



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 10:08 PM GMT

PDB ID : 3F8P
Title : Structure of Sulfolobus solfataricus TrxR-B3
Authors : Ruggiero, A.; Masullo, M.; Ruocco, M.R.; Arcari, P.; Zagari, A.; Vitagliano, L.
Deposited on : 2008-11-13
Resolution : 1.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

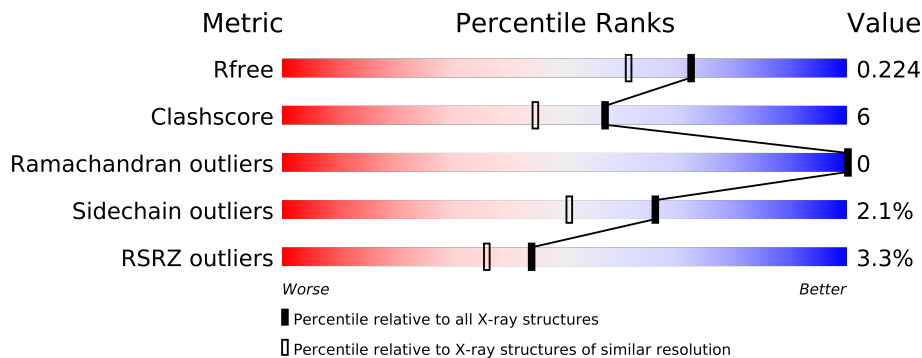
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.80 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	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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. 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	323	
1	B	323	
1	C	323	
1	D	323	

2 Entry composition i

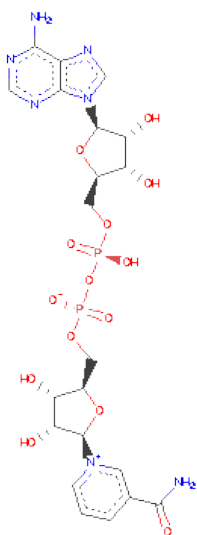
There are 5 unique types of molecules in this entry. The entry contains 9901 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Thioredoxin reductase (TrxB-3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2359	1518	391	444	6			
1	B	306	Total	C	N	O	S	0	0	0
			2351	1514	389	442	6			
1	C	308	Total	C	N	O	S	0	0	0
			2368	1524	393	445	6			
1	D	310	Total	C	N	O	S	0	0	0
			2382	1530	397	449	6			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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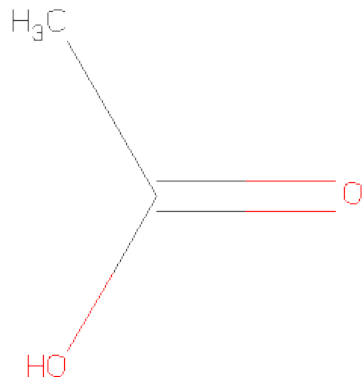
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			26	10	5	9	2		

- Molecule 3 is SULFATE ION (three-letter code: 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		
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	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

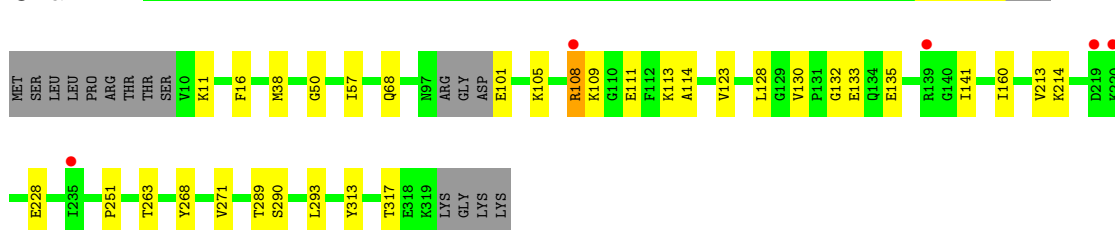
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	76	Total	O	0	0
			76	76		
5	B	73	Total	O	0	0
			73	73		
5	C	81	Total	O	0	0
			81	81		
5	D	70	Total	O	0	0
			70	70		

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.

