Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 11:39 PM EDT

PDB ID	:	2GBB
Title	:	Crystal structure of secreted chorismate mutase from Yersinia pestis
Authors	:	Ladner, J.E.; Reddy, P.T.; Nelson, B.C.; Robinson, H.; Kim, S.-K.
Deposited on	:	2006-03-10
Resolution	:	2.10 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 (i) 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 (1)) were used in the production of this report:

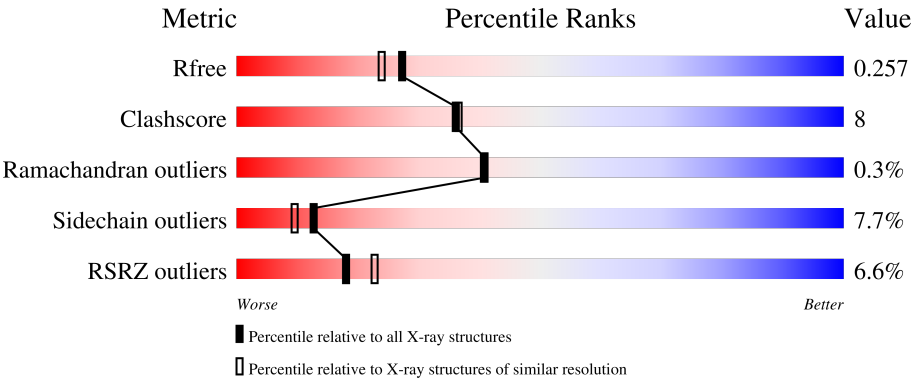
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	156	5% 82% 16%
1	B	156	6% 68% 26% 5%
1	C	156	9% 85% 14%
1	D	156	5% 72% 23%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	209	-	-	X	-
2	SO4	C	208	-	-	X	-
2	SO4	D	207	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5233 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.

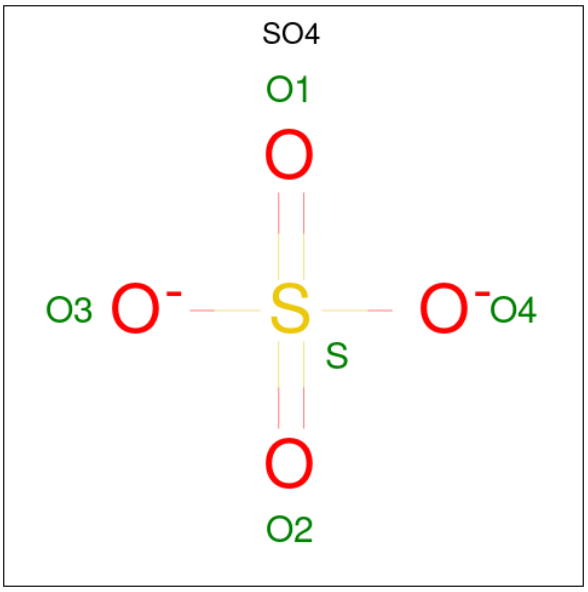
- Molecule 1 is a protein called putative chorismate mutase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	Se	0	4	0
			1248	781	217	244	2	4			
1	B	155	Total	C	N	O	S	Se	0	0	0
			1220	765	213	236	2	4			
1	C	156	Total	C	N	O	S	Se	0	0	0
			1229	770	215	238	2	4			
1	D	155	Total	C	N	O	S	Se	0	1	0
			1226	769	215	236	2	4			

There are 16 discrepancies between the modelled and reference sequences:

