



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:11 AM UTC

PDB ID : 2H5G / pdb_00002h5g
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 : 2006-05-26
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

<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

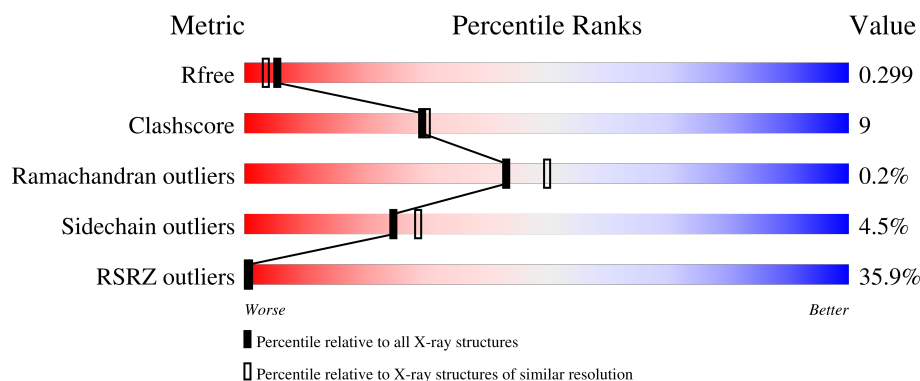
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (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 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	463	35% 71% 15% • 10%
1	B	463	29% 75% 15% • 8%

2 Entry composition

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 (CCD ID: 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		

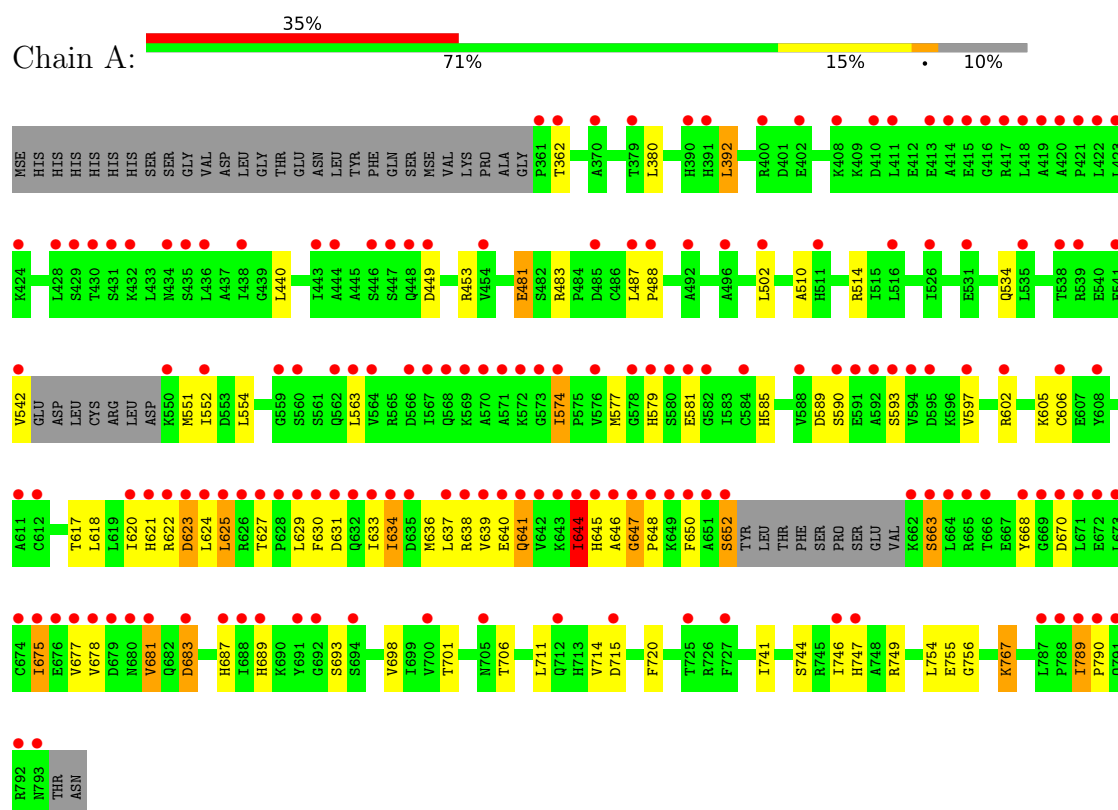
- Molecule 3 is water.

