



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:34 PM GMT

PDB ID : 2H5G  
Title : Crystal structure of human pyrroline-5-carboxylatesynthetase  
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 : 2006-05-26  
Resolution : 2.25 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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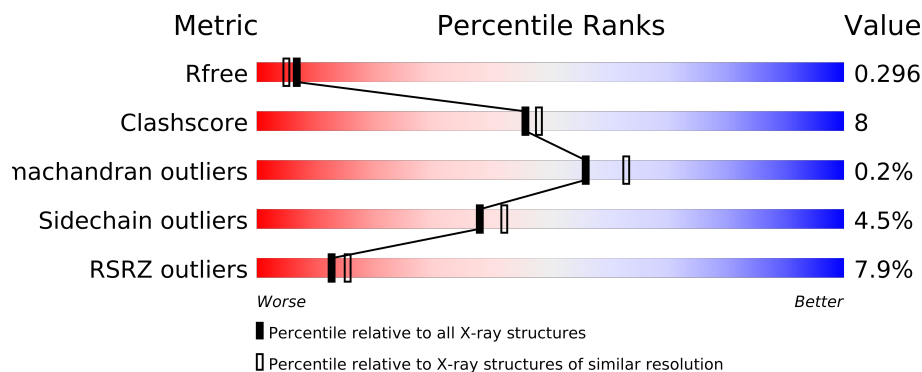
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1108 (2.28-2.24)
Clashscore	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (2.28-2.24)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	463	
1	B	463	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	B	306	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6695 atoms, of which 0 are hydrogen and 0 are deuterium.

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-carboxylatesynthetase.

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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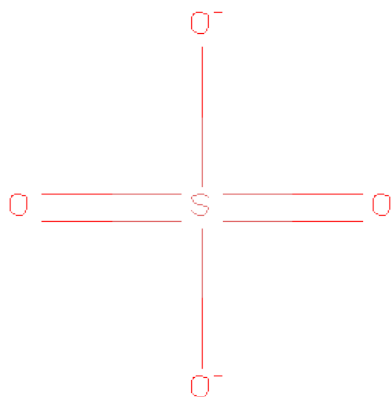
Chain	Residue	Modelled	Actual	Comment	Reference
A	358	PRO	-	CLONING ARTIFACT	UNP P54886
A	359	ALA	-	CLONING ARTIFACT	UNP P54886
A	360	GLY	-	CLONING ARTIFACT	UNP P54886
A	361	PRO	-	CLONING ARTIFACT	UNP P54886
A	369	MSE	MET	MODIFIED RESIDUE	UNP P54886
A	376	MSE	MET	MODIFIED RESIDUE	UNP P54886
A	551	MSE	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: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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	B	1	Total	O	S	0	0
			5	4	1		
2	B	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		

- Molecule 3 is water.

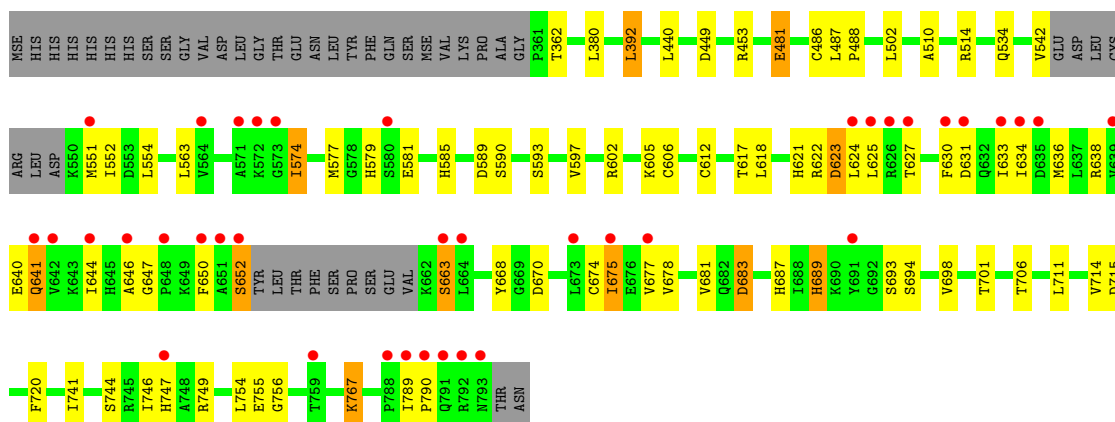
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	127	Total	O	0	3
			130	130		
3	B	150	Total	O	0	3
			152	152		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

