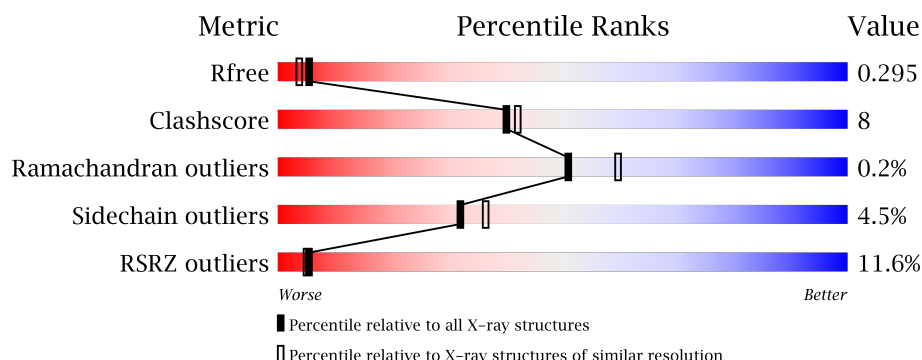
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1062 (2.26-2.26)
Clashscore	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)
RSRZ outliers	101464	1066 (2.26-2.26)

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	463	<div> <div>13%</div> <div> <div></div> <div>72%</div> <div>16%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	463	<div> <div>8%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>•</div> <div>8%</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6695 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 Delta 1-pyrroline-5-carboxylate synthetase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	Se	0	3	0
			3144	1981	553	598	6	6			
1	B	425	Total	C	N	O	S	Se	0	4	0
			3239	2038	566	622	7	6			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	333	MSE	-	INITIATING METHIONINE	UNP P54886
A	334	HIS	-	EXPRESSION TAG	UNP P54886
A	335	HIS	-	EXPRESSION TAG	UNP P54886
A	336	HIS	-	EXPRESSION TAG	UNP P54886
A	337	HIS	-	EXPRESSION TAG	UNP P54886
A	338	HIS	-	EXPRESSION TAG	UNP P54886
A	339	HIS	-	EXPRESSION TAG	UNP P54886
A	340	SER	-	CLONING ARTIFACT	UNP P54886
A	341	SER	-	CLONING ARTIFACT	UNP P54886
A	342	GLY	-	CLONING ARTIFACT	UNP P54886
A	343	VAL	-	CLONING ARTIFACT	UNP P54886
A	344	ASP	-	CLONING ARTIFACT	UNP P54886
A	345	LEU	-	CLONING ARTIFACT	UNP P54886
A	346	GLY	-	CLONING ARTIFACT	UNP P54886
A	347	THR	-	CLONING ARTIFACT	UNP P54886
A	348	GLU	-	CLONING ARTIFACT	UNP P54886
A	349	ASN	-	CLONING ARTIFACT	UNP P54886
A	350	LEU	-	CLONING ARTIFACT	UNP P54886
A	351	TYR	-	CLONING ARTIFACT	UNP P54886
A	352	PHE	-	CLONING ARTIFACT	UNP P54886
A	353	GLN	-	CLONING ARTIFACT	UNP P54886
A	354	SER	-	CLONING ARTIFACT	UNP P54886
A	355	MSE	-	CLONING ARTIFACT	UNP P54886
A	356	VAL	-	CLONING ARTIFACT	UNP P54886
A	357	LYS	-	CLONING ARTIFACT	UNP P54886

