Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:50 AM GMT

PDB ID	:	3N6H
Title	:	Crystal structure of Mandelate racemase/muconate lactonizing protein from Actinobacillus succinogenes 130Z complexed with magnesium/sulfate
Authors	:	Malashkevich, V.N.; Patskovsky, Y.; Toro, R.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2010-05-25
Resolution	:	2.30 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

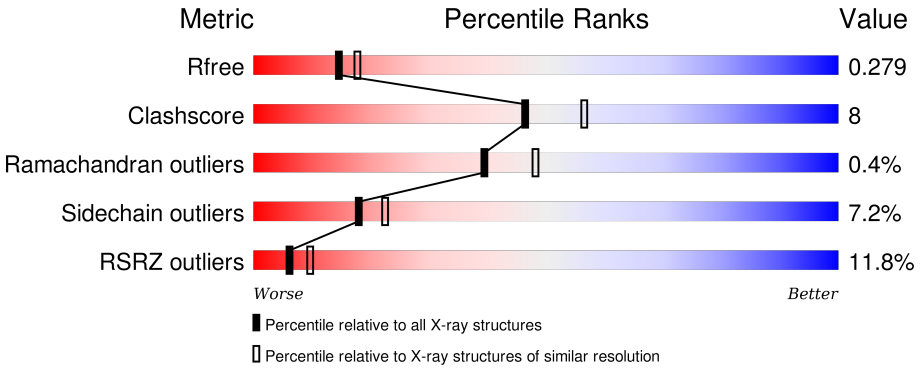
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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. 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	455	3% 72% 19% • 6%
1	B	455	% 77% 16% • 5%
1	C	455	13% 73% 19% • 6%
1	D	455	26% 74% 18% • 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13719 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 Mandelate racemase/muconate lactonizing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	Se	0	1	0
			3356	2136	581	619	6	14			
1	B	432	Total	C	N	O	S	Se	0	2	0
			3386	2155	587	624	6	14			
1	C	426	Total	C	N	O	S	Se	0	1	0
			3328	2117	577	614	6	14			
1	D	424	Total	C	N	O	S	Se	0	2	0
			3316	2108	574	614	6	14			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	EXPRESSION TAG	UNP A6VQF6
A	2	SER	-	EXPRESSION TAG	UNP A6VQF6
A	3	LEU	-	EXPRESSION TAG	UNP A6VQF6
A	448	GLU	-	EXPRESSION TAG	UNP A6VQF6
A	449	GLY	-	EXPRESSION TAG	UNP A6VQF6
A	450	HIS	-	EXPRESSION TAG	UNP A6VQF6
A	451	HIS	-	EXPRESSION TAG	UNP A6VQF6
A	452	HIS	-	EXPRESSION TAG	UNP A6VQF6
A	453	HIS	-	EXPRESSION TAG	UNP A6VQF6
A	454	HIS	-	EXPRESSION TAG	UNP A6VQF6
A	455	HIS	-	EXPRESSION TAG	UNP A6VQF6
B	1	MSE	-	EXPRESSION TAG	UNP A6VQF6
B	2	SER	-	EXPRESSION TAG	UNP A6VQF6
B	3	LEU	-	EXPRESSION TAG	UNP A6VQF6
B	448	GLU	-	EXPRESSION TAG	UNP A6VQF6
B	449	GLY	-	EXPRESSION TAG	UNP A6VQF6
B	450	HIS	-	EXPRESSION TAG	UNP A6VQF6
B	451	HIS	-	EXPRESSION TAG	UNP A6VQF6
B	452	HIS	-	EXPRESSION TAG	UNP A6VQF6
B	453	HIS	-	EXPRESSION TAG	UNP A6VQF6
B	454	HIS	-	EXPRESSION TAG	UNP A6VQF6