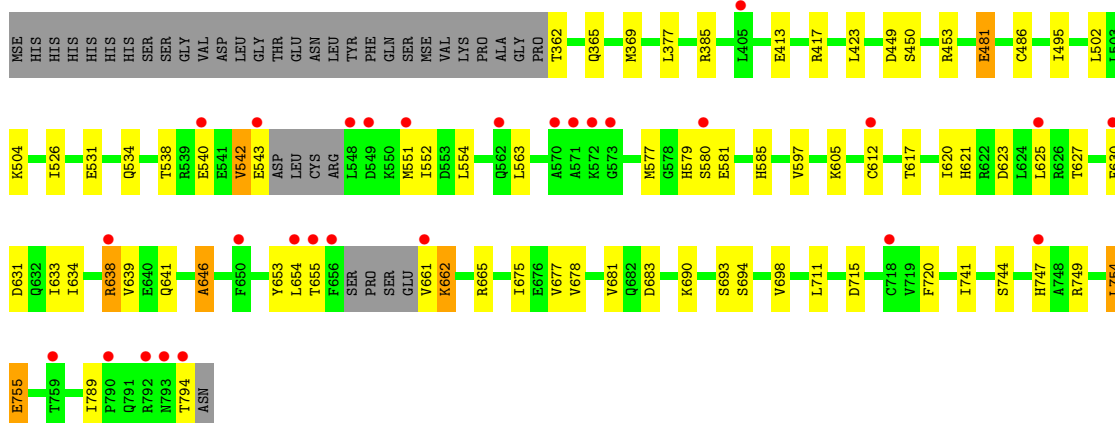
- Molecule 1: Delta 1-pyrroline-5-carboxylatesynthetase

Chain A: 



- Molecule 1: Delta 1-pyrroline-5-carboxylatesynthetase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.26 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.230 , 0.272 0.262 , 0.296	Depositor DCC
$R_{free}$ test set	2887 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.8	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	5 of 57127 reflections (0.009%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6695	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (105) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:577:MSE:HE1	1:B:747:HIS:HD2	1.46	0.79
1:B:369:MSE:HE2	1:B:534:GLN:HE22	1.48	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:B:661:VAL:HG13	1:B:662:LYS:H	1.60	0.67
1:A:670:ASP:HB2	3:A:74:HOH:O	1.94	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
1:B:715:ASP:O	1:B:749:ARG:NH2	2.37	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:631:ASP:O	1:B:634:ILE:HG13	2.14	0.47
1:A:678:VAL:HB	1:A:683:ASP:HB3	1.96	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:HB3	1:A:767:LYS:HE3	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:627:THR:CG2	1:A:630:PHE:H	2.31	0.43
1:A:602:ARG:HB2	1:A:636:MSE:SE	2.67	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:449:ASP:O	1:B:453:ARG:HB2	2.20	0.42
1:A:481:GLU:HG2	1:A:563:LEU:HD22	2.02	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: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:618:LEU:HD23	1:A:675:ILE:HG12	2.02	0.41
1:A:593:SER:O	1:A:597:VAL:HG23	2.21	0.41
1:A:606:CYS:SG	1:A:640:GLU:CG	3.04	0.40
1:A:392:LEU:HD13	1:A:440:LEU:HD21	2.03	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

### 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	414/463 (89%)	393 (95%)	21 (5%)	0	100	100
1	B	423/463 (91%)	406 (96%)	15 (4%)	2 (0%)	38	38
All	All	837/926 (90%)	799 (96%)	36 (4%)	2 (0%)	56	63