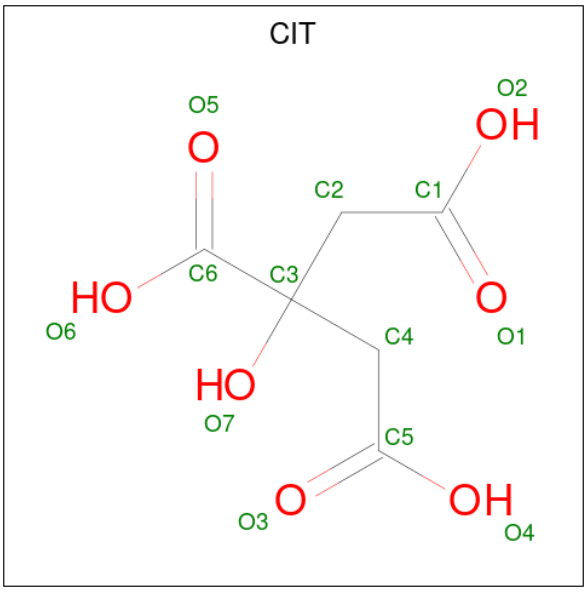
Chain	Residue	Modelled	Actual	Comment	Reference
A	47	MSE	MET	MODIFIED RESIDUE	GB 45435929
A	75	MSE	MET	MODIFIED RESIDUE	GB 45435929
A	92	MSE	MET	MODIFIED RESIDUE	GB 45435929
A	153	MSE	MET	MODIFIED RESIDUE	GB 45435929
B	47	MSE	MET	MODIFIED RESIDUE	GB 45435929
B	75	MSE	MET	MODIFIED RESIDUE	GB 45435929
B	92	MSE	MET	MODIFIED RESIDUE	GB 45435929
B	153	MSE	MET	MODIFIED RESIDUE	GB 45435929
C	47	MSE	MET	MODIFIED RESIDUE	GB 45435929
C	75	MSE	MET	MODIFIED RESIDUE	GB 45435929
C	92	MSE	MET	MODIFIED RESIDUE	GB 45435929
C	153	MSE	MET	MODIFIED RESIDUE	GB 45435929
D	47	MSE	MET	MODIFIED RESIDUE	GB 45435929
D	75	MSE	MET	MODIFIED RESIDUE	GB 45435929
D	92	MSE	MET	MODIFIED RESIDUE	GB 45435929
D	153	MSE	MET	MODIFIED RESIDUE	GB 45435929

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 6 7	0	0
3	B	1	Total C O 13 6 7	0	0
3	C	1	Total C O 13 6 7	0	0
3	D	1	Total C O 13 6 7	0	0

- Molecule 4 is water.

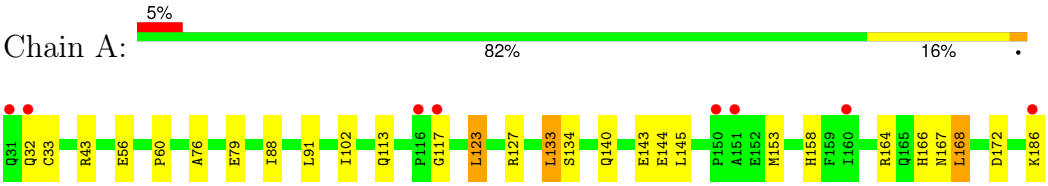
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	53	Total O 53 53	0	0
4	B	42	Total O 42 42	0	0
4	C	44	Total O 44 44	0	0
4	D	54	Total O 54 54	0	0

3 Residue-property plots (i)

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.

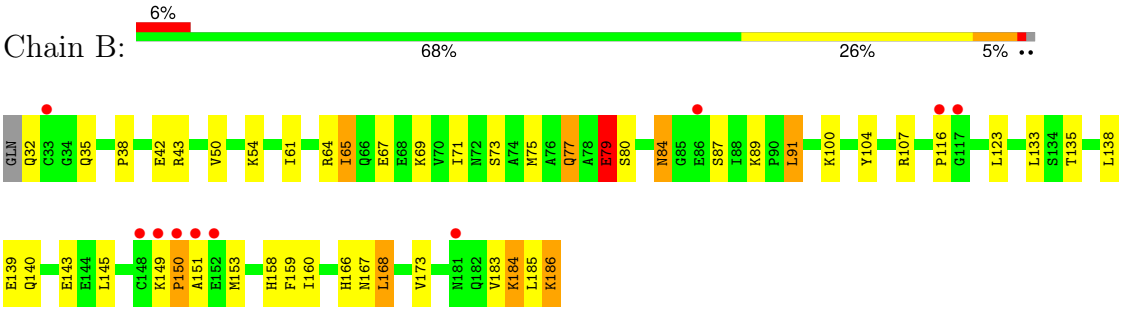
• Molecule 1: putative chorismate mutase

Chain A:



