



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 11:57 PM GMT

PDB ID : 1EV4
Title : RAT GLUTATHIONE S-TRANSFERASE A1-1: MUTANT W21F/F220Y
WITH GSO3 BOUND
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G.; Ibarra, C.; Atkins, W.M.
Deposited on : 2000-04-19
Resolution : 2.20 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>

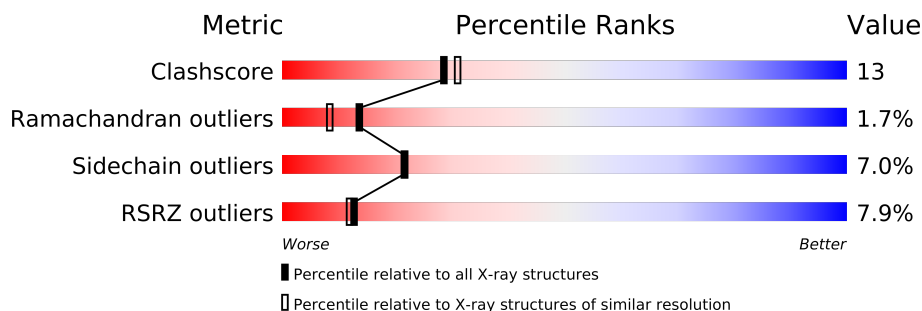
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.20 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))
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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	221	
1	C	221	
1	D	221	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5599 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 GLUTATHIONE S-TRANSFERASE A1-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1786	1152	299	324	11			
1	C	207	Total	C	N	O	S	0	0	0
			1664	1073	278	302	11			
1	D	221	Total	C	N	O	S	0	0	0
			1786	1152	299	324	11			

There are 9 discrepancies between the modelled and reference sequences:

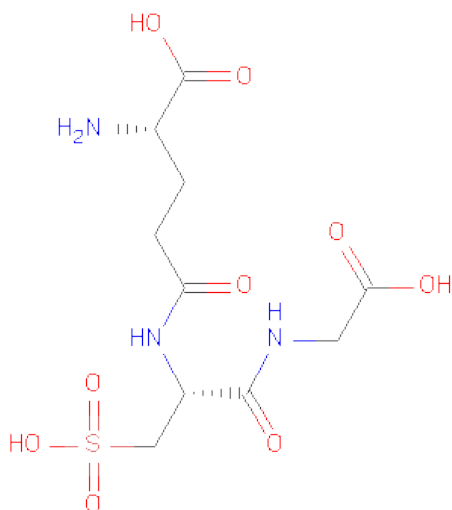
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	PHE	TRP	ENGINEERED	UNP P00502
A	96	SER	THR	CONFLICT	UNP P00502
A	220	TYR	PHE	ENGINEERED	UNP P00502
C	21	PHE	TRP	ENGINEERED	UNP P00502
C	96	SER	THR	CONFLICT	UNP P00502
C	220	TYR	PHE	ENGINEERED	UNP P00502
D	21	PHE	TRP	ENGINEERED	UNP P00502
D	96	SER	THR	CONFLICT	UNP P00502
D	220	TYR	PHE	ENGINEERED	UNP P00502

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



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

- Molecule 3 is GLUTATHIONE SULFONIC ACID (three-letter code: GTS) (formula: $C_{10}H_{17}N_3O_9S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			23	10	3	9	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	S	0	0
			23	10	3	9	1		
3	D	1	Total	C	N	O	S	0	0
			23	10	3	9	1		

- Molecule 4 is water.

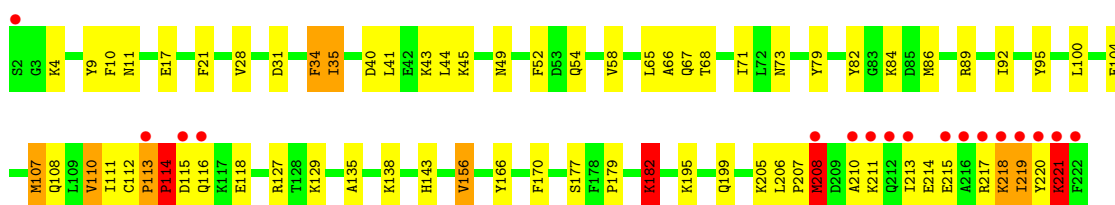
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	126	Total	O	0	0
			126	126		
4	C	56	Total	O	0	0
			56	56		
4	D	97	Total	O	0	0
			97	97		

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.

