



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:49 PM UTC

PDB ID : 3TFO / pdb_00003tfo
Title : Crystal structure of a putative 3-oxoacyl-(acyl-carrier-protein) reductase from *Sinorhizobium meliloti*
Authors : Agarwal, R.; Chamala, S.; Evans, B.; Foti, R.; Gizzi, A.; Hillerich, B.; Kar, A.; LaFleur, J.; Seidel, R.; Villigas, G.; Zencheck, W.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRG)
Deposited on : 2011-08-16
Resolution : 2.08 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

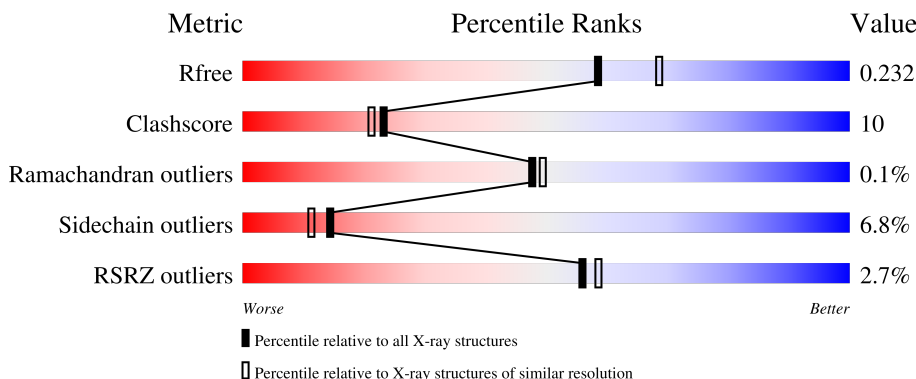
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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	264	
1	B	264	
1	C	264	
1	D	264	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6839 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 putative 3-oxoacyl-(acyl-carrier-protein) reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1552	975	276	295	6			
1	B	215	Total	C	N	O	S	0	0	0
			1542	969	274	293	6			
1	C	216	Total	C	N	O	S	0	0	0
			1559	977	281	296	5			
1	D	218	Total	C	N	O	S	0	0	0
			1564	982	279	297	6			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q92XI4
A	2	VAL	-	expression tag	UNP Q92XI4
A	243	ALA	-	expression tag	UNP Q92XI4
A	244	GLU	-	expression tag	UNP Q92XI4
A	245	ASN	-	expression tag	UNP Q92XI4
A	246	LEU	-	expression tag	UNP Q92XI4
A	247	TYR	-	expression tag	UNP Q92XI4
A	248	PHE	-	expression tag	UNP Q92XI4
A	249	GLN	-	expression tag	UNP Q92XI4
A	250	SER	-	expression tag	UNP Q92XI4
A	251	HIS	-	expression tag	UNP Q92XI4
A	252	HIS	-	expression tag	UNP Q92XI4
A	253	HIS	-	expression tag	UNP Q92XI4
A	254	HIS	-	expression tag	UNP Q92XI4
A	255	HIS	-	expression tag	UNP Q92XI4
A	256	HIS	-	expression tag	UNP Q92XI4
A	257	TRP	-	expression tag	UNP Q92XI4
A	258	SER	-	expression tag	UNP Q92XI4
A	259	HIS	-	expression tag	UNP Q92XI4
A	260	PRO	-	expression tag	UNP Q92XI4
A	261	GLN	-	expression tag	UNP Q92XI4