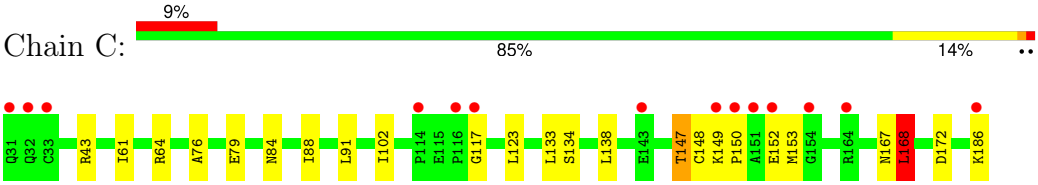
• Molecule 1: putative chorismate mutase

Chain B:



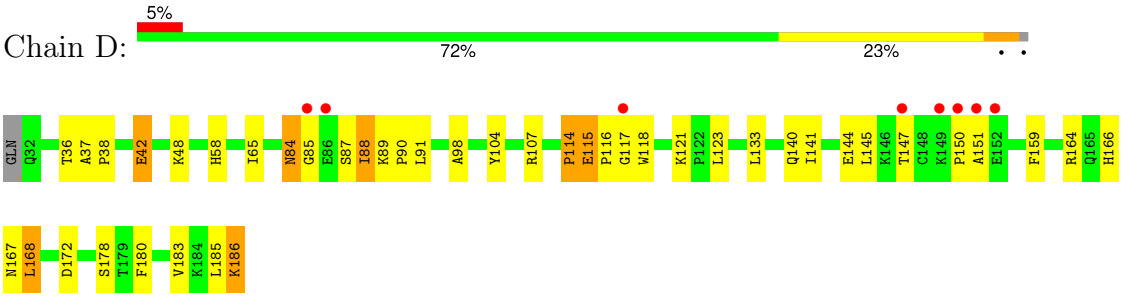
• Molecule 1: putative chorismate mutase

Chain C:



• Molecule 1: putative chorismate mutase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	89.01Å 144.09Å 116.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 29.16 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.5 (20.00-2.10) 97.5 (29.16-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.69 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.207 , 0.258 0.213 , 0.257	Depositor DCC
R_{free} test set	2213 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	30.4	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5233	wwPDB-VP
Average B, all atoms (Å^2)	35.0	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 79.51 % 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 5.4949e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, CIT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.94	2/1243 (0.2%)	0.85	0/1670
1	B	0.97	2/1237 (0.2%)	0.92	4/1664 (0.2%)
1	C	0.95	1/1246 (0.1%)	0.85	1/1676 (0.1%)
1	D	0.92	1/1234 (0.1%)	0.98	5/1659 (0.3%)
All	All	0.94	6/4960 (0.1%)	0.90	10/6669 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	1	3
All	All	1	6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	42	GLU	CG-CD	6.39	1.61	1.51
1	B	79	GLU	CD-OE1	5.99	1.32	1.25
1	A	113	GLN	CD-OE1	5.61	1.36	1.24
1	C	167	ASN	CG-OD1	5.29	1.35	1.24
1	B	77	GLN	CD-OE1	5.12	1.35	1.24
1	A	56	GLU	CD-OE2	5.12	1.31	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	115	GLU	N-CA-C	8.05	132.73	111.00
1	D	107	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	B	107	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	B	168	LEU	CA-CB-CG	6.46	130.16	115.30
1	B	43	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	D	85	GLY	N-CA-C	-5.93	98.27	113.10
1	C	168	LEU	CA-CB-CG	5.52	127.99	115.30
1	B	91	LEU	CB-CG-CD2	5.41	120.20	111.00
1	D	114	PRO	C-N-CA	5.36	135.11	121.70
1	D	114	PRO	O-C-N	-5.03	114.65	122.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	115	GLU	CA

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	GLY	Peptide
1	B	84	ASN	Peptide
1	C	117	GLY	Peptide
1	D	114	PRO	Peptide,Mainchain
1	D	84	ASN	Peptide

5.2 Too-close contacts (i)

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	1248	0	1237	13	0
1	B	1220	0	1219	22	0
1	C	1229	0	1227	17	0
1	D	1226	0	1222	27	0
2	A	25	0	0	5	0
2	B	15	0	0	1	0
2	C	20	0	0	3	0
2	D	5	0	0	2	0
3	A	13	0	5	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	13	0	5	1	0
3	C	13	0	5	0	0
3	D	13	0	5	1	0
4	A	53	0	0	1	0
4	B	42	0	0	1	0
4	C	44	0	0	1	0
4	D	54	0	0	3	0
All	All	5233	0	4925	80	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 8.