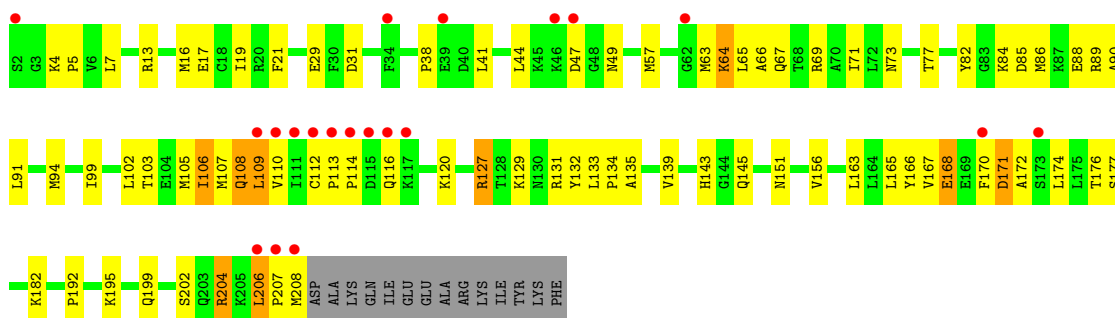
• Molecule 1: GLUTATHIONE S-TRANSFERASE A1-1

Chain A: 



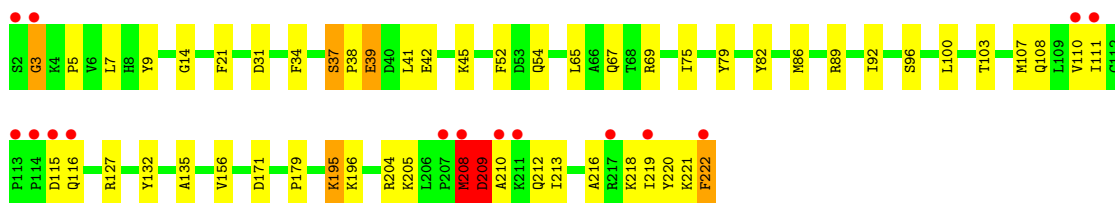
• Molecule 1: GLUTATHIONE S-TRANSFERASE A1-1

Chain C: 



• Molecule 1: GLUTATHIONE S-TRANSFERASE A1-1

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	84.60Å 275.20Å 70.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.82 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.20) 77.2 (19.82-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 1.80Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.218 , 0.285 0.240 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 74.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 61093 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5599	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: GTS, 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	0.66	0/1818	1.09	17/2440 (0.7%)
1	C	0.62	0/1694	1.01	5/2276 (0.2%)
1	D	0.61	0/1818	1.00	8/2440 (0.3%)
All	All	0.63	0/5330	1.03	30/7156 (0.4%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	222	PHE	N-CA-CB	-7.39	97.29	110.60
1	A	182	LYS	CB-CG-CD	7.20	130.32	111.60
1	D	31	ASP	CA-CB-CG	7.00	128.80	113.40
1	A	218	LYS	CB-CG-CD	6.81	129.30	111.60
1	A	170	PHE	N-CA-CB	-6.71	98.52	110.60
1	A	35	ILE	CG1-CB-CG2	6.70	126.13	111.40
1	C	206	LEU	N-CA-CB	-6.67	97.05	110.40
1	C	31	ASP	CA-CB-CG	6.43	127.54	113.40
1	A	107	MET	CB-CA-C	-6.42	97.56	110.40
1	A	4	LYS	N-CA-CB	-6.38	99.12	110.60
1	A	129	LYS	CB-CG-CD	-6.38	95.01	111.60
1	A	84	LYS	N-CA-CB	-6.26	99.33	110.60
1	A	208	MET	N-CA-CB	-6.14	99.54	110.60
1	D	37	SER	N-CA-CB	-5.99	101.52	110.50
1	A	4	LYS	CB-CG-CD	-5.76	96.61	111.60
1	C	206	LEU	CB-CA-C	5.76	121.15	110.20
1	C	105	MET	N-CA-CB	-5.71	100.31	110.60
1	A	34	PHE	CB-CA-C	-5.70	98.99	110.40
1	A	129	LYS	CG-CD-CE	5.62	128.77	111.90
1	A	31	ASP	CA-CB-CG	5.42	125.33	113.40
1	D	209	ASP	N-CA-CB	5.33	120.20	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	31	ASP	N-CA-CB	-5.28	101.11	110.60
1	D	39	GLU	N-CA-CB	5.17	119.91	110.60
1	A	221	LYS	CB-CG-CD	5.14	124.95	111.60
1	D	196	LYS	CB-CG-CD	-5.10	98.33	111.60
1	D	195	LYS	N-CA-CB	-5.10	101.42	110.60
1	D	7	LEU	CB-CG-CD1	-5.05	102.42	111.00
1	A	219	ILE	CG1-CB-CG2	-5.04	100.30	111.40
1	A	43	LYS	N-CA-CB	5.02	119.64	110.60
1	A	118	GLU	CB-CA-C	-5.00	100.40	110.40