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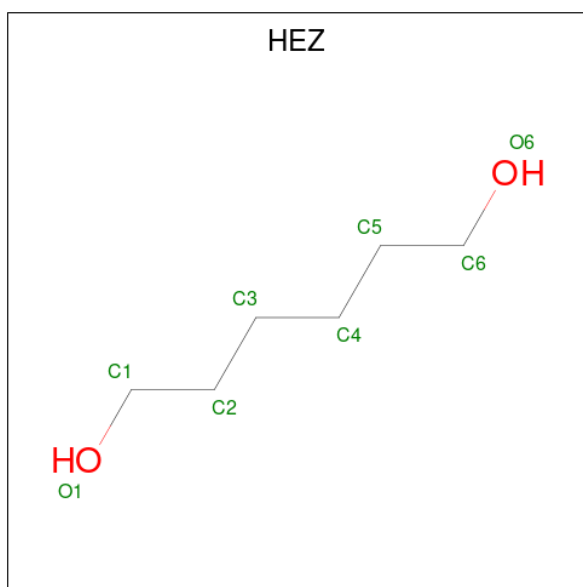
Chain	Residue	Modelled	Actual	Comment	Reference
A	262	PHE	-	expression tag	UNP Q92XI4
A	263	GLU	-	expression tag	UNP Q92XI4
A	264	LYS	-	expression tag	UNP Q92XI4
B	1	MET	-	expression tag	UNP Q92XI4
B	2	VAL	-	expression tag	UNP Q92XI4
B	243	ALA	-	expression tag	UNP Q92XI4
B	244	GLU	-	expression tag	UNP Q92XI4
B	245	ASN	-	expression tag	UNP Q92XI4
B	246	LEU	-	expression tag	UNP Q92XI4
B	247	TYR	-	expression tag	UNP Q92XI4
B	248	PHE	-	expression tag	UNP Q92XI4
B	249	GLN	-	expression tag	UNP Q92XI4
B	250	SER	-	expression tag	UNP Q92XI4
B	251	HIS	-	expression tag	UNP Q92XI4
B	252	HIS	-	expression tag	UNP Q92XI4
B	253	HIS	-	expression tag	UNP Q92XI4
B	254	HIS	-	expression tag	UNP Q92XI4
B	255	HIS	-	expression tag	UNP Q92XI4
B	256	HIS	-	expression tag	UNP Q92XI4
B	257	TRP	-	expression tag	UNP Q92XI4
B	258	SER	-	expression tag	UNP Q92XI4
B	259	HIS	-	expression tag	UNP Q92XI4
B	260	PRO	-	expression tag	UNP Q92XI4
B	261	GLN	-	expression tag	UNP Q92XI4
B	262	PHE	-	expression tag	UNP Q92XI4
B	263	GLU	-	expression tag	UNP Q92XI4
B	264	LYS	-	expression tag	UNP Q92XI4
C	1	MET	-	expression tag	UNP Q92XI4
C	2	VAL	-	expression tag	UNP Q92XI4
C	243	ALA	-	expression tag	UNP Q92XI4
C	244	GLU	-	expression tag	UNP Q92XI4
C	245	ASN	-	expression tag	UNP Q92XI4
C	246	LEU	-	expression tag	UNP Q92XI4
C	247	TYR	-	expression tag	UNP Q92XI4
C	248	PHE	-	expression tag	UNP Q92XI4
C	249	GLN	-	expression tag	UNP Q92XI4
C	250	SER	-	expression tag	UNP Q92XI4
C	251	HIS	-	expression tag	UNP Q92XI4
C	252	HIS	-	expression tag	UNP Q92XI4
C	253	HIS	-	expression tag	UNP Q92XI4
C	254	HIS	-	expression tag	UNP Q92XI4
C	255	HIS	-	expression tag	UNP Q92XI4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	256	HIS	-	expression tag	UNP Q92XI4
C	257	TRP	-	expression tag	UNP Q92XI4
C	258	SER	-	expression tag	UNP Q92XI4
C	259	HIS	-	expression tag	UNP Q92XI4
C	260	PRO	-	expression tag	UNP Q92XI4
C	261	GLN	-	expression tag	UNP Q92XI4
C	262	PHE	-	expression tag	UNP Q92XI4
C	263	GLU	-	expression tag	UNP Q92XI4
C	264	LYS	-	expression tag	UNP Q92XI4
D	1	MET	-	expression tag	UNP Q92XI4
D	2	VAL	-	expression tag	UNP Q92XI4
D	243	ALA	-	expression tag	UNP Q92XI4
D	244	GLU	-	expression tag	UNP Q92XI4
D	245	ASN	-	expression tag	UNP Q92XI4
D	246	LEU	-	expression tag	UNP Q92XI4
D	247	TYR	-	expression tag	UNP Q92XI4
D	248	PHE	-	expression tag	UNP Q92XI4
D	249	GLN	-	expression tag	UNP Q92XI4
D	250	SER	-	expression tag	UNP Q92XI4
D	251	HIS	-	expression tag	UNP Q92XI4
D	252	HIS	-	expression tag	UNP Q92XI4
D	253	HIS	-	expression tag	UNP Q92XI4
D	254	HIS	-	expression tag	UNP Q92XI4
D	255	HIS	-	expression tag	UNP Q92XI4
D	256	HIS	-	expression tag	UNP Q92XI4
D	257	TRP	-	expression tag	UNP Q92XI4
D	258	SER	-	expression tag	UNP Q92XI4
D	259	HIS	-	expression tag	UNP Q92XI4
D	260	PRO	-	expression tag	UNP Q92XI4
D	261	GLN	-	expression tag	UNP Q92XI4
D	262	PHE	-	expression tag	UNP Q92XI4
D	263	GLU	-	expression tag	UNP Q92XI4
D	264	LYS	-	expression tag	UNP Q92XI4

- Molecule 2 is HEXANE-1,6-DIOL (CCD ID: HEZ) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	C	1	Total	C	O	0	0
			8	6	2		

- 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	A	1	Total	O	S	0	0
			5	4	1		