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Chain	Residue	Modelled	Actual	Comment	Reference
A	358	PRO	-	CLONING ARTIFACT	UNP P54886
A	359	ALA	-	CLONING ARTIFACT	UNP P54886
A	360	GLY	-	CLONING ARTIFACT	UNP P54886
A	361	PRO	-	CLONING ARTIFACT	UNP P54886
A	369	MSE	MET	MODIFIED RESIDUE	UNP P54886
A	376	MSE	MET	MODIFIED RESIDUE	UNP P54886
A	551	MSE	MET	MODIFIED RESIDUE	UNP P54886
A	577	MSE	MET	MODIFIED RESIDUE	UNP P54886
A	586	MSE	MET	MODIFIED RESIDUE	UNP P54886
A	636	MSE	MET	MODIFIED RESIDUE	UNP P54886
B	333	MSE	-	INITIATING METHIONINE	UNP P54886
B	334	HIS	-	EXPRESSION TAG	UNP P54886
B	335	HIS	-	EXPRESSION TAG	UNP P54886
B	336	HIS	-	EXPRESSION TAG	UNP P54886
B	337	HIS	-	EXPRESSION TAG	UNP P54886
B	338	HIS	-	EXPRESSION TAG	UNP P54886
B	339	HIS	-	EXPRESSION TAG	UNP P54886
B	340	SER	-	CLONING ARTIFACT	UNP P54886
B	341	SER	-	CLONING ARTIFACT	UNP P54886
B	342	GLY	-	CLONING ARTIFACT	UNP P54886
B	343	VAL	-	CLONING ARTIFACT	UNP P54886
B	344	ASP	-	CLONING ARTIFACT	UNP P54886
B	345	LEU	-	CLONING ARTIFACT	UNP P54886
B	346	GLY	-	CLONING ARTIFACT	UNP P54886
B	347	THR	-	CLONING ARTIFACT	UNP P54886
B	348	GLU	-	CLONING ARTIFACT	UNP P54886
B	349	ASN	-	CLONING ARTIFACT	UNP P54886
B	350	LEU	-	CLONING ARTIFACT	UNP P54886
B	351	TYR	-	CLONING ARTIFACT	UNP P54886
B	352	PHE	-	CLONING ARTIFACT	UNP P54886
B	353	GLN	-	CLONING ARTIFACT	UNP P54886
B	354	SER	-	CLONING ARTIFACT	UNP P54886
B	355	MSE	-	CLONING ARTIFACT	UNP P54886
B	356	VAL	-	CLONING ARTIFACT	UNP P54886
B	357	LYS	-	CLONING ARTIFACT	UNP P54886
B	358	PRO	-	CLONING ARTIFACT	UNP P54886
B	359	ALA	-	CLONING ARTIFACT	UNP P54886
B	360	GLY	-	CLONING ARTIFACT	UNP P54886
B	361	PRO	-	CLONING ARTIFACT	UNP P54886
B	369	MSE	MET	MODIFIED RESIDUE	UNP P54886
B	376	MSE	MET	MODIFIED RESIDUE	UNP P54886
B	551	MSE	MET	MODIFIED RESIDUE	UNP P54886

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Chain	Residue	Modelled	Actual	Comment	Reference
B	577	MSE	MET	MODIFIED RESIDUE	UNP P54886
B	586	MSE	MET	MODIFIED RESIDUE	UNP P54886
B	636	MSE	MET	MODIFIED RESIDUE	UNP P54886

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	127	Total	O	0	3
			130	130		
3	B	150	Total	O	0	3
			152	152		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	122.02Å 137.40Å 72.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.56 – 2.25 46.56 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.1 (46.56-2.25) 98.1 (46.56-2.25)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.26 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.230 , 0.272 0.259 , 0.295	Depositor DCC
R_{free} test set	2887 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6695	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.64 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.7277e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.94	14/3196 (0.4%)	0.71	1/4327 (0.0%)
1	B	1.04	15/3299 (0.5%)	0.75	6/4464 (0.1%)
All	All	1.00	29/6495 (0.4%)	0.73	7/8791 (0.1%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	663	SER	CB-OG	20.46	1.68	1.42
1	B	653	TYR	CE2-CZ	19.32	1.63	1.38
1	B	653	TYR	CG-CD2	16.46	1.60	1.39
1	B	540	GLU	CD-OE1	16.13	1.43	1.25
1	A	542	VAL	C-O	13.78	1.49	1.23
1	B	413	GLU	CD-OE1	12.94	1.39	1.25
1	B	653	TYR	C-O	12.13	1.46	1.23
1	B	580	SER	CB-OG	11.96	1.57	1.42
1	B	653	TYR	C-N	11.35	1.60	1.34
1	B	653	TYR	CG-CD1	11.02	1.53	1.39
1	A	623	ASP	CG-OD2	10.22	1.48	1.25
1	B	413	GLU	CD-OE2	9.11	1.35	1.25
1	A	674	CYS	CB-SG	8.60	1.96	1.82
1	A	641	GLN	CD-OE1	8.50	1.42	1.24
1	A	652	SER	CB-OG	8.30	1.53	1.42
1	A	641	GLN	CB-CG	8.22	1.74	1.52
1	A	623	ASP	CG-OD1	8.06	1.43	1.25
1	B	540	GLU	CD-OE2	7.72	1.34	1.25
1	A	641	GLN	CD-NE2	7.51	1.51	1.32
1	A	675	ILE	CB-CG1	6.90	1.73	1.54
1	A	646	ALA	C-N	6.88	1.45	1.33
1	B	653	TYR	CE1-CZ	6.72	1.47	1.38
1	B	641	GLN	CB-CG	6.40	1.69	1.52
1	A	641	GLN	CG-CD	6.09	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	646	ALA	C-N	5.97	1.43	1.33
1	B	417	ARG	CZ-NH1	5.33	1.40	1.33
1	A	612	CYS	CB-SG	5.20	1.91	1.82
1	B	654	LEU	CB-CG	5.20	1.67	1.52
1	A	638	ARG	C-O	5.04	1.32	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	653	TYR	CB-CG-CD2	-9.39	115.37	121.00
1	B	653	TYR	CD1-CG-CD2	6.64	125.20	117.90
1	A	641	GLN	CG-CD-OE1	-5.76	110.08	121.60
1	B	653	TYR	CG-CD2-CE2	-5.75	116.70	121.30
1	B	653	TYR	CG-CD1-CE1	-5.52	116.88	121.30
1	B	638	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	B	653	TYR	O-C-N	5.24	131.09	122.70