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

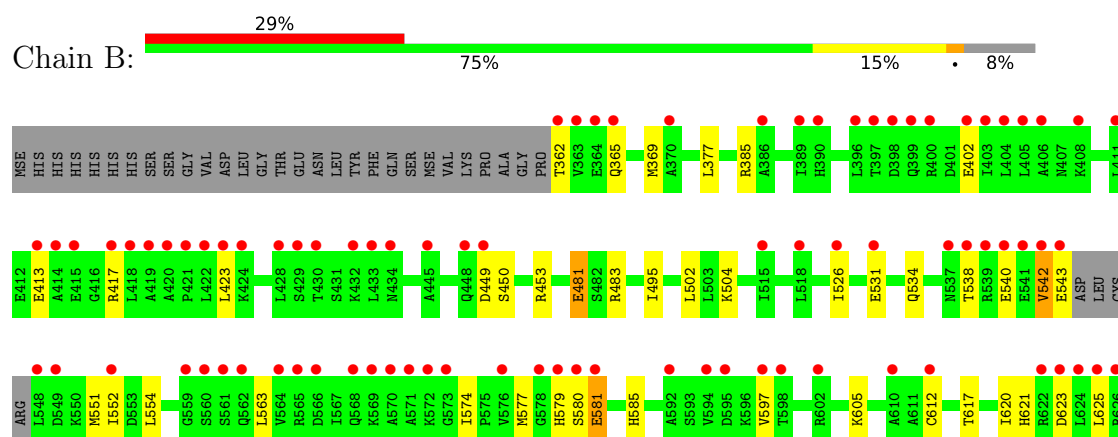
3 Residue-property plots

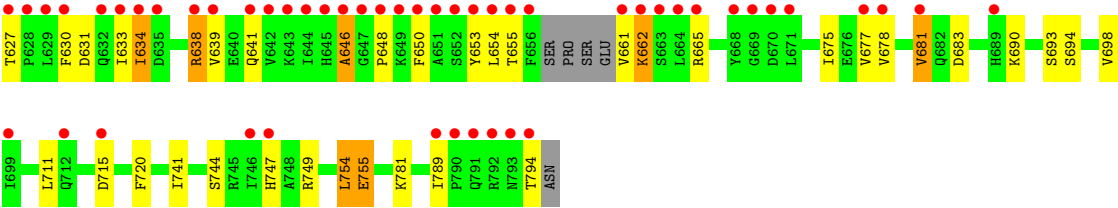
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Delta 1-pyrroline-5-carboxylate synthetase



- Molecule 1: Delta 1-pyrroline-5-carboxylate synthetase





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 0.262 , 0.299	Depositor DCC
R_{free} test set	2890 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.9	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.*

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

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	1.10	24/3196 (0.8%)	0.99	8/4327 (0.2%)
1	B	1.07	17/3299 (0.5%)	0.98	9/4464 (0.2%)
All	All	1.08	41/6495 (0.6%)	0.98	17/8791 (0.2%)