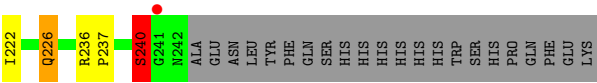
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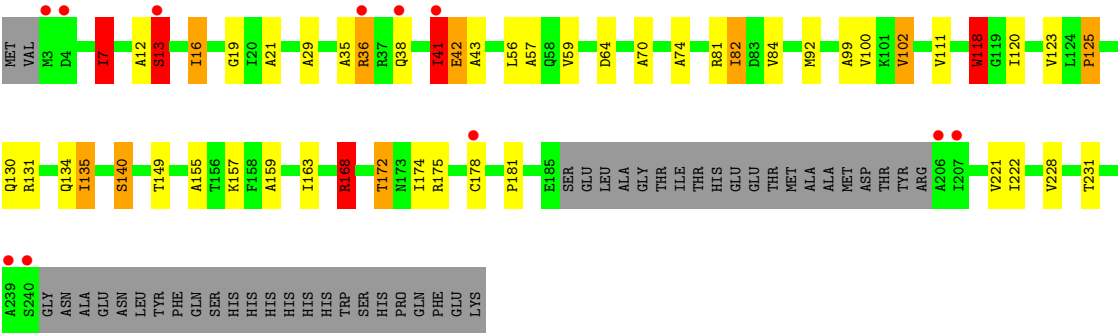
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	142	Total	O	0	0
			142	142		
4	B	137	Total	O	0	0
			137	137		
4	C	152	Total	O	0	0
			152	152		
4	D	120	Total	O	0	0
			120	120		



● Molecule 1: putative 3-oxoacyl-(acyl-carrier-protein) reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	108.55Å 108.55Å 207.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.08 – 2.08 48.08 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.08-2.08) 99.8 (48.08-2.08)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.26 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.176 , 0.219 (Not available) , 0.232	Depositor DCC
R_{free} test set	4270 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6839	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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, HEZ

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	1.84	21/1568 (1.3%)	1.32	14/2137 (0.7%)
1	B	1.79	15/1558 (1.0%)	1.39	9/2124 (0.4%)
1	C	1.74	24/1575 (1.5%)	1.37	8/2146 (0.4%)
1	D	1.83	18/1580 (1.1%)	1.39	13/2154 (0.6%)
All	All	1.80	78/6281 (1.2%)	1.37	44/8561 (0.5%)

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	41	ILE	CA-CB	9.24	1.65	1.54
1	B	20	ILE	CA-CB	8.84	1.65	1.54
1	C	92	MET	SD-CE	-8.53	1.58	1.79
1	A	109	ILE	CA-CB	8.52	1.64	1.54
1	A	113	ILE	CA-CB	8.12	1.62	1.55
1	B	150	ALA	CA-CB	7.97	1.64	1.53
1	A	81	ARG	N-CA	7.75	1.55	1.46
1	D	120	ILE	CA-CB	7.55	1.63	1.54
1	D	59	VAL	CA-CB	7.01	1.62	1.54
1	C	136	ILE	CA-CB	6.75	1.62	1.54
1	A	113	ILE	CG1-CD1	-6.39	1.26	1.51
1	B	147	VAL	CA-CB	6.30	1.62	1.54
1	D	118	TRP	N-CA	6.27	1.53	1.46
1	B	75	ALA	CA-CB	6.25	1.63	1.53
1	A	9	ILE	C-O	6.20	1.30	1.24
1	C	4	ASP	CA-CB	-6.19	1.41	1.53
1	B	37	ARG	CA-C	6.07	1.60	1.52
1	C	82	ILE	C-O	-6.01	1.17	1.24
1	C	22	ARG	N-CA	5.90	1.53	1.46
1	C	124	LEU	C-O	-5.86	1.19	1.24
1	B	151	ALA	CA-CB	5.84	1.62	1.53
1	C	69	ALA	CA-CB	5.83	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	ALA	CA-CB	-5.79	1.44	1.53
1	D	19	GLY	C-O	-5.78	1.16	1.23
1	B	124	LEU	C-O	-5.77	1.19	1.24
1	B	161	ARG	C-O	-5.75	1.17	1.24
1	A	135	ILE	C-O	5.71	1.30	1.24
1	C	76	VAL	CA-C	5.70	1.59	1.52
1	A	220	GLN	C-O	-5.67	1.17	1.24
1	D	99	ALA	CA-CB	5.65	1.63	1.53
1	D	74	ALA	CA-CB	-5.63	1.44	1.53
1	B	183	VAL	C-O	5.57	1.30	1.24
1	D	70	ALA	C-O	-5.55	1.17	1.24
1	C	141	ILE	CG1-CD1	-5.53	1.30	1.51
1	C	41	ILE	C-O	5.45	1.30	1.24
1	B	103	ASP	C-O	-5.43	1.17	1.24
1	C	136	ILE	CG1-CD1	-5.42	1.30	1.51
1	D	102	VAL	N-CA	-5.41	1.39	1.46
1	B	154	CYS	C-O	-5.39	1.17	1.24
1	D	135	ILE	CA-CB	5.39	1.61	1.54
1	A	98	ALA	CA-CB	5.38	1.62	1.53
1	C	6	VAL	CA-C	5.38	1.59	1.52
1	D	43	ALA	CA-CB	5.35	1.61	1.53
1	C	99	ALA	C-O	-5.34	1.17	1.24
1	B	157	LYS	C-O	-5.33	1.17	1.24
1	A	77	ASP	CA-C	-5.31	1.45	1.52
1	B	224	ALA	CA-CB	5.31	1.61	1.53
1	A	33	LEU	C-O	5.31	1.30	1.23
1	D	149	THR	CA-CB	5.30	1.60	1.54
1	C	135	ILE	CA-CB	5.30	1.61	1.54
1	C	114	LYS	C-O	-5.29	1.18	1.24
1	D	172	THR	CB-CG2	-5.29	1.35	1.52
1	D	82	ILE	C-O	-5.29	1.18	1.24
1	A	233	ILE	N-CA	-5.28	1.40	1.46
1	C	13	SER	C-O	-5.27	1.18	1.24
1	A	178	CYS	CA-CB	5.26	1.60	1.53
1	C	44	ILE	CA-CB	5.26	1.60	1.54
1	C	113	ILE	C-O	-5.22	1.18	1.23
1	C	123	VAL	C-O	-5.18	1.18	1.24
1	B	49	ARG	C-O	-5.17	1.18	1.24
1	A	136	ILE	CA-CB	-5.16	1.47	1.53
1	A	228	VAL	CA-CB	5.13	1.59	1.53
1	D	21	ALA	C-O	-5.12	1.18	1.24
1	A	60	LEU	C-O	-5.11	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	153	TYR	C-O	-5.11	1.18	1.24
1	C	162	ALA	C-O	-5.10	1.18	1.24
1	A	93	PRO	C-O	-5.09	1.18	1.23
1	D	16	ILE	C-O	-5.08	1.18	1.24
1	C	112	ASN	C-O	-5.08	1.18	1.24
1	C	12	ALA	C-O	-5.08	1.17	1.24
1	A	215	ALA	C-O	-5.05	1.18	1.24
1	D	125	PRO	C-O	-5.05	1.18	1.24
1	A	218	VAL	C-O	-5.04	1.18	1.24
1	C	217	ALA	C-O	-5.03	1.18	1.24
1	C	151	ALA	CA-CB	-5.02	1.45	1.53
1	A	29	ALA	CA-CB	5.02	1.61	1.53
1	A	23	GLU	C-O	-5.02	1.18	1.24
1	D	118	TRP	C-O	-5.01	1.18	1.24