All (80) 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:C:149:LYS:HB2	1:C:152:GLU:HG3	1.55	0.89
1:A:60:PRO:HA	2:A:209:SO4:O2	1.85	0.77
1:D:185:LEU:O	1:D:186:LYS:HB2	1.86	0.76
1:A:133:LEU:HD22	4:A:440:HOH:O	1.89	0.72
1:B:65:ILE:HG23	4:B:404:HOH:O	1.92	0.69
1:C:76:ALA:O	1:C:79:GLU:HB2	1.93	0.68
2:C:208:SO4:O4	1:D:104:TYR:HE1	1.76	0.68
1:D:42:GLU:OE2	4:D:332:HOH:O	2.13	0.66
1:B:71:ILE:O	1:B:75:MSE:HG3	1.96	0.65
1:B:150:PRO:HA	1:B:153:MSE:HB2	1.78	0.64
1:C:64:ARG:HH21	1:D:58[E]:HIS:CE1	2.15	0.64
1:C:64:ARG:NH2	1:D:58[E]:HIS:CE1	2.66	0.63
1:C:88:ILE:HD12	1:C:138:LEU:CD2	2.30	0.61
1:B:79:GLU:HG2	1:B:80:SER:N	2.17	0.60
1:D:84:ASN:O	1:D:87:SER:OG	2.05	0.59
1:B:160:ILE:HD13	1:B:173:VAL:HG11	1.84	0.59
1:A:158:HIS:HA	2:A:202:SO4:O3	2.03	0.58
3:D:194:CIT:O3	3:D:194:CIT:O7	2.15	0.58
3:B:192:CIT:O3	3:B:192:CIT:O7	2.19	0.56
1:C:61:ILE:N	2:C:208:SO4:O2	2.26	0.56
1:D:37:ALA:HB3	1:D:38:PRO:HD3	1.89	0.55
1:C:168:LEU:HD22	1:C:172:ASP:HB2	1.89	0.55
1:C:84:ASN:HB2	1:C:186:LYS:HB2	1.90	0.54
1:D:48:LYS:HG2	1:D:118:TRP:CE2	2.43	0.54
1:A:168:LEU:HD22	1:A:172:ASP:HB2	1.90	0.54
1:C:150:PRO:HA	1:C:153:MSE:HE3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ALA:O	1:A:79:GLU:HB2	2.08	0.52
1:C:147:THR:OG1	1:C:148:CYS:N	2.42	0.52
1:A:32:GLN:HG2	1:A:33:CYS:SG	2.49	0.52
1:C:88:ILE:HD12	1:C:138:LEU:HD21	1.91	0.51
1:A:60:PRO:CA	2:A:209:SO4:O2	2.58	0.51
1:D:116:PRO:HD2	2:D:207:SO4:O4	2.11	0.50
1:D:141:ILE:HG21	1:D:183:VAL:HG11	1.93	0.50
1:C:148:CYS:HB3	1:C:152:GLU:HB2	1.93	0.50
1:A:102:ILE:HD11	1:A:168:LEU:HG	1.94	0.50
1:D:117:GLY:N	2:D:207:SO4:O3	2.45	0.49
1:C:43:ARG:HE	1:C:134:SER:HB2	1.78	0.48
1:B:50:VAL:CG1	1:B:54:LYS:HE3	2.43	0.48
1:C:102:ILE:HD11	1:C:168:LEU:HG	1.95	0.48
1:D:164:ARG:HA	4:D:413:HOH:O	2.14	0.48
1:B:160:ILE:HD13	1:B:173:VAL:CG1	2.44	0.48
1:D:166:HIS:O	1:D:167:ASN:HB2	2.14	0.48
1:B:149:LYS:O	1:B:151:ALA:N	2.47	0.47
1:B:84:ASN:O	1:B:87:SER:OG	2.10	0.47