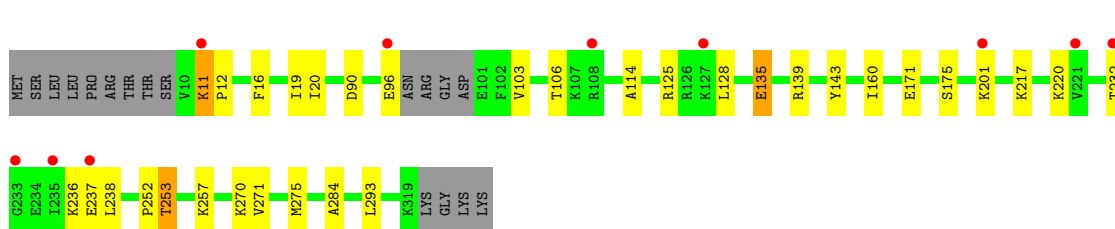
• Molecule 1: Thioredoxin reductase (TrxB-3)

Chain A:



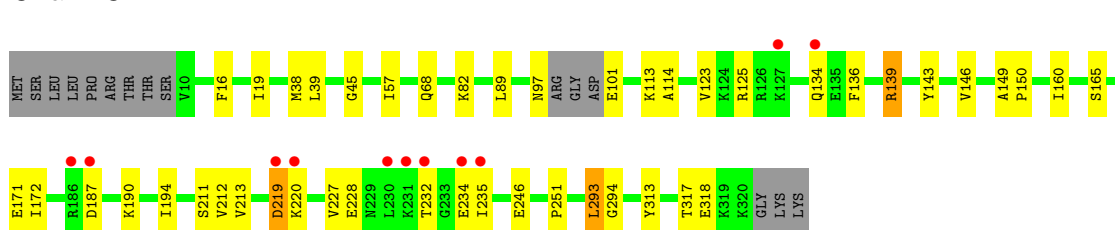
• Molecule 1: Thioredoxin reductase (TrxB-3)

Chain B:



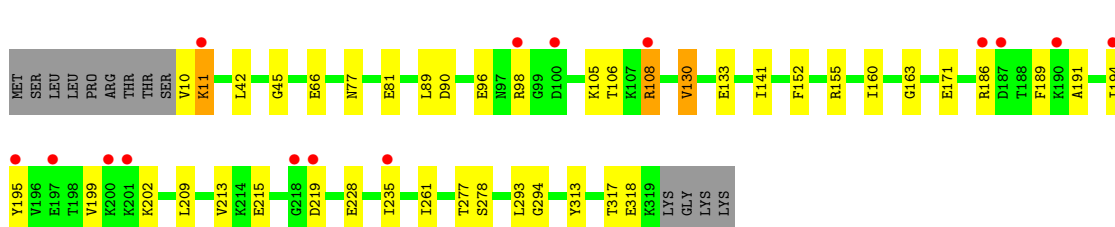
• Molecule 1: Thioredoxin reductase (TrxB-3)

Chain C:



• Molecule 1: Thioredoxin reductase (TrxB-3)

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.77Å 120.68Å 126.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.80 19.97 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-1.80) 98.1 (19.97-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.92 (at 1.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.200 , 0.237 0.199 , 0.224	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 37.3	EDS
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 108720 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9901	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: ACY, SO4, NAD

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	0.69	0/2399	0.78	0/3242
1	B	0.64	0/2391	0.76	0/3231
1	C	0.69	0/2408	0.79	0/3253
1	D	0.63	0/2423	0.77	0/3275
All	All	0.66	0/9621	0.77	0/13001

There are no bond length outliers.

There are no bond angle outliers.

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	2359	0	2417	33	0
1	B	2351	0	2411	23	0
1	C	2368	0	2430	33	0
1	D	2382	0	2438	44	0
2	A	27	0	12	1	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	26	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	15	0	0	0	0
3	B	10	0	0	0	0
3	D	5	0	0	0	0
4	B	4	0	3	0	0
5	A	76	0	0	0	0
5	B	73	0	0	0	0
5	C	81	0	0	0	0
5	D	70	0	0	2	0
All	All	9901	0	9747	124	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 6.