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	41	ILE	N-CA-CB	-11.17	98.11	110.51
1	B	123	VAL	N-CA-C	11.00	121.83	110.72
1	D	123	VAL	N-CA-C	10.00	120.82	110.72
1	A	2	VAL	N-CA-C	8.57	119.38	110.72
1	B	13	SER	N-CA-C	7.49	119.44	111.28
1	A	41	ILE	CA-CB-CG2	7.28	122.87	110.50
1	B	126	ILE	N-CA-CB	7.25	118.56	110.51
1	C	41	ILE	CB-CA-C	7.15	121.03	111.88
1	D	172	THR	N-CA-CB	-7.08	100.24	110.65
1	C	41	ILE	CA-CB-CG2	7.00	122.40	110.50
1	A	113	ILE	CB-CA-C	-6.94	105.81	111.71
1	A	113	ILE	CA-CB-CG1	6.93	122.18	110.40
1	A	41	ILE	CB-CA-C	6.80	120.68	111.97
1	C	141	ILE	CA-CB-CG2	6.75	121.97	110.50
1	A	109	ILE	N-CA-CB	6.65	118.33	110.55
1	D	41	ILE	CA-CB-CG2	6.48	121.51	110.50
1	C	240	SER	N-CA-C	6.40	118.78	111.11
1	B	47	GLU	N-CA-C	6.39	118.25	111.28
1	D	13	SER	N-CA-C	6.30	118.15	111.28
1	B	81	ARG	CB-CA-C	-6.17	98.86	110.16
1	A	77	ASP	CB-CA-C	-6.03	100.79	110.79
1	D	41	ILE	CB-CA-C	5.91	119.53	111.97
1	D	102	VAL	N-CA-CB	-5.91	100.55	110.65
1	D	228	VAL	N-CA-C	5.64	115.92	107.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	13	SER	N-CA-C	5.50	117.28	111.28
1	B	52	GLY	CA-C-N	-5.48	116.99	122.69
1	B	52	GLY	C-N-CA	-5.48	116.99	122.69
1	D	172	THR	CA-CB-CG2	5.47	119.79	110.50
1	A	124	LEU	CA-C-N	-5.43	113.44	119.19
1	A	124	LEU	C-N-CA	-5.43	113.44	119.19
1	B	90	GLY	N-CA-C	-5.40	100.39	113.18
1	D	111	VAL	N-CA-C	5.38	115.59	110.53
1	D	7	ILE	CB-CA-C	-5.34	103.21	110.42
1	A	38	GLN	N-CA-C	5.17	117.82	111.82
1	A	41	ILE	N-CA-C	5.14	115.36	110.42
1	A	231	THR	N-CA-C	5.11	116.84	111.28
1	A	101	LYS	CA-C-N	5.09	127.43	120.46
1	A	101	LYS	C-N-CA	5.09	127.43	120.46
1	D	92	MET	CA-C-N	-5.08	113.00	120.46
1	D	92	MET	C-N-CA	-5.08	113.00	120.46
1	D	168	ARG	CG-CD-NE	5.07	123.16	112.00
1	C	122	ALA	N-CA-C	5.05	116.86	111.36
1	B	80	GLY	N-CA-C	5.02	122.63	114.90
1	C	39	ALA	N-CA-C	5.00	116.42	111.07