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	1786	0	1852	52	0
1	C	1664	0	1726	55	0
1	D	1786	0	1852	31	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	23	0	14	1	0
3	C	23	0	14	0	0
3	D	23	0	14	1	0
4	A	126	0	0	16	0
4	C	56	0	0	10	0
4	D	97	0	0	6	0
All	All	5599	0	5472	135	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 13.

All (135) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:10:PHE:HA	4:A:790:HOH:O	1.63	0.97
1:A:86:MET:HA	4:A:757:HOH:O	1.73	0.87
1:C:206:LEU:HB3	1:C:207:PRO:HD2	1.66	0.76
1:C:91:LEU:HA	4:C:735:HOH:O	1.85	0.75
1:A:73:ASN:HB3	4:A:455:HOH:O	1.87	0.75
1:A:92:ILE:HG23	1:A:156:VAL:HG22	1.68	0.73
1:C:108:GLN:HE22	1:C:112:CYS:HB3	1.53	0.72
1:A:179:PRO:O	1:A:182:LYS:HG2	1.89	0.71
1:A:179:PRO:HA	1:A:182:LYS:HE2	1.73	0.70
1:A:208:MET:SD	1:A:208:MET:N	2.63	0.70
1:D:107:MET:O	1:D:110:VAL:HG12	1.93	0.69
1:C:7:LEU:HB3	1:C:16:MET:HE3	1.73	0.68
1:A:35:ILE:HB	4:A:790:HOH:O	1.93	0.67
1:A:210:ALA:HB3	1:A:211:LYS:NZ	2.09	0.67
1:C:29:GLU:HG2	4:C:557:HOH:O	1.94	0.67
1:C:109:LEU:HD23	1:C:110:VAL:HG13	1.78	0.65
1:A:104:GLU:HA	1:A:107:MET:HG2	1.78	0.65
1:C:112:CYS:SG	1:C:120:LYS:HD2	2.36	0.64
1:A:49:ASN:HB2	4:A:768:HOH:O	1.97	0.64
1:D:110:VAL:HG11	1:D:208:MET:HG3	1.81	0.62
1:D:209:ASP:HB3	1:D:212:GLN:HB2	1.82	0.60
1:C:65:LEU:HD13	1:C:71:ILE:HA	1.82	0.60
1:C:102:LEU:HD23	1:C:163:LEU:HD21	1.84	0.59
1:A:89:ARG:HB2	4:A:757:HOH:O	2.03	0.58
1:C:133:LEU:HB2	1:C:134:PRO:HD3	1.86	0.57
1:C:65:LEU:HB3	1:C:71:ILE:HG12	1.85	0.57
1:C:176:THR:HA	1:C:182:LYS:NZ	2.20	0.56
1:C:49:ASN:HB2	4:C:733:HOH:O	2.05	0.56
1:D:38:PRO:HD3	1:D:220:TYR:O	2.05	0.56
1:A:73:ASN:ND2	4:A:651:HOH:O	2.38	0.56
1:A:41:LEU:HD23	1:A:221:LYS:HG2	1.87	0.55
1:A:35:ILE:CB	4:A:790:HOH:O	2.53	0.55
1:A:177:SER:N	4:A:774:HOH:O	2.40	0.55
1:A:220:TYR:O	1:A:221:LYS:HB2	2.06	0.55
1:D:34:PHE:CZ	1:D:205:LYS:HE3	2.42	0.54
1:C:167:VAL:HG13	1:C:174:LEU:HD12	1.89	0.54
1:C:134:PRO:HD2	4:C:783:HOH:O	2.06	0.54
1:C:38:PRO:O	1:C:41:LEU:HB3	2.07	0.54
1:A:35:ILE:HG23	1:A:40:ASP:HB2	1.89	0.54
1:D:39:GLU:N	4:D:775:HOH:O	2.42	0.53
1:C:13:ARG:HH21	1:C:204:ARG:NH1	2.07	0.52