All (124) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:261:ILE:HG23	1:D:277:THR:HG21	1.43	0.96
1:D:228:GLU:HB2	1:D:235:ILE:HD13	1.48	0.92
1:D:202:LYS:HE2	1:D:202:LYS:HA	1.52	0.92
1:D:261:ILE:HG23	1:D:277:THR:CG2	2.03	0.88
1:D:277:THR:HG22	1:D:278:SER:H	1.43	0.82
1:A:289:THR:HG22	1:A:290:SER:N	1.96	0.80
1:C:101:GLU:OE2	1:C:113:LYS:HD3	1.82	0.80
1:D:228:GLU:HB2	1:D:235:ILE:CD1	2.11	0.80
1:A:57:ILE:HD11	1:A:68:GLN:NE2	1.98	0.79
1:A:313:TYR:OH	1:B:171:GLU:HG2	1.83	0.79
1:D:98:ARG:HG2	1:D:98:ARG:O	1.84	0.78
1:A:271:VAL:HG21	1:A:289:THR:HG21	1.65	0.77
1:A:50:GLY:HA2	2:A:4001:NAD:O3B	1.85	0.77
1:B:217:LYS:HE2	1:B:237:GLU:OE1	1.85	0.77
1:A:271:VAL:HG22	1:A:289:THR:CG2	2.14	0.76
1:A:271:VAL:CG2	1:A:289:THR:HG21	2.16	0.76
1:A:132:GLY:HA2	1:A:135:GLU:HG2	1.68	0.75
1:D:277:THR:HG22	1:D:278:SER:N	2.03	0.73
1:D:90:ASP:OD1	1:D:108:ARG:HD2	1.88	0.73
1:D:90:ASP:OD2	1:D:106:THR:HG22	1.88	0.73
1:C:136:PHE:HA	1:C:139:ARG:HG3	1.71	0.72
1:D:277:THR:HG23	5:D:5021:HOH:O	1.89	0.72
1:D:261:ILE:CG2	1:D:277:THR:HG21	2.19	0.72
1:D:202:LYS:CA	1:D:202:LYS:HE2	2.19	0.72
1:C:293:LEU:HD13	1:C:294:GLY:N	2.06	0.71
1:C:160:ILE:CD1	1:C:213:VAL:HG21	2.20	0.70
1:A:271:VAL:CG2	1:A:289:THR:CG2	2.70	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:160:ILE:HD13	1:C:213:VAL:HG21	1.73	0.69
1:B:125:ARG:HD2	1:B:143:TYR:CD2	2.28	0.68
1:A:289:THR:HG22	1:A:290:SER:H	1.58	0.67
1:D:160:ILE:HD11	1:D:213:VAL:HG21	1.77	0.65
1:D:293:LEU:HD13	1:D:294:GLY:N	2.11	0.65
1:B:232:THR:O	1:B:232:THR:HG22	1.96	0.65
1:D:10:VAL:C	1:D:11:LYS:HD2	2.18	0.63
1:B:139:ARG:HD2	1:B:220:LYS:O	2.00	0.61
1:D:277:THR:CG2	5:D:5021:HOH:O	2.48	0.61
1:A:132:GLY:HA2	1:A:135:GLU:CG	2.31	0.59
1:D:90:ASP:OD2	1:D:106:THR:CG2	2.50	0.59
1:A:160:ILE:CD1	1:A:213:VAL:HG21	2.33	0.59
1:C:212:VAL:O	1:C:227:VAL:HG23	2.03	0.58
1:A:108:ARG:NE	1:A:109:LYS:HE3	2.17	0.58
1:C:194:ILE:HG12	1:D:318:GLU:HG2	1.85	0.58
1:D:10:VAL:HG11	1:D:42:LEU:HD13	1.87	0.57
1:D:77:ASN:O	1:D:81:GLU:HG2	2.04	0.57