There are no chirality outliers.

There are no planarity outliers.

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	3144	0	3084	61	0
1	B	3239	0	3202	44	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
3	A	130	0	0	4	0
3	B	152	0	0	1	0
All	All	6695	0	6286	105	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 8.

All (105) 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:641:GLN:CB	1:A:641:GLN:CG	1.74	1.61
1:A:663:SER:CB	1:A:663:SER:OG	1.68	1.41
1:A:577:MSE:HE2	1:A:747[B]:HIS:CD2	1.71	1.26
1:A:577:MSE:HE1	1:A:747[A]:HIS:ND1	1.62	1.14
1:A:502:LEU:HD23	1:A:534:GLN:HB2	1.33	1.05
1:A:577:MSE:CE	1:A:747[B]:HIS:CD2	2.40	1.04
1:B:543:GLU:O	1:B:543:GLU:HG3	1.59	1.01
1:B:577:MSE:HE1	1:B:747:HIS:CD2	1.97	1.00
1:A:755:GLU:OE1	3:A:290:HOH:O	1.95	0.83
1:A:502:LEU:CD2	1:A:534:GLN:HB2	2.09	0.81
1:B:543:GLU:O	1:B:543:GLU:CG	2.29	0.80
1:B:551:MSE:HE2	1:B:552:ILE:HD11	1.62	0.80
1:B:369:MSE:HE2	1:B:534:GLN:HE22	1.48	0.79
1:B:577:MSE:HE1	1:B:747:HIS:HD2	1.46	0.79
1:A:577:MSE:HE2	1:A:747[B]:HIS:HD2	1.43	0.79
1:A:551:MSE:HE2	1:A:552:ILE:HD11	1.64	0.78
1:A:621:HIS:HD2	1:A:623:ASP:H	1.29	0.78
1:A:640:GLU:HG3	3:A:99:HOH:O	1.84	0.75
1:A:606:CYS:SG	1:A:640:GLU:HG2	2.26	0.75
1:B:620:ILE:HD13	1:B:630:PHE:HE1	1.55	0.72
1:B:502:LEU:HD23	1:B:534:GLN:HB2	1.72	0.71
1:A:746:ILE:O	1:A:747[B]:HIS:CG	2.44	0.70
1:B:369:MSE:HE3	1:B:531:GLU:HG2	1.74	0.70
1:B:369:MSE:HE2	1:B:534:GLN:NE2	2.06	0.69
1:A:624:LEU:O	1:A:627:THR:HG22	1.93	0.69
1:B:597:VAL:HG11	1:B:633:ILE:HD11	1.75	0.68
1:B:504:LYS:HE2	1:B:538:THR:HA	1.74	0.67
1:A:621:HIS:CD2	1:A:623:ASP:H	2.11	0.67
1:A:670:ASP:HB2	3:A:74:HOH:O	1.94	0.67
1:B:661:VAL:HG13	1:B:662:LYS:H	1.60	0.67
1:A:747[A]:HIS:HE1	1:A:756:GLY:O	1.78	0.65
1:A:641:GLN:CA	1:A:641:GLN:CG	2.70	0.64
1:B:620:ILE:HD12	1:B:675:ILE:HG23	1.80	0.63
1:A:689[A]:HIS:HE1	1:A:714:VAL:HA	1.64	0.63
1:B:698:VAL:HG22	1:B:720:PHE:HB2	1.81	0.63
1:A:698:VAL:HG22	1:A:720:PHE:HB2	1.81	0.62
1:B:665:ARG:NH1	1:B:690:LYS:O	2.33	0.61
1:B:551:MSE:HB3	1:B:552:ILE:HD12	1.83	0.60
1:A:487:LEU:HB3	1:A:488:PRO:HD3	1.85	0.59
1:B:577:MSE:CE	1:B:747:HIS:HD2	2.16	0.59
1:B:577:MSE:CE	1:B:747:HIS:CD2	2.81	0.58
1:A:627:THR:HG23	1:A:630:PHE:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:ASP:O	1:B:749:ARG:NH2	2.37	0.56
1:A:597:VAL:HG11	1:A:633:ILE:HD11	1.88	0.56
1:A:641:GLN:CD	1:A:641:GLN:CB	2.71	0.55
1:B:362:THR:HG23	1:B:365:GLN:H	1.72	0.55
1:A:590:SER:HB3	1:A:621:HIS:CD2	2.42	0.54
1:B:621:HIS:HD2	1:B:623:ASP:H	1.57	0.53
1:B:646:ALA:O	1:B:661:VAL:HB	2.09	0.53
1:A:663:SER:CB	1:A:663:SER:HG	2.12	0.52
1:A:715:ASP:O	1:A:749:ARG:NH2	2.42	0.52