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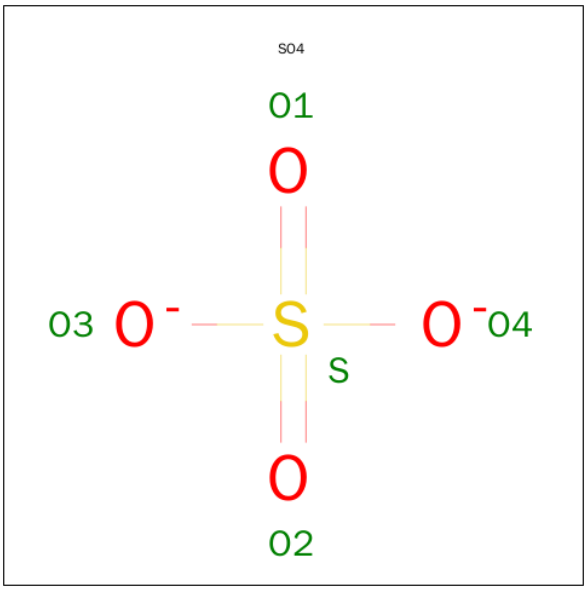
Chain	Residue	Modelled	Actual	Comment	Reference
B	455	HIS	-	EXPRESSION TAG	UNP A6VQF6
C	1	MSE	-	EXPRESSION TAG	UNP A6VQF6
C	2	SER	-	EXPRESSION TAG	UNP A6VQF6
C	3	LEU	-	EXPRESSION TAG	UNP A6VQF6
C	448	GLU	-	EXPRESSION TAG	UNP A6VQF6
C	449	GLY	-	EXPRESSION TAG	UNP A6VQF6
C	450	HIS	-	EXPRESSION TAG	UNP A6VQF6
C	451	HIS	-	EXPRESSION TAG	UNP A6VQF6
C	452	HIS	-	EXPRESSION TAG	UNP A6VQF6
C	453	HIS	-	EXPRESSION TAG	UNP A6VQF6
C	454	HIS	-	EXPRESSION TAG	UNP A6VQF6
C	455	HIS	-	EXPRESSION TAG	UNP A6VQF6
D	1	MSE	-	EXPRESSION TAG	UNP A6VQF6
D	2	SER	-	EXPRESSION TAG	UNP A6VQF6
D	3	LEU	-	EXPRESSION TAG	UNP A6VQF6
D	448	GLU	-	EXPRESSION TAG	UNP A6VQF6
D	449	GLY	-	EXPRESSION TAG	UNP A6VQF6
D	450	HIS	-	EXPRESSION TAG	UNP A6VQF6
D	451	HIS	-	EXPRESSION TAG	UNP A6VQF6
D	452	HIS	-	EXPRESSION TAG	UNP A6VQF6
D	453	HIS	-	EXPRESSION TAG	UNP A6VQF6
D	454	HIS	-	EXPRESSION TAG	UNP A6VQF6
D	455	HIS	-	EXPRESSION TAG	UNP A6VQF6

- 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	B	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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0

- Molecule 5 is water.

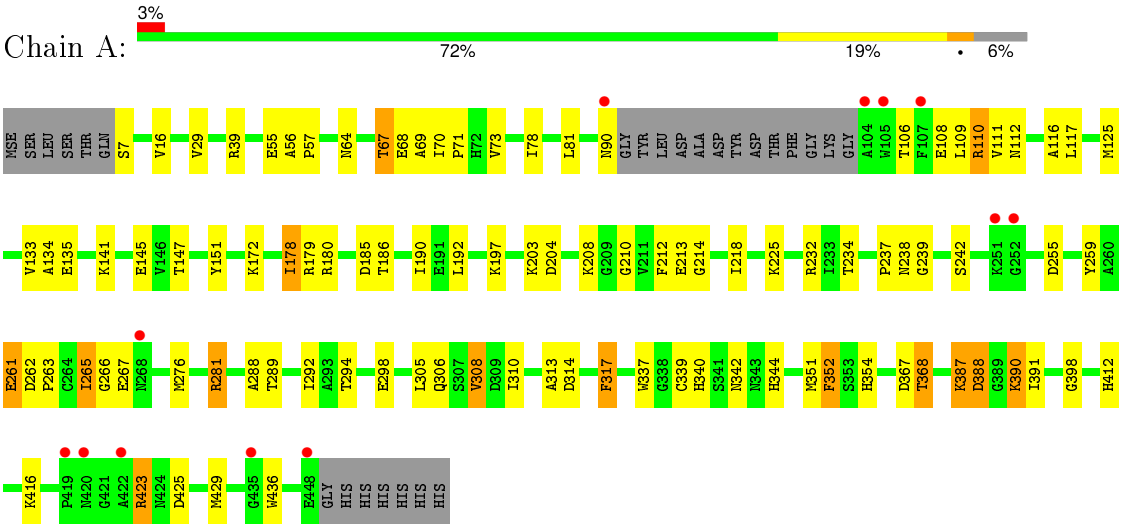
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	150	Total O 150 150	0	0
5	B	105	Total O 105 105	0	0
5	C	41	Total O 41 41	0	0
5	D	12	Total O 12 12	0	0

3 Residue-property plots (i)

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.