1:D:228:GLU:CB	1:D:235:ILE:HD13	2.29	0.56
1:C:313:TYR:OH	1:D:171:GLU:HG3	2.05	0.56
1:A:101:GLU:OE2	1:A:113:LYS:HD3	2.07	0.55
1:A:289:THR:CG2	1:A:290:SER:N	2.67	0.55
1:D:163:GLY:C	1:D:191:ALA:HB2	2.26	0.55
1:C:57:ILE:HD11	1:C:68:GLN:HE21	1.72	0.55
1:C:136:PHE:CA	1:C:139:ARG:HG3	2.36	0.54
1:A:108:ARG:CD	1:A:109:LYS:HE3	2.37	0.54
1:C:82:LYS:NZ	1:D:66:GLU:OE2	2.41	0.54
1:B:11:LYS:NZ	1:B:11:LYS:HB2	2.22	0.54
1:B:135:GLU:N	1:B:135:GLU:OE1	2.41	0.53
1:A:105:LYS:HE2	1:A:111:GLU:OE2	2.08	0.53
1:D:98:ARG:O	1:D:98:ARG:CG	2.56	0.53
1:C:125:ARG:HD2	1:C:143:TYR:CD2	2.44	0.53
1:A:317:THR:HB	1:B:171:GLU:OE2	2.09	0.52
1:A:57:ILE:CD1	1:A:68:GLN:NE2	2.70	0.52
1:A:214:LYS:HE3	1:A:228:GLU:OE1	2.10	0.51
1:C:228:GLU:HB2	1:C:235:ILE:HD12	1.92	0.51
1:C:228:GLU:HB2	1:C:235:ILE:CD1	2.41	0.51
1:D:277:THR:CG2	1:D:278:SER:H	2.20	0.50
1:D:293:LEU:C	1:D:293:LEU:HD13	2.32	0.50
1:A:128:LEU:HG	1:A:130:VAL:HG13	1.92	0.50
1:D:96:GLU:OE2	1:D:105:LYS:HE3	2.12	0.50
1:A:160:ILE:HD11	1:A:213:VAL:HG21	1.94	0.50
1:A:108:ARG:HE	1:A:109:LYS:HE3	1.76	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:189:PHE:CZ	1:D:209:LEU:HD21	2.47	0.50
1:C:194:ILE:CG1	1:D:318:GLU:HG2	2.41	0.49
1:B:270:LYS:HD2	1:B:271:VAL:N	2.27	0.49
1:D:277:THR:CG2	1:D:278:SER:N	2.75	0.49
1:D:133:GLU:HA	1:D:141:ILE:CD1	2.42	0.49
1:B:253:THR:HG22	1:B:257:LYS:HE3	1.94	0.49
1:A:133:GLU:HA	1:A:141:ILE:CD1	2.43	0.49
1:C:125:ARG:HH11	1:C:125:ARG:HG3	1.78	0.49
1:D:195:TYR:O	1:D:199:VAL:HG23	2.12	0.48
1:C:136:PHE:C	1:C:139:ARG:HG3	2.33	0.48
1:C:146:VAL:HA	1:C:172:ILE:HD13	1.95	0.48
1:A:289:THR:CG2	1:A:290:SER:H	2.24	0.47
1:B:232:THR:CG2	1:B:232:THR:O	2.61	0.47
1:B:96:GLU:HB3	1:B:103:VAL:HB	1.96	0.47
1:D:90:ASP:CG	1:D:106:THR:HG22	2.34	0.47
1:C:171:GLU:HG3	1:D:313:TYR:OH	2.15	0.47
1:B:236:LYS:HE2	1:B:238:LEU:HD23	1.96	0.47
1:B:16:PHE:O	1:B:114:ALA:HA	2.14	0.47
1:C:318:GLU:HG2	1:D:194:ILE:HD11	1.95	0.47
1:A:123:VAL:HG12	1:A:251:PRO:HA	1.97	0.47
1:C:165:SER:OG	1:C:246:GLU:OE1	2.33	0.46