1:A:577:MSE:HE2	1:A:747[B]:HIS:NE2	2.19	0.52
1:A:681:VAL:HG21	1:A:706:THR:HG23	1.92	0.51
1:A:647:GLY:O	1:A:650:PHE:HB3	2.10	0.51
1:A:644:ILE:HG13	1:A:644:ILE:O	2.10	0.51
1:B:661:VAL:HG13	1:B:662:LYS:N	2.27	0.49
1:A:551:MSE:HE2	1:A:552:ILE:CD1	2.40	0.48
1:B:481:GLU:HG2	1:B:563:LEU:HD22	1.94	0.48
1:A:747[A]:HIS:CE1	1:A:756:GLY:O	2.63	0.48
1:B:620:ILE:HD13	1:B:630:PHE:CE1	2.41	0.47
1:B:661:VAL:O	1:B:662:LYS:CB	2.62	0.47
1:A:744:SER:O	1:A:749:ARG:HD2	2.14	0.47
1:A:678:VAL:HB	1:A:683:ASP:HB3	1.96	0.47
1:B:631:ASP:O	1:B:634:ILE:HG13	2.14	0.47
1:A:581:GLU:HG3	1:A:693:SER:CB	2.45	0.47
1:B:450:SER:HB3	1:B:754:LEU:HD11	1.97	0.47
1:B:579:HIS:HD2	1:B:741:ILE:O	1.98	0.47
1:A:579:HIS:HD2	1:A:741:ILE:O	1.98	0.46
1:A:767:LYS:HE3	1:A:767:LYS:HB3	1.58	0.46
1:A:502:LEU:CD2	1:A:534:GLN:CB	2.90	0.46
1:A:621:HIS:HD2	1:A:623:ASP:N	2.07	0.46
1:A:631:ASP:O	1:A:634:ILE:HG13	2.16	0.46
1:A:585:HIS:CD2	1:A:617:THR:HB	2.52	0.45
1:B:377:LEU:HD21	1:B:495:ILE:HA	1.98	0.45
1:B:579:HIS:CE1	1:B:612[B]:CYS:SG	3.10	0.45
1:B:755:GLU:HG3	3:B:209:HOH:O	2.17	0.44
1:B:638:ARG:HG3	1:B:639:VAL:N	2.33	0.44
1:A:668:TYR:HB3	1:A:670:ASP:OD1	2.18	0.44
1:A:602:ARG:HB2	1:A:636:MSE:SE	2.67	0.43
1:A:627:THR:CG2	1:A:630:PHE:H	2.31	0.43
1:B:581:GLU:HG3	1:B:693:SER:HB2	2.01	0.43
1:A:789:ILE:HA	1:A:790:PRO:HD2	1.73	0.43
1:B:581:GLU:HG3	1:B:693:SER:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:GLU:HG3	1:A:693:SER:HB3	2.00	0.42
1:A:574:ILE:H	1:A:574:ILE:HG12	1.65	0.42
1:B:597:VAL:CG1	1:B:633:ILE:HD11	2.47	0.42
1:A:622:ARG:HA	1:A:625:LEU:HD23	2.02	0.42
1:B:542:VAL:HG12	1:B:542:VAL:O	2.20	0.42
1:A:481:GLU:HG2	1:A:563:LEU:HD22	2.02	0.42
1:B:449:ASP:O	1:B:453:ARG:HB2	2.20	0.42
1:A:510:ALA:O	1:A:514:ARG:HB2	2.20	0.42
1:B:385:ARG:HD2	1:B:495:ILE:O	2.20	0.41
1:B:744:SER:O	1:B:749:ARG:HD2	2.20	0.41
1:A:687:HIS:HE1	3:A:175:HOH:O	2.02	0.41
1:B:585:HIS:CD2	1:B:617:THR:HB	2.56	0.41
1:B:678:VAL:HB	1:B:683:ASP:HB3	2.01	0.41
1:A:618:LEU:HD23	1:A:675:ILE:HG12	2.02	0.41
1:A:663:SER:CA	1:A:663:SER:OG	2.56	0.41
1:A:625:LEU:HD21	1:A:677:VAL:HG22	2.02	0.41
1:A:593:SER:O	1:A:597:VAL:HG23	2.21	0.41
1:A:392:LEU:HD13	1:A:440:LEU:HD21	2.03	0.40
1:A:606:CYS:SG	1:A:640:GLU:CG	3.04	0.40
1:A:589:ASP:HB3	1:A:701:THR:HB	2.03	0.40
1:A:449:ASP:O	1:A:453:ARG:HB2	2.21	0.40
1:B:625:LEU:HD21	1:B:677:VAL:HG22	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	414/463 (89%)	393 (95%)	21 (5%)	0	100	100
1	B	423/463 (91%)	406 (96%)	15 (4%)	2 (0%)	32	33
All	All	837/926 (90%)	799 (96%)	36 (4%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	662	LYS
1	B	542	VAL