1:D:96:SER:O	1:D:100:LEU:HD22	2.09	0.52
1:A:207:PRO:HD2	4:A:570:HOH:O	2.08	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:195:LYS:HE3	4:A:699:HOH:O	2.09	0.51
1:C:108:GLN:NE2	1:C:112:CYS:HB3	2.25	0.51
1:D:218:LYS:HA	1:D:221:LYS:HD2	1.92	0.51
1:A:220:TYR:O	3:A:230:GTS:HA32	2.10	0.51
1:C:47:ASP:HB2	4:C:733:HOH:O	2.10	0.51
1:D:3:GLY:O	1:D:5:PRO:HD3	2.11	0.51
1:A:66:ALA:O	1:A:67:GLN:HB2	2.11	0.51
1:C:106:ILE:O	1:C:109:LEU:HD22	2.10	0.51
1:A:215:GLU:O	1:A:218:LYS:HG3	2.10	0.51
1:A:210:ALA:O	1:A:213:ILE:HG22	2.11	0.50
1:C:73:ASN:HB2	4:C:601:HOH:O	2.11	0.50
1:A:41:LEU:HD23	1:A:219:ILE:O	2.11	0.50
1:A:34:PHE:CZ	1:A:205:LYS:HE3	2.47	0.50
1:C:103:THR:O	1:C:107:MET:HG2	2.12	0.50
1:D:92:ILE:HG23	1:D:156:VAL:HG13	1.94	0.50
1:C:145:GLN:HB3	1:C:151:ASN:OD1	2.11	0.49
1:C:131:ARG:N	4:C:783:HOH:O	2.43	0.49
1:D:216:ALA:HA	1:D:219:ILE:HD12	1.94	0.49
1:A:113:PRO:HB2	1:A:116:GLN:NE2	2.28	0.49
1:A:52:PHE:O	1:A:54:GLN:HG3	2.13	0.48
1:A:89:ARG:HD2	4:A:456:HOH:O	2.12	0.48
1:C:66:ALA:O	1:C:67:GLN:HB2	2.13	0.48
1:A:210:ALA:HB3	1:A:211:LYS:HZ2	1.78	0.48
1:D:9:TYR:OH	1:D:14:GLY:HA3	2.13	0.48
1:D:34:PHE:HZ	1:D:205:LYS:CE	2.27	0.48
1:C:135:ALA:O	1:C:139:VAL:HG23	2.14	0.48
1:C:13:ARG:HH21	1:C:204:ARG:HH12	1.63	0.47
1:C:113:PRO:HD2	1:C:116:GLN:OE1	2.13	0.47
1:A:110:VAL:HG23	1:A:111:ILE:HD12	1.97	0.47
1:C:4:LYS:HD2	4:C:582:HOH:O	2.14	0.47
1:A:95:TYR:HB2	1:A:156:VAL:HG11	1.97	0.47
1:D:110:VAL:HG13	1:D:111:ILE:HG13	1.97	0.47
1:C:99:ILE:HG23	1:C:163:LEU:HD22	1.97	0.47
1:C:90:ALA:HA	4:D:342:HOH:O	2.14	0.47
1:A:218:LYS:HG3	1:A:219:ILE:N	2.30	0.46
1:D:34:PHE:HB2	4:D:562:HOH:O	2.15	0.46
1:A:195:LYS:O	1:A:199:GLN:HG3	2.15	0.46
1:C:163:LEU:O	1:C:167:VAL:HG23	2.15	0.46
1:D:195:LYS:HD2	4:D:734:HOH:O	2.15	0.46
1:C:17:GLU:HG2	1:C:166:TYR:OH	2.14	0.46
1:A:210:ALA:C	1:A:213:ILE:HG22	2.36	0.46
1:C:69:ARG:CZ	1:D:69:ARG:NH1	2.79	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:179:PRO:HG3	4:D:793:HOH:O	2.15	0.46
1:C:16:MET:SD	1:C:19:ILE:HD12	2.56	0.46
1:D:34:PHE:CZ	1:D:205:LYS:CE	2.98	0.46
1:D:41:LEU:HG	1:D:45:LYS:HE3	1.97	0.46
1:C:63:MET:C	1:C:64:LYS:HD2	2.36	0.46