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%)	35	38
1	B	346/389 (89%)	331 (96%)	15 (4%)	40	45
All	All	674/778 (87%)	643 (95%)	31 (5%)	38	41

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
1	B	605	LYS
1	B	627	THR
1	B	655	THR

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Mol	Chain	Res	Type
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 chains 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	0.16	0	6,6,6	0.32	0
2	SO4	A	302	-	4,4,4	0.58	0	6,6,6	0.60	0
2	SO4	A	305	-	4,4,4	0.13	0	6,6,6	0.21	0
2	SO4	B	303	-	4,4,4	0.17	0	6,6,6	0.33	0
2	SO4	B	304	-	4,4,4	0.34	0	6,6,6	0.32	0
2	SO4	B	306	-	4,4,4	0.21	0	6,6,6	0.37	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.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	417/463 (90%)	0.63	38 (9%) 9 11	30, 59, 83, 100	0
1	B	425/463 (91%)	0.47	28 (6%) 18 21	31, 58, 82, 103	0
All	All	842/926 (90%)	0.55	66 (7%) 13 16	30, 58, 83, 103	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	655	THR	7.8
1	A	626	ARG	7.2
1	A	650	PHE	6.4
1	B	654	LEU	5.4
1	A	639	VAL	5.1
1	A	652	SER	5.1
1	B	549	ASP	4.8
1	B	794	THR	4.6
1	A	747[A]	HIS	4.6
1	A	630	PHE	4.6
1	A	573	GLY	4.6
1	A	651	ALA	4.3
1	A	625	LEU	4.3
1	B	572	LYS	4.2
1	A	644	ILE	4.2
1	B	656	PHE	4.2
1	A	572	LYS	4.1
1	A	571	ALA	3.9
1	B	661	VAL	3.9
1	A	631	ASP	3.8
1	A	677	VAL	3.6
1	A	664	LEU	3.6
1	B	548	LEU	3.5
1	B	573	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	570	ALA	3.4
1	A	675	ILE	3.4
1	A	646	ALA	3.3
1	A	790	PRO	3.2
1	A	580	SER	3.2
1	B	571	ALA	3.1
1	A	691	TYR	3.0
1	A	791	GLN	3.0
1	B	650	PHE	2.9
1	A	793	ASN	2.9
1	B	405	LEU	2.9
1	A	627	THR	2.9
1	A	564	VAL	2.9
1	A	634	ILE	2.8
1	A	789	ILE	2.8
1	A	673	LEU	2.8
1	A	648	PRO	2.7
1	B	759	THR	2.7
1	B	562	GLN	2.6
1	A	642	VAL	2.5
1	B	790	PRO	2.5
1	A	663	SER	2.5
1	B	793	ASN	2.5
1	A	792	ARG	2.4
1	A	635	ASP	2.3
1	B	792	ARG	2.3
1	B	747	HIS	2.3
1	A	641	GLN	2.3
1	B	625	LEU	2.2
1	A	551	MSE	2.2
1	B	718	CYS	2.2
1	B	551	MSE	2.2
1	B	612[A]	CYS	2.2
1	B	638	ARG	2.2
1	B	543	GLU	2.2
1	A	633	ILE	2.1
1	B	630	PHE	2.1
1	A	759	THR	2.1
1	B	580	SER	2.1
1	A	624	LEU	2.0
1	B	540	GLU	2.0
1	A	788	PRO	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 ⓘ

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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	B	306	5/5	0.36	13.83	75,83,90,91	0
2	SO4	A	302	5/5	0.20	1.63	52,58,79,85	0
2	SO4	A	305	5/5	0.18	0.49	94,95,99,100	0
2	SO4	B	304	5/5	0.12	-1.27	52,59,78,79	0
2	SO4	A	301	5/5	0.08	-1.66	52,54,57,60	0
2	SO4	B	303	5/5	0.06	-2.68	50,51,57,59	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.