1:B:90:ASP:OD2	1:B:106:THR:HB	2.15	0.46
1:A:38:MET:HG2	1:B:175:SER:HB3	1.97	0.46
1:C:19:ILE:HD12	1:C:114:ALA:HB2	1.98	0.46
1:C:57:ILE:CD1	1:C:68:GLN:NE2	2.79	0.46
1:C:57:ILE:HD11	1:C:68:GLN:NE2	2.31	0.46
1:A:271:VAL:HG13	1:A:289:THR:HG23	1.99	0.45
1:A:293:LEU:HD23	1:A:293:LEU:C	2.37	0.45
1:D:160:ILE:CD1	1:D:213:VAL:HG21	2.44	0.45
1:C:219:ASP:HB3	1:C:220:LYS:H	1.50	0.45
1:B:19:ILE:HG13	1:B:114:ALA:HB2	1.99	0.45
1:C:232:THR:CG2	1:C:234:GLU:HB2	2.47	0.45
1:A:160:ILE:HD13	1:A:213:VAL:HG21	1.98	0.44
1:C:313:TYR:O	1:C:317:THR:HG23	2.18	0.44
1:A:16:PHE:O	1:A:114:ALA:HA	2.18	0.43
1:D:90:ASP:HB3	1:D:106:THR:HG21	2.00	0.43
1:B:217:LYS:CE	1:B:237:GLU:OE1	2.62	0.43
1:C:123:VAL:HG12	1:C:251:PRO:HA	2.00	0.43
1:C:211:SER:HB3	1:C:227:VAL:CG2	2.49	0.42
1:B:11:LYS:HG3	1:B:12:PRO:HD2	2.01	0.42
1:C:149:ALA:HB3	1:C:150:PRO:HD3	2.02	0.42
1:C:16:PHE:O	1:C:114:ALA:HA	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:313:TYR:O	1:D:317:THR:HG23	2.20	0.41
1:B:201:LYS:HE3	1:B:201:LYS:HB2	1.88	0.41
1:A:108:ARG:HG2	1:A:109:LYS:HG2	2.01	0.41
1:C:45:GLY:O	1:C:89:LEU:HA	2.21	0.41
1:D:130:VAL:CG2	1:D:215:GLU:HA	2.51	0.41
1:D:152:PHE:HA	1:D:155:ARG:HD3	2.02	0.41
1:D:81:GLU:HA	1:D:81:GLU:OE1	2.19	0.41
1:A:263:THR:HA	1:A:268:TYR:O	2.20	0.40
1:D:45:GLY:O	1:D:89:LEU:HA	2.21	0.40
1:B:128:LEU:HD21	1:B:160:ILE:HD13	2.02	0.40
1:C:39:LEU:HD11	1:C:313:TYR:HA	2.03	0.40
1:B:253:THR:CG2	1:B:257:LYS:HE3	2.51	0.40
1:B:275:MET:HB3	1:B:284:ALA: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	303/323 (94%)	296 (98%)	7 (2%)	0	100	100
1	B	302/323 (94%)	293 (97%)	9 (3%)	0	100	100
1	C	304/323 (94%)	299 (98%)	5 (2%)	0	100	100
1	D	308/323 (95%)	302 (98%)	6 (2%)	0	100	100
All	All	1217/1292 (94%)	1190 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	253/267 (95%)	251 (99%)	2 (1%)	89	85
1	B	252/267 (94%)	246 (98%)	6 (2%)	61	44
1	C	254/267 (95%)	246 (97%)	8 (3%)	52	33
1	D	255/267 (96%)	250 (98%)	5 (2%)	68	53
All	All	1014/1068 (95%)	993 (98%)	21 (2%)	66	51