1:D:132:TYR:O	1:D:135:ALA:HB3	2.16	0.46
1:A:135:ALA:O	1:A:138:LYS:HB3	2.16	0.46
1:A:104:GLU:O	1:A:108:GLN:HG3	2.16	0.45
1:D:37:SER:HA	1:D:220:TYR:O	2.16	0.45
1:A:218:LYS:HG3	1:A:219:ILE:H	1.81	0.45
1:C:86:MET:HA	1:C:89:ARG:HE	1.82	0.45
1:C:13:ARG:HB2	1:C:208:MET:SD	2.56	0.45
1:C:77:THR:HG21	1:D:89:ARG:HH22	1.82	0.45
1:A:35:ILE:N	4:A:790:HOH:O	2.46	0.45
1:C:94:MET:HB3	4:C:735:HOH:O	2.14	0.45
1:A:68:THR:N	4:A:742:HOH:O	2.48	0.45
1:A:206:LEU:HG	4:A:591:HOH:O	2.17	0.45
1:D:75:ILE:HG23	1:D:79:TYR:CD2	2.52	0.44
1:A:89:ARG:HB3	4:A:456:HOH:O	2.17	0.44
1:C:5:PRO:HD2	1:C:29:GLU:O	2.18	0.44
1:C:202:SER:OG	1:C:204:ARG:HB3	2.18	0.44
1:A:112:CYS:HA	1:A:113:PRO:HD3	1.86	0.44
1:A:58:VAL:HG23	1:A:71:ILE:HD13	2.00	0.44
1:A:17:GLU:HG2	1:A:166:TYR:OH	2.17	0.43
1:A:213:ILE:O	1:A:217:ARG:HG3	2.18	0.43
1:C:7:LEU:HD13	1:C:16:MET:SD	2.59	0.43
1:A:11:ASN:HD22	1:A:205:LYS:HE3	1.82	0.43
1:D:52:PHE:O	1:D:54:GLN:HG3	2.18	0.43
1:C:165:LEU:O	1:C:168:GLU:HB3	2.18	0.43
1:D:103:THR:O	1:D:107:MET:HG2	2.19	0.43
1:A:41:LEU:O	1:A:45:LYS:HG3	2.19	0.43
1:C:57:MET:HA	1:C:65:LEU:O	2.18	0.42
1:C:195:LYS:O	1:C:199:GLN:HG3	2.19	0.42
1:C:129:LYS:HE3	1:C:129:LYS:HB2	1.79	0.42
1:C:143:HIS:CE1	1:C:145:GLN:HB2	2.54	0.42
1:D:67:GLN:HA	3:D:250:GTS:O11	2.19	0.42
1:A:28:VAL:HG21	1:A:79:TYR:CZ	2.55	0.42
1:C:127:ARG:O	1:C:131:ARG:HB3	2.20	0.41
1:C:132:TYR:N	4:C:783:HOH:O	2.53	0.41
1:A:112:CYS:O	1:A:114:PRO:HD3	2.20	0.41
1:C:112:CYS:CB	1:C:120:LYS:HD2	2.51	0.41
1:A:215:GLU:O	1:A:219:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:39:GLU:HG3	4:D:775:HOH:O	2.20	0.41
1:C:77:THR:HG21	1:D:86:MET:HB3	2.01	0.41
1:C:170:PHE:O	1:C:171:ASP:HB2	2.20	0.41
1:D:110:VAL:O	1:D:213:ILE:HD12	2.21	0.41
1:A:9:TYR:CG	1:A:10:PHE:N	2.89	0.41
1:D:218:LYS:HB3	1:D:218:LYS:HE2	1.77	0.40
1:C:86:MET:N	1:C:89:ARG:HH21	2.18	0.40
1:C:85:ASP:OD1	1:C:88:GLU:HG3	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	219/221 (99%)	199 (91%)	16 (7%)	4 (2%)	13	7
1	C	205/221 (93%)	186 (91%)	17 (8%)	2 (1%)	22	18
1	D	219/221 (99%)	203 (93%)	11 (5%)	5 (2%)	10	5
All	All	643/663 (97%)	588 (91%)	44 (7%)	11 (2%)	14	8