1:D:36:THR:HG21	1:D:180:PHE:CE1	2.48	0.47
2:A:209:SO4:O3	1:B:61:ILE:HB	2.15	0.47
1:D:150:PRO:HA	4:D:470:HOH:O	2.16	0.46
1:D:98:ALA:HB1	1:D:168:LEU:HD21	1.98	0.46
1:D:88:ILE:HD13	1:D:183:VAL:HG22	1.97	0.45
1:D:186:LYS:O	1:D:186:LYS:CE	2.65	0.45
2:C:208:SO4:O4	4:C:303:HOH:O	2.21	0.45
1:D:89:LYS:HB3	1:D:90:PRO:HD3	1.99	0.45
1:B:158:HIS:CD2	1:D:121:LYS:HE3	2.53	0.44
1:A:140:GLN:O	1:A:144:GLU:HG3	2.18	0.44
1:D:186:LYS:O	1:D:186:LYS:NZ	2.50	0.44
1:B:38:PRO:O	1:B:42:GLU:HG3	2.17	0.43
1:A:123:LEU:HD22	1:A:127:ARG:HG3	2.00	0.43
1:B:32:GLN:O	1:B:140:GLN:NE2	2.51	0.43
1:D:168:LEU:HD22	1:D:172:ASP:HB2	1.99	0.43
1:B:71:ILE:HG21	1:B:89:LYS:HE2	2.01	0.43
1:B:77:GLN:OE1	1:B:138:LEU:HD12	2.18	0.43
1:D:168:LEU:HD22	1:D:172:ASP:CB	2.49	0.43
1:D:186:LYS:HB3	1:D:186:LYS:HE3	1.58	0.43
1:D:115:GLU:N	1:D:116:PRO:HD3	2.34	0.42
3:A:191:CIT:O3	3:A:191:CIT:O7	2.31	0.42
1:C:168:LEU:HD22	1:C:172:ASP:CB	2.48	0.42
1:B:67:GLU:OE2	1:B:100:LYS:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:PRO:HD2	2:B:203:SO4:O1	2.20	0.42
1:A:166:HIS:O	1:A:167:ASN:HB2	2.19	0.41
2:A:209:SO4:O3	1:B:104:TYR:HE1	2.03	0.41
1:A:144:GLU:OE1	1:A:153:MSE:HG2	2.21	0.41
1:C:88:ILE:CD1	1:C:138:LEU:CD2	2.97	0.41
1:A:43:ARG:HE	1:A:134:SER:HB2	1.86	0.41
1:D:38:PRO:O	1:D:42:GLU:HG2	2.20	0.41
1:B:139:GLU:O	1:B:143:GLU:HG3	2.21	0.41
1:B:166:HIS:O	1:B:167:ASN:HB2	2.21	0.41
1:B:183:VAL:O	1:B:184:LYS:HE3	2.21	0.40
1:D:140:GLN:O	1:D:144:GLU:HG3	2.22	0.40
1:B:185:LEU:O	1:B:186:LYS:HB2	2.21	0.40
1:C:88:ILE:CD1	1:C:138:LEU:HD22	2.51	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	158/156 (101%)	155 (98%)	3 (2%)	0	100	100
1	B	153/156 (98%)	149 (97%)	3 (2%)	1 (1%)	22	18
1	C	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
1	D	154/156 (99%)	147 (96%)	6 (4%)	1 (1%)	25	21
All	All	619/624 (99%)	600 (97%)	17 (3%)	2 (0%)	41	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	150	PRO
1	D	151	ALA