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	1552	0	1599	36	0
1	B	1542	0	1585	31	0
1	C	1559	0	1610	35	0
1	D	1564	0	1608	33	0
2	A	8	0	14	2	0
2	C	8	0	14	0	0
3	A	15	0	0	1	0
3	B	15	0	0	1	0
3	C	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	10	0	0	1	0
4	A	142	0	0	10	0
4	B	137	0	0	8	0
4	C	152	0	0	5	0
4	D	120	0	0	3	0
All	All	6839	0	6430	131	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (131) 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:D:36:ARG:HH11	1:D:36:ARG:HG3	1.03	1.13
4:A:560:HOH:O	1:B:231:THR:HG21	1.50	1.07
1:A:1:MET:O	1:A:5:LYS:HE2	1.61	1.00
1:D:36:ARG:HH11	1:D:36:ARG:CG	1.76	0.98
1:C:92:MET:HE2	1:C:153:TYR:CE2	2.03	0.93
1:A:41:ILE:HG23	1:A:57:ALA:HB1	1.53	0.91
1:D:36:ARG:HG3	1:D:36:ARG:NH1	1.84	0.88
1:A:113:ILE:HD11	1:A:156:THR:HA	1.55	0.87
1:A:2:VAL:HG23	1:A:223:GLU:CG	2.07	0.85
1:C:73:GLN:HG2	4:C:312:HOH:O	1.79	0.81
1:C:41:ILE:HG22	1:C:57:ALA:HB1	1.64	0.80
1:C:92:MET:CE	1:C:153:TYR:CE2	2.66	0.78
1:B:178:CYS:HB3	4:B:434:HOH:O	1.82	0.77
1:A:219:ARG:NH2	3:A:266:SO4:O3	2.20	0.75
1:C:4:ASP:CB	4:C:470:HOH:O	2.35	0.75
1:C:41:ILE:CG2	1:C:57:ALA:HB1	2.17	0.74
1:D:100:VAL:O	1:D:100:VAL:HG12	1.88	0.73
1:C:92:MET:HE3	1:C:153:TYR:CZ	2.24	0.73
1:D:131:ARG:HD2	4:D:682:HOH:O	1.88	0.73
1:C:82:ILE:H	1:C:130:GLN:HE22	1.37	0.73
1:B:82:ILE:H	1:B:130:GLN:HE22	1.39	0.70
1:A:2:VAL:HG23	1:A:223:GLU:HG3	1.73	0.69
1:C:81:ARG:HG2	1:C:81:ARG:NH1	2.08	0.69
1:D:41:ILE:CG2	1:D:57:ALA:HB1	2.23	0.68
1:A:145:SER:HB3	4:A:302:HOH:O	1.94	0.67
1:A:2:VAL:HG23	1:A:223:GLU:HG2	1.75	0.67
1:A:113:ILE:HD11	1:A:156:THR:CA	2.23	0.67
1:B:102:VAL:HG22	1:D:118:TRP:CZ3	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:GLN:HE22	1:C:222:ILE:HA	1.59	0.66
1:A:77:ASP:HB3	4:A:349:HOH:O	1.96	0.66
1:C:35:ALA:HB3	1:C:41:ILE:HG13	1.77	0.66
1:B:100:VAL:HG12	4:B:268:HOH:O	1.95	0.65
1:C:81:ARG:HG2	1:C:81:ARG:HH11	1.61	0.64
1:A:226:GLN:HG2	4:A:319:HOH:O	1.97	0.64
1:B:178:CYS:CB	4:B:434:HOH:O	2.41	0.64
1:A:82:ILE:H	1:A:130:GLN:HE22	1.45	0.64
1:A:220:GLN:NE2	2:A:265:HEZ:H21	2.12	0.63
1:A:77:ASP:CB	4:A:349:HOH:O	2.47	0.63
1:B:36:ARG:O	1:B:59:VAL:HG23	1.99	0.63
1:A:1:MET:O	1:A:5:LYS:CE	2.43	0.60
1:A:50:ASP:HB2	4:A:391:HOH:O	2.02	0.60
1:D:134:GLN:HE22	1:D:222:ILE:HA	1.67	0.59
1:D:41:ILE:HG23	1:D:57:ALA:HB1	1.84	0.59
1:A:77:ASP:CG	4:A:349:HOH:O	2.46	0.58
1:A:43:ALA:O	1:A:47:GLU:HG3	2.02	0.58
1:D:36:ARG:CG	1:D:36:ARG:NH1	2.47	0.58
1:C:37:ARG:CB	4:C:382:HOH:O	2.51	0.58
1:C:33:LEU:HB3	1:C:41:ILE:HD12	1.85	0.57
1:B:100:VAL:HG12	1:B:100:VAL:O	2.05	0.57
4:B:384:HOH:O	1:D:125:PRO:HG3	2.04	0.57
1:B:22:ARG:NH2	1:B:47:GLU:OE1	2.29	0.56
1:C:92:MET:CE	1:C:153:TYR:CZ	2.86	0.56
1:D:82:ILE:H	1:D:130:GLN:HE22	1.52	0.56
1:A:49:ARG:NH2	4:A:446:HOH:O	2.39	0.55
1:C:35:ALA:CB	1:C:41:ILE:HG13	2.38	0.53
1:C:13:SER:HB2	3:C:266:SO4:O4	2.08	0.53
1:D:41:ILE:HG22	1:D:57:ALA:HB1	1.89	0.53
1:B:87:ASN:HB2	1:B:137:ASN:HD22	1.73	0.53
1:A:134:GLN:HE22	1:A:222:ILE:HA	1.73	0.52
1:D:131:ARG:CD	4:D:682:HOH:O	2.54	0.52
1:A:168:ARG:HD3	1:A:231:THR:HG21	1.93	0.51
1:B:107:ARG:HD3	4:B:278:HOH:O	2.10	0.51
1:A:226:GLN:CG	4:A:319:HOH:O	2.55	0.51
1:D:12:ALA:C	1:D:41:ILE:HD11	2.36	0.50
1:B:56:LEU:HD23	4:B:335:HOH:O	2.12	0.50