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	653	TYR	C-N	17.16	1.60	1.33
1	B	653	TYR	C-O	16.77	1.46	1.24
1	A	663	SER	CB-OG	13.35	1.68	1.42
1	A	542	VAL	C-O	12.99	1.49	1.23
1	A	623	ASP	CG-OD2	12.37	1.48	1.25
1	B	653	TYR	CE2-CZ	10.59	1.63	1.38
1	B	653	TYR	CG-CD2	10.09	1.60	1.39
1	A	641	GLN	CD-OE1	10.05	1.42	1.23
1	A	675	ILE	CB-CG1	9.97	1.73	1.53
1	A	623	ASP	CG-OD1	9.76	1.43	1.25
1	B	540	GLU	CD-OE1	9.49	1.43	1.25
1	A	641	GLN	CD-NE2	8.75	1.51	1.33
1	A	646	ALA	C-N	8.02	1.45	1.33
1	B	580	SER	CB-OG	7.82	1.57	1.42
1	B	413	GLU	CD-OE1	7.65	1.39	1.25
1	A	646	ALA	C-O	7.46	1.32	1.24
1	A	648	PRO	C-N	7.44	1.43	1.33
1	A	641	GLN	CB-CG	7.43	1.74	1.52
1	B	654	LEU	CB-CG	7.09	1.67	1.53
1	B	646	ALA	C-N	6.91	1.43	1.33
1	A	645	HIS	N-CA	6.91	1.54	1.46
1	A	638	ARG	C-O	6.87	1.32	1.24
1	B	653	TYR	CG-CD1	6.73	1.53	1.39
1	A	620	ILE	C-N	6.49	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	648	PRO	C-N	6.45	1.42	1.33
1	B	650	PHE	C-O	6.40	1.32	1.24
1	A	638	ARG	C-N	6.18	1.41	1.33
1	A	625	LEU	C-O	6.18	1.31	1.24
1	A	641	GLN	C-N	6.16	1.42	1.33
1	A	637	LEU	C-O	5.89	1.31	1.24
1	B	641	GLN	CB-CG	5.79	1.69	1.52
1	A	644	ILE	CA-C	5.78	1.59	1.52
1	B	634	ILE	CA-CB	5.68	1.61	1.54
1	A	634	ILE	CA-CB	5.45	1.61	1.54
1	A	652	SER	CB-OG	5.45	1.53	1.42
1	B	413	GLU	CD-OE2	5.43	1.35	1.25
1	A	641	GLN	CG-CD	5.21	1.65	1.52
1	B	638	ARG	NE-CZ	5.17	1.38	1.33
1	B	417	ARG	CZ-NH1	5.17	1.40	1.32
1	A	637	LEU	N-CA	5.07	1.52	1.46
1	A	637	LEU	C-N	5.04	1.41	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	641	GLN	OE1-CD-NE2	10.40	133.00	122.60
1	B	653	TYR	O-C-N	6.81	131.09	122.37
1	B	483	ARG	CA-C-N	-6.73	112.70	119.56
1	B	483	ARG	C-N-CA	-6.73	112.70	119.56
1	B	681	VAL	CB-CA-C	-6.62	103.37	112.04
1	B	581	GLU	N-CA-C	6.38	118.84	108.76
1	B	574	ILE	N-CA-C	6.26	114.01	108.63
1	B	653	TYR	CA-C-N	-6.19	112.70	122.73
1	B	653	TYR	C-N-CA	-6.19	112.70	122.73
1	A	483	ARG	CA-C-N	-6.16	113.28	119.56
1	A	483	ARG	C-N-CA	-6.16	113.28	119.56
1	A	641	GLN	CG-CD-OE1	-5.36	110.08	120.80
1	A	647	GLY	CA-C-N	5.32	126.50	119.84
1	A	647	GLY	C-N-CA	5.32	126.50	119.84
1	A	789	ILE	CA-C-N	5.25	126.40	119.84
1	A	789	ILE	C-N-CA	5.25	126.40	119.84
1	B	654	LEU	N-CA-C	5.00	117.60	109.24

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	63	0
1	B	3239	0	3202	46	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	2	0
All	All	6695	0	6286	109	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 9.

All (109) 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:HG3	1:B:543:GLU:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG	1:A:641:GLN:CA	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:641:GLN:CB	1:A:641:GLN:CD	2.71	0.59
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
1:A:597:VAL:HG11	1:A:633:ILE:HD11	1.88	0.56
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: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:663:SER:CB	1:A:663:SER:HG	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:369:MSE:HG2	1:B:531:GLU:CD	2.42	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
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:781:LYS:NZ	3:B:102:HOH:O	2.47	0.41
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:625:LEU:HD21	1:A:677:VAL:HG22	2.02	0.41
1:A:629:LEU:C	1:A:629:LEU:HD23	2.46	0.41
1:A:663:SER:OG	1:A:663:SER:CA	2.56	0.41
1:A:593:SER:O	1:A:597:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:622:ARG:C	1:A:624:LEU:H	2.29	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%)	24	24
All	All	837/926 (90%)	799 (96%)	36 (4%)	2 (0%)	43	50