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	328/389 (84%)	312 (95%)	16 (5%)	29	32
1	B	346/389 (89%)	331 (96%)	15 (4%)	33	39
All	All	674/778 (87%)	643 (95%)	31 (5%)	32	35

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	362	THR
1	A	380	LEU
1	A	392	LEU
1	A	481	GLU
1	A	486	CYS
1	A	554	LEU
1	A	574	ILE
1	A	605	LYS
1	A	652	SER
1	A	683	ASP
1	A	689[A]	HIS
1	A	689[B]	HIS
1	A	694	SER
1	A	711	LEU
1	A	754	LEU
1	A	767	LYS
1	B	423	LEU
1	B	481	GLU
1	B	486	CYS
1	B	526	ILE
1	B	554	LEU

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Mol	Chain	Res	Type
1	B	605	LYS
1	B	627	THR
1	B	655	THR
1	B	681	VAL
1	B	694	SER
1	B	711	LEU
1	B	754	LEU
1	B	755	GLU
1	B	789	ILE
1	B	794	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	579	HIS
1	B	366	GLN
1	B	399	GLN
1	B	534	GLN
1	B	579	HIS
1	B	621	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 ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	301	-	4,4,4	0.18	0	6,6,6	0.37	0
2	SO4	A	302	-	4,4,4	0.55	0	6,6,6	0.33	0
2	SO4	A	305	-	4,4,4	0.19	0	6,6,6	0.19	0
2	SO4	B	303	-	4,4,4	0.21	0	6,6,6	0.44	0
2	SO4	B	304	-	4,4,4	0.34	0	6,6,6	0.41	0
2	SO4	B	306	-	4,4,4	0.18	0	6,6,6	0.39	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
2	SO4	A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	A	302	-	-	0/0/0/0	0/0/0/0
2	SO4	A	305	-	-	0/0/0/0	0/0/0/0
2	SO4	B	303	-	-	0/0/0/0	0/0/0/0
2	SO4	B	304	-	-	0/0/0/0	0/0/0/0
2	SO4	B	306	-	-	0/0/0/0	0/0/0/0