1:B:30:LYS:HD3	1:B:79:TRP:CD1	2.47	0.49
1:C:226:GLN:HG2	4:C:332:HOH:O	2.11	0.49
1:D:64:ASP:OD1	1:D:64:ASP:C	2.55	0.49
1:B:64:ASP:OD1	1:B:64:ASP:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:ALA:O	1:C:56:LEU:HD23	2.13	0.49
1:B:127:MET:HB3	1:B:174:ILE:HD12	1.93	0.49
1:D:13:SER:HB2	3:D:265:SO4:O3	2.12	0.49
1:A:130:GLN:O	1:A:131:ARG:HB2	2.13	0.48
1:B:178:CYS:SG	4:B:434:HOH:O	2.59	0.48
1:B:127:MET:HB3	1:B:174:ILE:CD1	2.44	0.48
1:A:92:MET:HG3	1:A:153:TYR:CD1	2.48	0.47
1:A:2:VAL:HG12	1:A:29:ALA:HB2	1.95	0.47
1:C:127:MET:HB3	1:C:174:ILE:CD1	2.45	0.47
1:C:81:ARG:HH11	1:C:81:ARG:CG	2.27	0.47
1:C:127:MET:HB3	1:C:174:ILE:HD12	1.97	0.47
1:D:100:VAL:O	1:D:100:VAL:CG1	2.61	0.46
1:C:10:THR:O	1:C:88:ASN:HB3	2.15	0.46
1:A:12:ALA:C	1:A:41:ILE:HD11	2.41	0.46
1:D:35:ALA:HB3	1:D:41:ILE:HG12	1.97	0.46
1:D:38:GLN:HE21	1:D:42:GLU:HG3	1.81	0.46
1:D:140:SER:HA	1:D:181:PRO:HD2	1.97	0.46
1:D:157:LYS:HA	1:D:157:LYS:HD2	1.60	0.46
1:C:120:ILE:O	1:C:124:LEU:HB2	2.16	0.45
1:D:168:ARG:HH11	1:D:168:ARG:HD2	1.66	0.45
1:B:102:VAL:HG22	1:D:118:TRP:HZ3	1.81	0.45
1:A:50:ASP:CB	4:A:391:HOH:O	2.63	0.45
1:B:39:ALA:N	3:B:266:SO4:O3	2.46	0.44
1:B:232:GLU:HG3	4:B:325:HOH:O	2.17	0.44
1:C:41:ILE:HG23	1:C:57:ALA:HB1	1.97	0.44
1:C:140:SER:HB3	1:C:157:LYS:HG3	1.99	0.44
1:D:118:TRP:HA	1:D:118:TRP:CE3	2.53	0.43
1:A:13:SER:HA	1:A:41:ILE:CD1	2.48	0.43
1:C:141:ILE:HG12	1:C:236:ARG:NH1	2.33	0.43
1:B:123:VAL:HG13	1:B:127:MET:HE3	1.99	0.43
2:A:265:HEZ:H51	1:B:220:GLN:NE2	2.33	0.43
1:B:233:ILE:HG22	1:B:235:ILE:HG13	2.01	0.43
1:B:180:ASN:ND2	1:B:232:GLU:OE2	2.50	0.43
1:D:118:TRP:HA	1:D:118:TRP:HE3	1.83	0.43
1:B:41:ILE:HD12	1:B:57:ALA:HB1	2.01	0.43
1:B:61:ASP:OD1	1:B:61:ASP:C	2.62	0.42
1:C:161:ARG:HH11	1:C:161:ARG:HD3	1.71	0.42
1:A:2:VAL:CG2	1:A:223:GLU:HG3	2.45	0.42
1:A:13:SER:HA	1:A:41:ILE:HD12	2.02	0.42
1:B:118:TRP:HA	1:B:118:TRP:CE3	2.54	0.42
1:A:141:ILE:HD12	1:A:236:ARG:CZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:TRP:HA	1:B:118:TRP:HE3	1.84	0.41
1:B:76:VAL:O	1:B:80:GLY:HA2	2.20	0.41
1:C:140:SER:H	1:C:180:ASN:HD22	1.69	0.41
1:D:36:ARG:HH11	1:D:36:ARG:CB	2.31	0.41
1:D:7:ILE:HG13	1:D:29:ALA:HB1	2.01	0.41
1:D:159:ALA:O	1:D:163:ILE:HG12	2.21	0.41
1:C:237:PRO:O	1:C:240:SER:HB2	2.21	0.41
1:D:100:VAL:HG12	4:D:321:HOH:O	2.20	0.41
1:A:135:ILE:HD12	1:A:167:LEU:HD21	2.03	0.41
1:B:123:VAL:CG1	1:B:127:MET:HE3	2.51	0.41
1:A:2:VAL:HG12	1:A:2:VAL:O	2.21	0.40
1:A:163:ILE:HG13	1:C:155:ALA:HB2	2.02	0.40
1:B:163:ILE:HG13	1:D:155:ALA:HB2	2.02	0.40
1:A:141:ILE:HD12	1:A:141:ILE:HG23	1.80	0.40
1:C:4:ASP:N	4:C:661:HOH:O	2.54	0.40
1:C:16:ILE:HD11	1:C:184:VAL:HG21	2.03	0.40
1:C:41:ILE:HA	1:C:41:ILE:HD13	1.77	0.40
1:D:7:ILE:HD13	1:D:84:VAL:HB	2.03	0.40
1:A:140:SER:HA	1:A:181:PRO:HD2	2.03	0.40
1:C:236:ARG:HH11	1:C:236:ARG:HD3	1.74	0.40
1:D:134:GLN:HA	1:D:175:ARG:O	2.21	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	212/264 (80%)	207 (98%)	5 (2%)	0	100	100
1	B	211/264 (80%)	207 (98%)	3 (1%)	1 (0%)	24	21
1	C	212/264 (80%)	208 (98%)	4 (2%)	0	100	100
1	D	214/264 (81%)	209 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	849/1056 (80%)	831 (98%)	17 (2%)	1 (0%)	48	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	15	GLY