All (2) Ramachandran outliers are listed below:

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

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	328/389 (84%)	313 (95%)	15 (5%)	24	28
1	B	346/389 (89%)	331 (96%)	15 (4%)	26	31
All	All	674/778 (87%)	644 (96%)	30 (4%)	24	29

All (30) 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	554	LEU
1	A	574	ILE
1	A	605	LYS
1	A	639	VAL
1	A	644	ILE
1	A	652	SER
1	A	681	VAL
1	A	683	ASP
1	A	711	LEU
1	A	754	LEU
1	A	767	LYS
1	B	402	GLU
1	B	423	LEU
1	B	481	GLU
1	B	526	ILE
1	B	554	LEU
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

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	687	HIS
1	B	366	GLN
1	B	399	GLN
1	B	534	GLN
1	B	579	HIS
1	B	621	HIS
1	B	632	GLN

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 oligosaccharides 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	305	-	4,4,4	0.26	0	6,6,6	0.21	0
2	SO4	B	303	-	4,4,4	0.28	0	6,6,6	0.47	0
2	SO4	A	302	-	4,4,4	0.57	0	6,6,6	0.37	0
2	SO4	B	306	-	4,4,4	0.25	0	6,6,6	0.39	0
2	SO4	A	301	-	4,4,4	0.25	0	6,6,6	0.38	0
2	SO4	B	304	-	4,4,4	0.37	0	6,6,6	0.43	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](#)

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%)	1.88	163 (39%) 1 0	30, 59, 83, 100	3 (0%)
1	B	419/463 (90%)	1.76	135 (32%) 1 0	31, 58, 83, 103	4 (0%)
All	All	830/926 (89%)	1.82	298 (35%) 1 0	30, 58, 83, 103	7 (0%)