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	108	ARG
1	B	11	LYS
1	B	20	ILE
1	B	135	GLU
1	B	252	PRO
1	B	253	THR
1	B	293	LEU
1	C	38	MET
1	C	97	ASN
1	C	134	GLN
1	C	139	ARG
1	C	187	ASP
1	C	190	LYS
1	C	219	ASP
1	C	293	LEU
1	D	11	LYS
1	D	108	ARG
1	D	130	VAL
1	D	186	ARG
1	D	219	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	134	GLN
1	A	184	HIS
1	B	68	GLN
1	B	134	GLN
1	C	68	GLN

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Mol	Chain	Res	Type
1	C	77	ASN
1	C	210	ASN
1	D	68	GLN
1	D	77	ASN
1	D	134	GLN

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 ⓘ

11 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	NAD	A	4001	-	29,29,48	2.15	7 (24%)	45,45,73	1.26	4 (8%)
3	SO4	A	4157	-	4,4,4	3.51	2 (50%)	6,6,6	1.03	0
3	SO4	A	4159	-	4,4,4	3.20	2 (50%)	6,6,6	0.86	0
3	SO4	A	4160	-	4,4,4	3.51	2 (50%)	6,6,6	0.86	0
4	ACY	B	1501	-	3,3,3	1.28	0	3,3,3	1.18	0
2	NAD	B	4002	-	29,29,48	1.99	4 (13%)	45,45,73	0.86	1 (2%)
3	SO4	B	4158	-	4,4,4	3.34	2 (50%)	6,6,6	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	B	4161	-	4,4,4	3.47	2 (50%)	6,6,6	0.83	0
2	NAD	C	4003	-	29,29,48	1.64	4 (13%)	45,45,73	1.22	3 (6%)
2	NAD	D	4004	-	26,28,48	1.44	6 (23%)	38,42,73	1.12	3 (7%)
3	SO4	D	4162	-	4,4,4	3.39	2 (50%)	6,6,6	0.80	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	NAD	A	4001	-	-	0/16/32/62	0/1/3/5
3	SO4	A	4157	-	-	0/0/0/0	0/0/0/0
3	SO4	A	4159	-	-	0/0/0/0	0/0/0/0
3	SO4	A	4160	-	-	0/0/0/0	0/0/0/0
4	ACY	B	1501	-	-	0/0/0/0	0/0/0/0
2	NAD	B	4002	-	-	0/16/32/62	0/1/3/5
3	SO4	B	4158	-	-	0/0/0/0	0/0/0/0
3	SO4	B	4161	-	-	0/0/0/0	0/0/0/0
2	NAD	C	4003	-	-	0/16/32/62	0/1/3/5
2	NAD	D	4004	-	-	0/13/31/62	0/1/3/5
3	SO4	D	4162	-	-	0/0/0/0	0/0/0/0

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4002	NAD	PN-O5D	7.94	1.65	1.51
2	A	4001	NAD	PN-O5D	7.11	1.63	1.51
2	C	4003	NAD	PN-O5D	6.85	1.63	1.51
2	A	4001	NAD	PN-O1N	-5.96	1.40	1.51
3	B	4161	SO4	O3-S	-5.13	1.29	1.47
3	A	4157	SO4	O3-S	-5.03	1.30	1.47
3	A	4160	SO4	O1-S	4.94	1.63	1.47
3	A	4160	SO4	O3-S	-4.92	1.30	1.47
3	A	4157	SO4	O1-S	4.81	1.62	1.47
3	D	4162	SO4	O1-S	4.78	1.62	1.47
3	B	4158	SO4	O1-S	4.68	1.62	1.47
3	B	4158	SO4	O3-S	-4.67	1.31	1.47
3	A	4159	SO4	O3-S	-4.63	1.31	1.47
3	D	4162	SO4	O3-S	-4.56	1.31	1.47
3	B	4161	SO4	O1-S	4.54	1.61	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4002	NAD	C2B-C1B	-4.43	1.47	1.53
3	A	4159	SO4	O1-S	4.29	1.61	1.47
2	D	4004	NAD	C4A-N3A	3.58	1.41	1.35
2	A	4001	NAD	PN-O2N	-3.39	1.46	1.51
2	B	4002	NAD	PN-O1N	-3.00	1.46	1.51
2	D	4004	NAD	O3B-C3B	2.85	1.49	1.43
2	D	4004	NAD	C2B-C1B	-2.63	1.49	1.53
2	D	4004	NAD	PN-O1N	2.59	1.49	1.46
2	D	4004	NAD	C8A-N9A	2.48	1.40	1.36
2	A	4001	NAD	C2B-C3B	-2.44	1.46	1.53
2	B	4002	NAD	C4A-N3A	2.36	1.39	1.35
2	C	4003	NAD	C8A-N9A	2.31	1.40	1.36
2	A	4001	NAD	O4B-C4B	-2.19	1.39	1.45
2	C	4003	NAD	O3B-C3B	2.17	1.48	1.43
2	A	4001	NAD	C1B-N9A	-2.14	1.42	1.48
2	C	4003	NAD	C2A-N3A	2.10	1.36	1.32
2	D	4004	NAD	O4B-C4B	-2.03	1.40	1.45
2	A	4001	NAD	C2B-C1B	-2.01	1.50	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4001	NAD	C4B-O4B-C1B	-4.41	104.96	109.75
2	C	4003	NAD	O4B-C1B-N9A	-4.32	104.42	108.44
2	D	4004	NAD	O4B-C1B-N9A	-2.76	105.87	108.44
2	D	4004	NAD	C4A-C5A-N7A	2.76	111.88	109.52
2	A	4001	NAD	C4A-C5A-N7A	2.56	111.71	109.52
2	C	4003	NAD	O4B-C1B-C2B	-2.44	103.03	106.77
2	A	4001	NAD	N3A-C2A-N1A	-2.44	126.67	128.71
2	B	4002	NAD	C4B-O4B-C1B	-2.34	107.21	109.75
2	C	4003	NAD	N3A-C2A-N1A	-2.26	126.82	128.71
2	A	4001	NAD	O2N-PN-O3	2.23	113.14	105.27
2	D	4004	NAD	C2B-C1B-N9A	2.12	118.72	113.27