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	PRO
1	A	221	LYS
1	D	208	MET
1	C	171	ASP
1	D	210	ALA
1	D	209	ASP
1	C	172	ALA
1	D	171	ASP
1	A	110	VAL
1	A	113	PRO
1	D	3	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	195/195 (100%)	181 (93%)	14 (7%)	21	20
1	C	183/195 (94%)	168 (92%)	15 (8%)	17	15
1	D	195/195 (100%)	184 (94%)	11 (6%)	30	33
All	All	573/585 (98%)	533 (93%)	40 (7%)	21	22

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	PHE
1	A	44	LEU
1	A	65	LEU
1	A	82	TYR
1	A	100	LEU
1	A	114	PRO
1	A	115	ASP
1	A	127	ARG
1	A	143	HIS
1	A	156	VAL
1	A	182	LYS
1	A	208	MET
1	A	214	GLU
1	A	221	LYS
1	C	21	PHE
1	C	44	LEU
1	C	64	LYS
1	C	82	TYR
1	C	84	LYS
1	C	106	ILE
1	C	108	GLN
1	C	109	LEU
1	C	114	PRO
1	C	127	ARG
1	C	156	VAL
1	C	168	GLU
1	C	177	SER

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Mol	Chain	Res	Type
1	C	192	PRO
1	C	204	ARG
1	D	21	PHE
1	D	42	GLU
1	D	65	LEU
1	D	82	TYR
1	D	108	GLN
1	D	115	ASP
1	D	116	GLN
1	D	127	ARG
1	D	204	ARG
1	D	208	MET
1	D	222	PHE

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	11	ASN
1	A	116	GLN
1	A	199	GLN
1	C	108	GLN
1	C	193	ASN
1	C	199	GLN
1	D	36	GLN
1	D	49	ASN
1	D	108	GLN
1	D	193	ASN
1	D	199	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

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	$\# Z > 2$
3	GTS	A	230	-	22,22,22	1.18	3 (13%)	30,30,30	1.38	3 (10%)
2	SO4	A	260	-	4,4,4	1.16	0	6,6,6	0.34	0
3	GTS	C	240	-	22,22,22	1.16	1 (4%)	30,30,30	1.43	4 (13%)
2	SO4	C	261	-	4,4,4	0.97	0	6,6,6	0.20	0
3	GTS	D	250	-	22,22,22	1.17	3 (13%)	30,30,30	1.42	5 (16%)
2	SO4	D	262	-	4,4,4	0.94	0	6,6,6	0.18	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
3	GTS	A	230	-	-	0/27/27/27	0/0/0/0
2	SO4	A	260	-	-	0/0/0/0	0/0/0/0
3	GTS	C	240	-	-	0/27/27/27	0/0/0/0
2	SO4	C	261	-	-	0/0/0/0	0/0/0/0
3	GTS	D	250	-	-	0/27/27/27	0/0/0/0
2	SO4	D	262	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	230	GTS	CB2-SG2	4.07	1.82	1.77
3	C	240	GTS	CB2-SG2	4.07	1.82	1.77
3	D	250	GTS	CB2-SG2	3.04	1.81	1.77
3	D	250	GTS	O31-C3	-2.18	1.22	1.30
3	D	250	GTS	O12-C1	-2.13	1.22	1.30
3	A	230	GTS	O31-C3	-2.07	1.23	1.30
3	A	230	GTS	O12-C1	-2.02	1.23	1.30