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	128/128 (100%)	119 (93%)	9 (7%)	15 12
1	B	131/128 (102%)	116 (88%)	15 (12%)	5 3
1	C	132/128 (103%)	127 (96%)	5 (4%)	33 34
1	D	130/128 (102%)	119 (92%)	11 (8%)	10 7
All	All	521/512 (102%)	481 (92%)	40 (8%)	13 9

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

Mol	Chain	Res	Type
1	A	88	ILE
1	A	91	LEU
1	A	123	LEU
1	A	133	LEU
1	A	143	GLU
1	A	145	LEU
1	A	164	ARG
1	A	168	LEU
1	A	186	LYS
1	B	35	GLN
1	B	64	ARG
1	B	65	ILE
1	B	69	LYS
1	B	73	SER
1	B	79	GLU
1	B	91	LEU
1	B	123	LEU
1	B	133	LEU
1	B	135	THR
1	B	145	LEU
1	B	159	PHE
1	B	168	LEU
1	B	184	LYS
1	B	186	LYS

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Mol	Chain	Res	Type
1	C	91	LEU
1	C	123	LEU
1	C	133	LEU
1	C	147	THR
1	C	168	LEU
1	D	65	ILE
1	D	88	ILE
1	D	91	LEU
1	D	123	LEU
1	D	133	LEU
1	D	145	LEU
1	D	147	THR
1	D	159	PHE
1	D	168	LEU
1	D	178	SER
1	D	186	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

17 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	CIT	B	192	-	12,12,12	1.65	3 (25%)	17,17,17	2.39	7 (41%)
2	SO4	C	206	-	4,4,4	0.28	0	6,6,6	0.17	0
3	CIT	A	191	-	12,12,12	1.21	1 (8%)	17,17,17	1.62	2 (11%)
2	SO4	B	197	-	4,4,4	0.34	0	6,6,6	0.34	0
2	SO4	B	203	-	4,4,4	0.21	0	6,6,6	0.17	0
2	SO4	A	200	-	4,4,4	0.18	0	6,6,6	0.12	0
3	CIT	D	194	-	12,12,12	1.73	4 (33%)	17,17,17	2.41	10 (58%)
2	SO4	A	209	-	4,4,4	0.56	0	6,6,6	0.66	0
2	SO4	C	208	-	4,4,4	0.58	0	6,6,6	1.20	0
2	SO4	B	204	-	4,4,4	0.26	0	6,6,6	0.27	0
3	CIT	C	193	-	12,12,12	1.40	2 (16%)	17,17,17	1.58	3 (17%)
2	SO4	A	201	-	4,4,4	0.27	0	6,6,6	0.32	0
2	SO4	A	202	-	4,4,4	0.35	0	6,6,6	0.22	0
2	SO4	D	207	-	4,4,4	0.27	0	6,6,6	0.15	0
2	SO4	C	205	-	4,4,4	0.27	0	6,6,6	0.22	0
2	SO4	C	199	-	4,4,4	0.35	0	6,6,6	0.38	0
2	SO4	A	198	-	4,4,4	0.22	0	6,6,6	0.48	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	CIT	B	192	-	-	2/16/16/16	-
3	CIT	D	194	-	-	2/16/16/16	-
3	CIT	C	193	-	-	3/16/16/16	-
3	CIT	A	191	-	-	2/16/16/16	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	194	CIT	C4-C3	-3.53	1.49	1.54
3	B	192	CIT	C4-C3	-3.11	1.50	1.54
3	C	193	CIT	O7-C3	2.60	1.48	1.43
3	B	192	CIT	O4-C5	-2.49	1.22	1.30
3	D	194	CIT	O4-C5	-2.37	1.23	1.30
3	D	194	CIT	O3-C5	2.26	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	194	CIT	O7-C3	2.14	1.47	1.43
3	C	193	CIT	O3-C5	2.06	1.28	1.22
3	B	192	CIT	O7-C3	2.06	1.47	1.43
3	A	191	CIT	O7-C3	2.03	1.47	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	192	CIT	O7-C3-C6	-4.81	102.13	108.96
3	D	194	CIT	O6-C6-C3	4.63	122.03	113.14
3	C	193	CIT	O6-C6-C3	4.62	122.00	113.14
3	A	191	CIT	O6-C6-C3	4.42	121.62	113.14
3	D	194	CIT	C3-C4-C5	-3.92	103.21	113.92
3	B	192	CIT	C3-C4-C5	-3.64	103.97	113.92
3	B	192	CIT	O6-C6-C3	3.59	120.03	113.14
3	B	192	CIT	O4-C5-O3	-3.21	115.07	123.33
3	D	194	CIT	O7-C3-C2	3.00	116.23	109.38
3	B	192	CIT	O2-C1-C2	2.89	123.49	114.35
3	B	192	CIT	O5-C6-C3	-2.83	116.61	122.09
3	D	194	CIT	O7-C3-C4	-2.82	102.94	109.38
3	D	194	CIT	O2-C1-C2	2.74	123.03	114.35
3	D	194	CIT	O4-C5-O3	-2.71	116.36	123.33
3	D	194	CIT	O1-C1-C2	-2.71	115.28	122.95
3	D	194	CIT	O3-C5-C4	2.43	129.83	122.95
3	D	194	CIT	O5-C6-C3	-2.36	117.53	122.09
3	A	191	CIT	O7-C3-C6	-2.29	105.71	108.96
3	B	192	CIT	C3-C2-C1	-2.27	107.70	113.92
3	C	193	CIT	O5-C6-C3	-2.17	117.89	122.09
3	C	193	CIT	O2-C1-C2	2.09	120.97	114.35
3	D	194	CIT	O7-C3-C6	-2.03	106.08	108.96