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	158/204 (78%)	150 (95%)	8 (5%)	21	20
1	B	156/204 (76%)	150 (96%)	6 (4%)	29	30
1	C	159/204 (78%)	148 (93%)	11 (7%)	14	11
1	D	158/204 (78%)	140 (89%)	18 (11%)	5	3
All	All	631/816 (77%)	588 (93%)	43 (7%)	14	11

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ILE
1	A	102	VAL
1	A	109	ILE
1	A	118	TRP
1	A	168	ARG
1	A	172	THR
1	A	174	ILE
1	A	226	GLN
1	B	56	LEU
1	B	102	VAL
1	B	123	VAL
1	B	126	ILE
1	B	140	SER
1	B	221	VAL

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Mol	Chain	Res	Type
1	C	13	SER
1	C	26	VAL
1	C	38	GLN
1	C	44	ILE
1	C	56	LEU
1	C	118	TRP
1	C	141	ILE
1	C	171	SER
1	C	221	VAL
1	C	226	GLN
1	C	240	SER
1	D	7	ILE
1	D	13	SER
1	D	16	ILE
1	D	36	ARG
1	D	41	ILE
1	D	42	GLU
1	D	56	LEU
1	D	81	ARG
1	D	102	VAL
1	D	118	TRP
1	D	135	ILE
1	D	140	SER
1	D	168	ARG
1	D	172	THR
1	D	174	ILE
1	D	178	CYS
1	D	221	VAL
1	D	231	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	73	GLN
1	A	87	ASN
1	A	130	GLN
1	A	134	GLN
1	A	220	GLN
1	B	87	ASN
1	B	130	GLN
1	B	137	ASN