All (298) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	548	LEU	8.7
1	B	655	THR	8.2
1	A	644	ILE	7.8
1	A	542	VAL	7.2
1	B	661	VAL	7.1
1	A	652	SER	6.8
1	A	626	ARG	6.8
1	A	634	ILE	6.6
1	A	793	ASN	6.6
1	A	747[A]	HIS	6.3
1	B	430	THR	6.2
1	B	656	PHE	6.0
1	A	430	THR	6.0
1	B	362	THR	5.5
1	A	677	VAL	5.5
1	A	662	LYS	5.3
1	B	650	PHE	5.3
1	A	635	ASP	5.3
1	A	573	GLY	5.3
1	A	638	ARG	5.3
1	B	654	LEU	5.2
1	A	639	VAL	5.2
1	B	573	GLY	5.1
1	A	572	LYS	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	625	LEU	5.0
1	B	653	TYR	5.0
1	A	650	PHE	5.0
1	B	794	THR	5.0
1	B	549	ASP	5.0
1	A	651	ALA	5.0
1	A	623	ASP	4.9
1	A	641	GLN	4.8
1	A	791	GLN	4.8
1	B	634	ILE	4.7
1	B	580	SER	4.7
1	B	747	HIS	4.7
1	A	642	VAL	4.6
1	B	792	ARG	4.6
1	A	571	ALA	4.5
1	B	390	HIS	4.5
1	B	542	VAL	4.5
1	A	627	THR	4.4
1	B	644	ILE	4.4
1	B	541	GLU	4.4
1	B	626	ARG	4.3
1	A	646	ALA	4.2
1	A	630	PHE	4.2
1	A	539	ARG	4.2
1	A	789	ILE	4.1
1	A	429	SER	4.1
1	B	543	GLU	4.1
1	B	571	ALA	4.1
1	A	790	PRO	4.1
1	A	792	ARG	4.0
1	B	539	ARG	4.0
1	A	640	GLU	4.0
1	A	622	ARG	4.0
1	A	675	ILE	4.0
1	B	405	LEU	4.0
1	B	639	VAL	4.0
1	B	562	GLN	3.9
1	B	365	GLN	3.9
1	B	651	ALA	3.9
1	B	630	PHE	3.8
1	A	594	VAL	3.8
1	A	621	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	564	VAL	3.8
1	A	788	PRO	3.8
1	B	649	LYS	3.8
1	B	581	GLU	3.8
1	A	612	CYS	3.8
1	A	628	PRO	3.7
1	A	671	LEU	3.7
1	A	580	SER	3.7
1	B	570	ALA	3.7
1	B	625	LEU	3.7
1	A	678	VAL	3.7
1	B	627	THR	3.7
1	B	414	ALA	3.7
1	B	689	HIS	3.7
1	B	572	LYS	3.7
1	A	402	GLU	3.6
1	B	652	SER	3.6
1	A	415	GLU	3.6
1	B	791	GLN	3.6
1	A	637	LEU	3.6
1	B	612[A]	CYS	3.6
1	A	581	GLU	3.6
1	B	638	ARG	3.5
1	A	578	GLY	3.5
1	A	390[A]	HIS	3.5
1	B	540	GLU	3.5
1	A	361	PRO	3.5
1	B	398	ASP	3.5
1	A	689[A]	HIS	3.5
1	A	691	TYR	3.5
1	A	434	ASN	3.5
1	A	419	ALA	3.4
1	B	421	PRO	3.4
1	B	411	LEU	3.4
1	B	418	LEU	3.4
1	A	570	ALA	3.4
1	A	550	LYS	3.4
1	A	432	LYS	3.4
1	A	649	LYS	3.4
1	A	566	ASP	3.4
1	B	400	ARG	3.3
1	A	663	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	647	GLY	3.3
1	B	646	ALA	3.3
1	A	665	ARG	3.3
1	B	629	LEU	3.3
1	A	579	HIS	3.3
1	A	362	THR	3.3
1	A	590	SER	3.3
1	A	559	GLY	3.2
1	B	648	PRO	3.2
1	A	568	GLN	3.2
1	B	628	PRO	3.2
1	B	429	SER	3.2
1	A	418	LEU	3.2
1	A	541	GLU	3.2
1	B	423	LEU	3.2
1	B	632	GLN	3.1
1	A	574	ILE	3.1
1	B	559	GLY	3.1
1	B	578	GLY	3.1
1	A	602	ARG	3.1
1	A	681	VAL	3.1
1	B	642	VAL	3.1
1	B	681	VAL	3.1
1	B	789	ILE	3.1
1	A	417	ARG	3.1
1	B	790	PRO	3.1
1	B	428	LEU	3.1
1	A	431	SER	3.0
1	B	568	GLN	3.0
1	A	670	ASP	3.0
1	A	631	ASP	3.0
1	B	610	ALA	3.0
1	A	624	LEU	3.0
1	A	632	GLN	3.0
1	B	624	LEU	3.0
1	B	449	ASP	3.0
1	A	421	PRO	3.0
1	A	645	HIS	2.9
1	A	562	GLN	2.9
1	A	449	ASP	2.9
1	B	665	ARG	2.9
1	A	712	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	400	ARG	2.9
1	A	629	LEU	2.9
1	A	673	LEU	2.9
1	A	668	TYR	2.9
1	B	552	ILE	2.9
1	A	416	GLY	2.8
1	A	643	LYS	2.8