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 ⓘ

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	411/463 (88%)	0.88	60 (14%) 3 3	30, 59, 83, 100	0
1	B	419/463 (90%)	0.69	36 (8%) 11 12	31, 58, 83, 103	0
All	All	830/926 (89%)	0.78	96 (11%) 5 5	30, 58, 83, 103	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	655	THR	9.2
1	A	626	ARG	7.6
1	B	549	ASP	6.7
1	A	650	PHE	6.1
1	A	625	LEU	6.0
1	A	747[A]	HIS	5.7
1	B	654	LEU	5.4
1	A	651	ALA	5.0
1	A	639	VAL	5.0
1	A	572	LYS	4.6
1	B	661	VAL	4.6
1	B	794	THR	4.6
1	A	652	SER	4.6
1	A	630	PHE	4.6
1	B	656	PHE	4.5
1	B	793	ASN	4.5
1	A	580	SER	4.2
1	B	548	LEU	4.2
1	B	572	LYS	4.2
1	A	791	GLN	4.1
1	A	627	THR	4.1
1	A	644	ILE	4.0
1	A	631	ASP	3.9
1	B	570	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	793	ASN	3.9
1	A	790	PRO	3.7
1	A	573	GLY	3.6
1	A	539	ARG	3.5
1	A	792	ARG	3.4
1	A	648	PRO	3.4
1	A	675	ILE	3.4
1	B	405	LEU	3.3
1	A	677	VAL	3.3
1	B	573	GLY	3.2
1	B	759	THR	3.2
1	B	562	GLN	3.1
1	A	511	HIS	3.1
1	A	663	SER	3.1
1	B	792	ARG	3.0
1	A	647	GLY	3.0
1	A	634	ILE	3.0
1	A	646	ALA	3.0
1	B	650	PHE	3.0
1	B	542	VAL	3.0
1	A	571	ALA	3.0
1	B	541	GLU	2.9
1	A	633	ILE	2.9
1	A	665	ARG	2.9
1	A	691	TYR	2.9
1	B	537	ASN	2.8
1	A	673	LEU	2.8
1	B	718	CYS	2.8
1	B	791	GLN	2.7
1	A	581	GLU	2.7
1	B	571	ALA	2.7
1	B	365	GLN	2.6
1	A	486	CYS	2.6
1	B	580	SER	2.6
1	A	538	THR	2.6
1	A	727	PHE	2.6
1	B	612[A]	CYS	2.5
1	A	629	LEU	2.5
1	A	789	ILE	2.5
1	B	543	GLU	2.4
1	A	788	PRO	2.4
1	B	790	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	730	GLY	2.4
1	A	620	ILE	2.4
1	A	664	LEU	2.4
1	B	748	ALA	2.4
1	B	493	LEU	2.3
1	A	759	THR	2.3
1	B	429	SER	2.3
1	A	542	VAL	2.3
1	B	630	PHE	2.3
1	A	641	GLN	2.3
1	A	493	LEU	2.3
1	B	363	VAL	2.2
1	A	638	ARG	2.2
1	A	668	TYR	2.2
1	B	717	ALA	2.2
1	A	559	GLY	2.1
1	A	649	LYS	2.1
1	B	568	GLN	2.1
1	B	731	TYR	2.1
1	A	560	SER	2.1
1	A	632	GLN	2.1
1	A	635	ASP	2.1
1	A	449	ASP	2.0
1	A	730	GLY	2.0
1	A	496	ALA	2.0
1	A	410	ASP	2.0
1	A	718	CYS	2.0
1	A	624	LEU	2.0
1	A	492	ALA	2.0
1	A	662	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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	SO4	B	304	5/5	0.93	0.13	-1.36	52,59,78,79	0
2	SO4	A	301	5/5	0.97	0.10	-1.54	52,54,57,60	0
2	SO4	B	303	5/5	0.98	0.08	-2.74	50,51,57,59	0
2	SO4	A	302	5/5	0.90	0.20	-	52,58,79,85	0
2	SO4	A	305	5/5	0.91	0.21	-	94,95,99,100	0
2	SO4	B	306	5/5	0.79	0.46	-	75,83,90,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.