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Mol	Chain	Res	Type
1	B	169	GLN
1	B	173	ASN
1	B	220	GLN
1	C	87	ASN
1	C	130	GLN
1	C	134	GLN
1	C	180	ASN
1	D	38	GLN
1	D	87	ASN
1	D	88	ASN
1	D	130	GLN
1	D	134	GLN
1	D	169	GLN
1	D	210	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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	HEZ	C	265	-	7,7,7	0.53	0	6,6,6	1.11	1 (16%)
3	SO4	B	267	-	4,4,4	0.81	0	6,6,6	1.28	0
3	SO4	A	268	-	4,4,4	0.41	0	6,6,6	0.55	0
3	SO4	D	265	-	4,4,4	0.36	0	6,6,6	0.71	0
3	SO4	A	267	-	4,4,4	0.12	0	6,6,6	0.47	0
3	SO4	B	266	-	4,4,4	0.47	0	6,6,6	0.32	0
3	SO4	C	266	-	4,4,4	0.19	0	6,6,6	1.08	0
3	SO4	C	267	-	4,4,4	0.43	0	6,6,6	0.31	0
2	HEZ	A	265	-	7,7,7	1.09	1 (14%)	6,6,6	0.98	0
3	SO4	D	266	-	4,4,4	0.26	0	6,6,6	0.51	0
3	SO4	C	268	-	4,4,4	0.57	0	6,6,6	0.86	0
3	SO4	B	265	-	4,4,4	0.44	0	6,6,6	0.90	0
3	SO4	A	266	-	4,4,4	1.08	0	6,6,6	1.52	1 (16%)

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	HEZ	C	265	-	-	1/5/5/5	-
2	HEZ	A	265	-	-	3/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	265	HEZ	O1-C1	2.16	1.53	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	266	SO4	O4-S-O3	-3.16	91.11	108.54
2	C	265	HEZ	C5-C4-C3	-2.24	103.03	114.37

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	265	HEZ	C2-C3-C4-C5
2	A	265	HEZ	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	C	265	HEZ	O1-C1-C2-C3
2	A	265	HEZ	C3-C4-C5-C6

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	265	SO4	1	0
3	B	266	SO4	1	0
3	C	266	SO4	1	0
2	A	265	HEZ	2	0
3	A	266	SO4	1	0

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	216/264 (81%)	-0.14	5 (2%) 61 64	20, 30, 45, 56	0
1	B	215/264 (81%)	-0.14	3 (1%) 73 76	23, 31, 43, 55	0
1	C	216/264 (81%)	-0.20	4 (1%) 66 69	20, 29, 42, 57	0
1	D	218/264 (82%)	-0.02	11 (5%) 34 35	22, 31, 46, 58	0
All	All	865/1056 (81%)	-0.12	23 (2%) 56 58	20, 30, 44, 58	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4	ASP	4.5
1	D	240	SER	4.0
1	D	206	ALA	3.6
1	C	4	ASP	3.5
1	A	239	ALA	3.2
1	C	51	ALA	3.0
1	D	207	ILE	2.8
1	B	207	ILE	2.7
1	A	3	MET	2.6
1	B	36	ARG	2.6
1	D	41	ILE	2.5
1	C	241	GLY	2.5
1	D	178	CYS	2.5
1	D	3	MET	2.3
1	D	38	GLN	2.3
1	A	66	HIS	2.3
1	D	239	ALA	2.3
1	D	36	ARG	2.2
1	B	126	ILE	2.2
1	D	13	SER	2.1
1	A	2	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	81	ARG	2.1
1	A	52	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	267	5/5	0.52	0.23	69,69,77,78	0
3	SO4	D	265	5/5	0.76	0.22	39,40,45,45	5
3	SO4	B	266	5/5	0.77	0.12	83,85,86,86	0
3	SO4	C	266	5/5	0.82	0.30	32,35,37,39	5
3	SO4	D	266	5/5	0.87	0.17	50,52,54,55	5
3	SO4	C	267	5/5	0.89	0.18	41,44,47,48	5
2	HEZ	C	265	8/8	0.91	0.13	35,42,52,53	0
3	SO4	A	268	5/5	0.91	0.15	33,35,37,39	5
3	SO4	A	266	5/5	0.92	0.12	29,38,43,45	1
2	HEZ	A	265	8/8	0.92	0.14	40,42,47,49	0
3	SO4	B	265	5/5	0.94	0.16	30,35,36,36	5
3	SO4	C	268	5/5	0.95	0.09	47,48,52,57	0
3	SO4	A	267	5/5	0.98	0.10	42,45,48,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.