1	B	518	LEU	2.8
1	B	531	GLU	2.8
1	A	620	ILE	2.8
1	A	666	THR	2.8
1	B	633	ILE	2.8
1	A	428	LEU	2.8
1	B	420	ALA	2.8
1	A	567	ILE	2.8
1	B	746	ILE	2.8
1	B	561	SER	2.8
1	A	448	GLN	2.8
1	A	423	LEU	2.8
1	B	402	GLU	2.8
1	A	538	THR	2.8
1	B	793	ASN	2.8
1	A	593	SER	2.8
1	A	591	GLU	2.8
1	B	715	ASP	2.7
1	A	582	GLY	2.7
1	B	386	ALA	2.7
1	B	417	ARG	2.7
1	A	746	ILE	2.7
1	B	669	GLY	2.7
1	B	662	LYS	2.7
1	A	511	HIS	2.7
1	A	633	ILE	2.7
1	B	413	GLU	2.7
1	B	622	ARG	2.7
1	B	677	VAL	2.7
1	A	787	LEU	2.7
1	B	419	ALA	2.6
1	B	623	ASP	2.6
1	A	420	ALA	2.6
1	B	602[A]	ARG	2.6
1	A	692	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	565	ARG	2.6
1	B	537	ASN	2.6
1	B	670	ASP	2.6
1	A	438	ILE	2.6
1	B	645	HIS	2.6
1	A	410	ASP	2.6
1	B	538	THR	2.6
1	B	526	ILE	2.5
1	A	664	LEU	2.5
1	A	485	ASP	2.5
1	B	635	ASP	2.5
1	B	397	THR	2.5
1	B	668	TYR	2.5
1	A	414	ALA	2.5
1	A	611	ALA	2.5
1	B	434[A]	ASN	2.5
1	A	648	PRO	2.5
1	B	641	GLN	2.5
1	A	413	GLU	2.5
1	A	727	PHE	2.5
1	A	597	VAL	2.5
1	B	399	GLN	2.5
1	A	700	VAL	2.4
1	B	664	LEU	2.4
1	A	680	ASN	2.4
1	A	370	ALA	2.4
1	B	592	ALA	2.4
1	B	647	GLY	2.4
1	B	370	ALA	2.4
1	A	560	SER	2.4
1	B	560	SER	2.4
1	A	526	ILE	2.4
1	A	552	ILE	2.4
1	A	584	CYS	2.4
1	B	363	VAL	2.4
1	A	436	LEU	2.4
1	B	433	LEU	2.4
1	B	579	HIS	2.4
1	A	502	LEU	2.3
1	B	422	LEU	2.3
1	B	595	ASP	2.3
1	A	588	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	415	GLU	2.3
1	A	674	CYS	2.3
1	A	679	ASP	2.3
1	A	391	HIS	2.3
1	B	364	GLU	2.3
1	B	445	ALA	2.3
1	A	447	SER	2.3
1	A	672	GLU	2.3
1	A	676	GLU	2.3
1	A	487	LEU	2.2
1	A	516	LEU	2.2
1	A	446	SER	2.2
1	A	694	SER	2.2
1	B	432	LYS	2.2
1	B	564	VAL	2.2
1	B	712	GLN	2.2
1	A	608	TYR	2.2
1	B	403	ILE	2.2
1	B	404	LEU	2.2
1	B	597	VAL	2.2
1	A	683	ASP	2.2
1	A	715	ASP	2.2
1	A	408	LYS	2.2
1	B	424	LYS	2.2
1	B	448	GLN	2.2
1	B	569	LYS	2.2
1	A	435	SER	2.2
1	A	411	LEU	2.2
1	B	699	ILE	2.2
1	B	408	LYS	2.2
1	A	687	HIS	2.2
1	A	492	ALA	2.2
1	B	406	ALA	2.2
1	B	389	ILE	2.1
1	A	576	VAL	2.1
1	B	678	VAL	2.1
1	A	424	LYS	2.1
1	B	643	LYS	2.1
1	A	669	GLY	2.1
1	A	379	THR	2.1
1	B	663	SER	2.1
1	A	535	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	671	LEU	2.1
1	B	576	VAL	2.1
1	A	592	ALA	2.1
1	A	422	LEU	2.1
1	A	688	ILE	2.1
1	B	396	LEU	2.1
1	B	515	ILE	2.1
1	B	566	ASP	2.1
1	A	488	PRO	2.1
1	A	606	CYS	2.1
1	A	444	ALA	2.1
1	A	496	ALA	2.1
1	A	569	LYS	2.1
1	A	454	VAL	2.1
1	A	563	LEU	2.0
1	A	595	ASP	2.0
1	B	594	VAL	2.0
1	A	531	GLU	2.0
1	A	725	THR	2.0
1	B	598	THR	2.0
1	A	705	ASN	2.0
1	A	443	ILE	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
2	SO4	B	306	5/5	0.72	0.17	75,83,90,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	305	5/5	0.78	0.14	94,95,99,100	0
2	SO4	A	302	5/5	0.81	0.14	52,58,79,85	0
2	SO4	B	304	5/5	0.89	0.12	52,59,78,79	0
2	SO4	A	301	5/5	0.97	0.11	52,54,57,60	0
2	SO4	B	303	5/5	0.98	0.11	50,51,57,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.