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	240	GTS	O3S-SG2-CB2	4.59	111.55	105.64
3	A	230	GTS	O3S-SG2-CB2	4.42	111.33	105.64
3	D	250	GTS	O3S-SG2-CB2	4.35	111.24	105.64
3	D	250	GTS	CG1-CB1-CA1	-2.80	109.20	114.43
3	D	250	GTS	C1-CA1-N1	-2.52	105.20	109.36
3	A	230	GTS	C1-CA1-N1	-2.47	105.28	109.36
3	C	240	GTS	CA2-CB2-SG2	2.36	118.25	114.66
3	D	250	GTS	O1S-SG2-CB2	2.36	111.16	107.03
3	C	240	GTS	O1S-SG2-CB2	2.31	111.08	107.03
3	A	230	GTS	O1S-SG2-CB2	2.22	110.93	107.03
3	D	250	GTS	CB2-CA2-C2	-2.13	104.93	109.83
3	C	240	GTS	CG1-CB1-CA1	-2.12	110.47	114.43

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	221/221 (100%)	0.08	17 (7%)	13 13	16, 27, 95, 100	0
1	C	207/221 (93%)	0.46	20 (9%)	8 7	26, 47, 88, 100	0
1	D	221/221 (100%)	0.05	15 (6%)	17 16	23, 35, 81, 100	0
All	All	649/663 (97%)	0.19	52 (8%)	13 11	16, 38, 86, 100	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	216	ALA	21.6
1	A	222	PHE	10.4
1	A	219	ILE	9.4
1	C	2	SER	9.1
1	A	211	LYS	8.3
1	A	212	GLN	7.5
1	C	112	CYS	7.5
1	A	220	TYR	7.4
1	D	2	SER	6.7
1	D	222	PHE	6.4
1	A	2	SER	6.2
1	A	215	GLU	6.0
1	C	113	PRO	5.8
1	C	207	PRO	5.6
1	D	3	GLY	5.6
1	A	217	ARG	5.5
1	A	221	LYS	5.5
1	C	115	ASP	5.3
1	C	208	MET	5.0
1	A	213	ILE	4.3
1	C	116	GLN	4.2
1	C	114	PRO	3.7
1	A	208	MET	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	208	MET	3.6
1	D	114	PRO	3.6
1	A	115	ASP	3.4
1	A	210	ALA	3.4
1	C	39	GLU	3.4
1	C	109	LEU	3.4
1	C	170	PHE	3.3
1	C	111	ILE	3.2
1	C	110	VAL	3.2
1	C	206	LEU	3.1
1	C	34	PHE	3.1
1	A	113	PRO	3.1
1	D	217	ARG	3.0
1	D	115	ASP	2.9
1	C	173	SER	2.8
1	D	116	GLN	2.7
1	D	211	LYS	2.5
1	D	207	PRO	2.4
1	C	46	LYS	2.4
1	D	113	PRO	2.4
1	C	117	LYS	2.4
1	D	219	ILE	2.4
1	D	210	ALA	2.2
1	A	218	LYS	2.2
1	D	111	ILE	2.2
1	C	62	GLY	2.1
1	C	47	ASP	2.1
1	D	110	VAL	2.1
1	A	116	GLN	2.1

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(\AA^2)	Q<0.9
3	GTS	C	240	23/23	0.14	0.55	29,60,80,83	0
3	GTS	D	250	23/23	0.11	-0.05	26,39,56,58	0
3	GTS	A	230	23/23	0.12	-0.24	16,33,51,59	0
2	SO4	C	261	5/5	0.14	-0.44	74,74,75,77	0
2	SO4	D	262	5/5	0.12	-0.48	81,81,83,85	0
2	SO4	A	260	5/5	0.09	-0.49	40,42,47,49	0

6.5 Other polymers

There are no such residues in this entry.