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, 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	307/323 (95%)	-0.03	5 (1%) 68 64	6, 18, 36, 45	0
1	B	306/323 (94%)	0.26	10 (3%) 44 36	8, 23, 42, 54	0
1	C	308/323 (95%)	0.06	11 (3%) 41 33	7, 18, 41, 57	0
1	D	310/323 (95%)	0.14	15 (4%) 29 23	7, 20, 46, 56	0
All	All	1231/1292 (95%)	0.11	41 (3%) 44 36	6, 20, 42, 57	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	194	ILE	5.5
1	D	200	LYS	5.1
1	B	11	LYS	4.7
1	C	127	LYS	4.0
1	C	219	ASP	3.6
1	D	98	ARG	3.4
1	B	127	LYS	3.3
1	C	235	ILE	3.3
1	B	235	ILE	3.1
1	A	219	ASP	3.1
1	D	201	LYS	3.1
1	A	220	LYS	3.0
1	D	11	LYS	3.0
1	B	108	ARG	2.9
1	C	230	LEU	2.9
1	C	187	ASP	2.9
1	A	108	ARG	2.9
1	B	201	LYS	2.7
1	C	186	ARG	2.7
1	C	232	THR	2.6
1	C	234	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	220	LYS	2.5
1	B	96	GLU	2.4
1	B	237	GLU	2.4
1	C	134	GLN	2.4
1	C	231	LYS	2.4
1	D	187	ASP	2.4
1	A	235	ILE	2.3
1	D	186	ARG	2.3
1	D	195	TYR	2.2
1	B	232	THR	2.2
1	D	190	LYS	2.2
1	D	197	GLU	2.1
1	D	100	ASP	2.1
1	D	219	ASP	2.1
1	D	218	GLY	2.1
1	B	233	GLY	2.1
1	D	235	ILE	2.0
1	B	221	VAL	2.0
1	A	139	ARG	2.0
1	D	108	ARG	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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	ACY	B	1501	4/4	0.16	1.58	25,29,29,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SO4	A	4157	5/5	0.16	0.52	55,55,56,57	0
3	SO4	A	4160	5/5	0.18	0.34	56,56,57,57	0
3	SO4	B	4158	5/5	0.14	0.27	44,44,45,48	0
3	SO4	A	4159	5/5	0.11	-0.16	47,48,49,50	0
3	SO4	B	4161	5/5	0.10	-0.38	46,47,48,49	0
3	SO4	D	4162	5/5	0.11	-0.41	41,42,43,43	0
2	NAD	D	4004	26/44	0.08	-0.51	10,14,18,18	0
2	NAD	B	4002	27/44	0.09	-0.63	14,23,26,32	0
2	NAD	A	4001	27/44	0.09	-0.65	10,14,18,35	0
2	NAD	C	4003	27/44	0.07	-0.89	10,12,16,21	0

6.5 Other polymers

There are no such residues in this entry.