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	193	CIT	C2-C3-C4-C5
3	B	192	CIT	C6-C3-C4-C5
3	C	193	CIT	C6-C3-C4-C5
3	D	194	CIT	C6-C3-C4-C5
3	D	194	CIT	C2-C3-C4-C5
3	A	191	CIT	C6-C3-C4-C5
3	A	191	CIT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	B	192	CIT	C2-C3-C4-C5
3	C	193	CIT	O7-C3-C4-C5

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	192	CIT	1	0
3	A	191	CIT	1	0
2	B	203	SO4	1	0
3	D	194	CIT	1	0
2	A	209	SO4	4	0
2	C	208	SO4	3	0
2	A	202	SO4	1	0
2	D	207	SO4	2	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, 95^{th} 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	152/156 (97%)	0.06	8 (5%) 26 32	20, 30, 56, 66	0
1	B	151/156 (96%)	0.25	10 (6%) 18 23	19, 33, 65, 81	0
1	C	152/156 (97%)	0.18	14 (9%) 9 11	20, 32, 68, 78	0
1	D	151/156 (96%)	0.14	8 (5%) 26 32	18, 33, 57, 75	0
All	All	606/624 (97%)	0.16	40 (6%) 18 23	18, 32, 62, 81	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	151	ALA	9.8
1	B	150	PRO	8.0
1	D	151	ALA	7.0
1	B	149	LYS	6.0
1	A	31	GLN	6.0
1	C	117	GLY	5.6
1	D	150	PRO	5.2
1	C	31	GLN	4.9
1	C	32	GLN	4.8
1	B	33	CYS	4.7
1	A	117	GLY	4.4
1	C	150	PRO	4.4
1	C	151	ALA	4.4
1	A	151	ALA	4.0
1	D	149	LYS	4.0
1	A	116	PRO	3.8
1	B	148	CYS	3.8
1	C	116	PRO	3.7
1	D	152	GLU	3.6
1	B	152	GLU	3.4
1	C	152	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	86	GLU	3.0
1	B	86	GLU	2.9
1	A	150	PRO	2.8
1	A	186	LYS	2.7
1	A	160	ILE	2.7
1	C	186	LYS	2.6
1	A	32	GLN	2.6
1	B	116	PRO	2.5
1	D	85	GLY	2.5
1	C	33	CYS	2.4
1	C	149	LYS	2.3
1	C	154	GLY	2.3
1	D	117	GLY	2.2
1	D	147	THR	2.1
1	B	117	GLY	2.1
1	B	181	ASN	2.1
1	C	114	PRO	2.1
1	C	143	GLU	2.0
1	C	164	ARG	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 monosaccharides 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, 95^{th} 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	A	201	5/5	0.83	0.28	44,45,47,48	5
2	SO4	A	202	5/5	0.83	0.16	51,52,53,54	5
3	CIT	C	193	13/13	0.86	0.14	39,48,52,54	0
3	CIT	A	191	13/13	0.87	0.14	42,49,52,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	C	206	5/5	0.87	0.20	59,59,61,61	5
3	CIT	D	194	13/13	0.87	0.13	27,32,34,34	0
2	SO4	B	197	5/5	0.88	0.14	36,36,38,41	5
2	SO4	B	204	5/5	0.89	0.17	43,44,45,47	5
2	SO4	C	199	5/5	0.90	0.14	35,36,37,40	5
2	SO4	C	205	5/5	0.91	0.17	47,48,49,50	5
2	SO4	A	198	5/5	0.92	0.15	41,43,44,45	5
2	SO4	D	207	5/5	0.93	0.29	56,56,57,57	5
2	SO4	B	203	5/5	0.93	0.36	49,50,50,50	5
3	CIT	B	192	13/13	0.94	0.10	23,32,38,39	0
2	SO4	A	200	5/5	0.95	0.16	46,48,48,49	5
2	SO4	C	208	5/5	0.96	0.45	11,19,22,22	0
2	SO4	A	209	5/5	0.97	0.50	9,22,24,27	0

6.5 Other polymers (i)

There are no such residues in this entry.