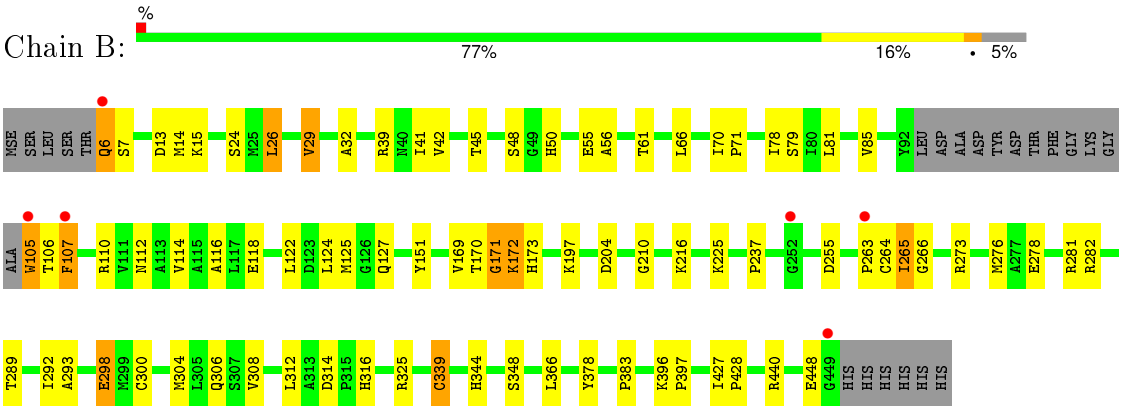
- Molecule 1: Mandelate racemase/muconate lactonizing protein

Chain A:



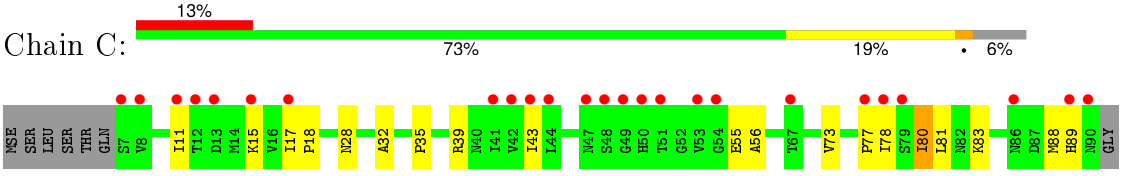
- Molecule 1: Mandelate racemase/muconate lactonizing protein

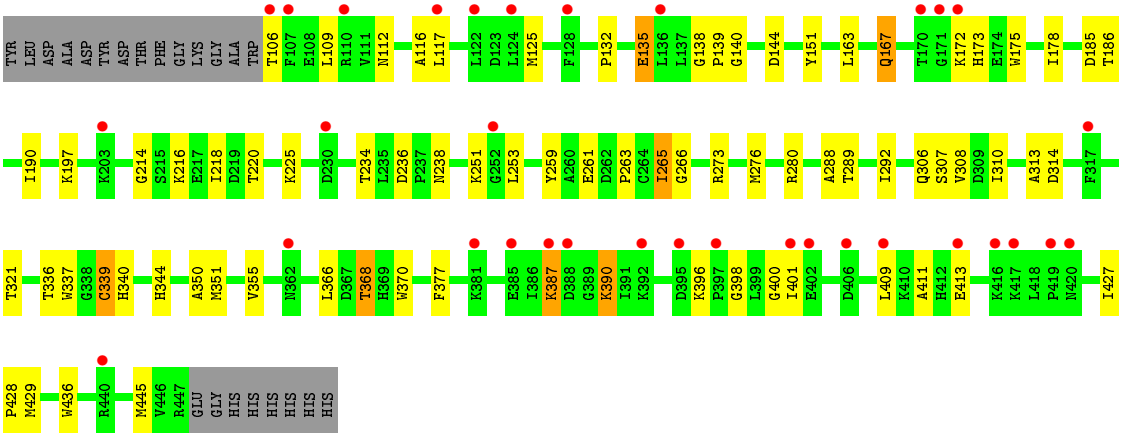
Chain B:



- Molecule 1: Mandelate racemase/muconate lactonizing protein

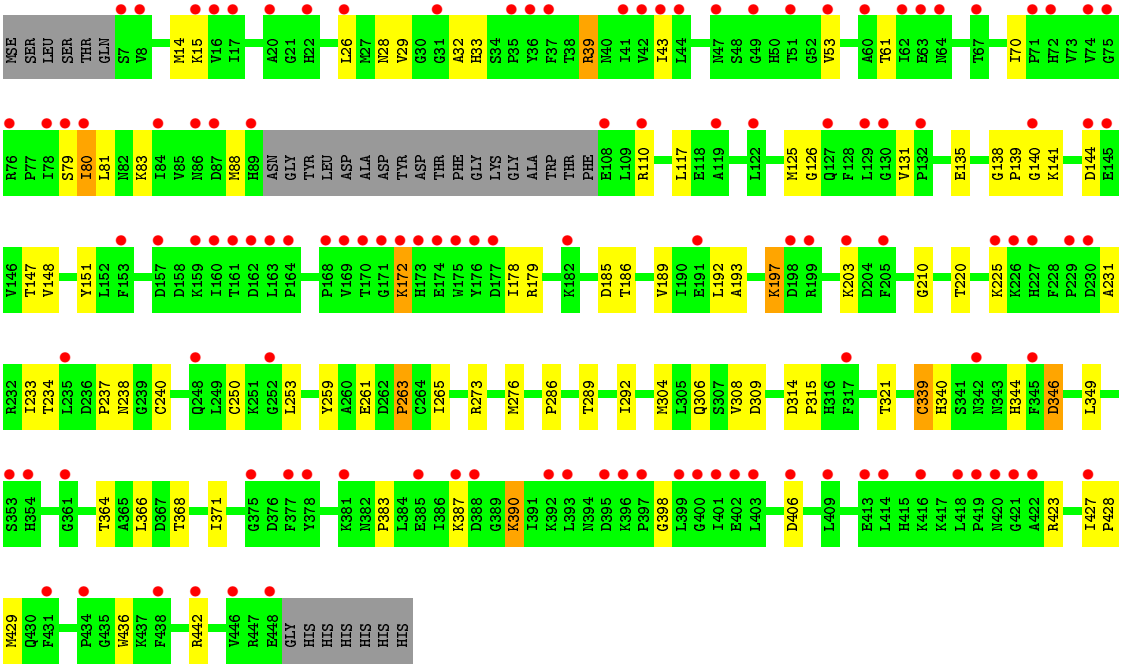
Chain C:





• Molecule 1: Mandelate racemase/muconate lactonizing protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	97.40Å 85.88Å 112.42Å 90.00° 96.03° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	77.9 (20.00-2.30) 77.9 (20.00-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.219 , 0.278 0.220 , 0.279	Depositor DCC
R_{free} test set	1907 reflections (3.08%)	DCC
Wilson B-factor (Å^2)	35.1	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 63797 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13719	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, SO4, CL

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	0.49	0/3428	0.61	0/4632
1	B	0.44	0/3463	0.58	0/4679
1	C	0.38	0/3398	0.52	0/4590
1	D	0.37	0/3388	0.50	0/4576
All	All	0.43	0/13677	0.56	0/18477

There are no bond length outliers.

There are no bond angle outliers.

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	3356	0	3307	65	0
1	B	3386	0	3330	46	0
1	C	3328	0	3286	47	0
1	D	3316	0	3274	46	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	B	1	0	0	0	0
5	A	150	0	0	3	0
5	B	105	0	0	3	0
5	C	41	0	0	1	0
5	D	12	0	0	1	0
All	All	13719	0	13197	201	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 (201) 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:26:LEU:HB2	1:D:33:HIS:CD2	1.96	1.00
1:D:79:SER:HA	1:D:125:MSE:HE1	1.45	0.98
1:A:306:GLN:HG3	1:C:306:GLN:HG3	1.55	0.88
1:D:26:LEU:HB2	1:D:33:HIS:HD2	1.36	0.87
1:B:298:GLU:HG2	5:B:536:HOH:O	1.78	0.82
1:B:172:LYS:HG2	1:B:173:HIS:H	1.47	0.79
1:D:314:ASP:HB2	1:D:340:HIS:HB3	1.66	0.78
1:A:314:ASP:OD1	1:A:340:HIS:HD2	1.68	0.76
1:D:29:VAL:HG21	1:D:238:ASN:HB2	1.68	0.76
1:A:237:PRO:HG2	1:A:263:PRO:HA	1.69	0.75
1:C:173:HIS:HD2	1:C:175:TRP:H	1.35	0.73
1:A:135:GLU:HG3	1:A:141:LYS:H	1.54	0.72
1:B:107:PHE:N	1:B:107:PHE:CD2	2.59	0.71
1:A:39:ARG:HD2	1:A:344:HIS:HA	1.73	0.70
1:C:310:ILE:HG12	1:C:336:THR:HB	1.74	0.70
1:A:29:VAL:HG22	1:A:210:GLY:HA3	1.74	0.69
1:A:289:THR:HG22	1:A:308:VAL:HG11	1.75	0.69
1:B:339:CYS:HB2	1:B:366:LEU:HD22	1.75	0.68
1:D:427:ILE:HB	1:D:428:PRO:HD3	1.75	0.68
1:A:317:PHE:N	1:A:317:PHE:HD1	1.91	0.68
1:A:281:ARG:HH11	1:A:281:ARG:HG2	1.59	0.68
1:C:56:ALA:HB2	1:C:116:ALA:HB2	1.77	0.67
1:A:317:PHE:N	1:A:317:PHE:CD1	2.63	0.66
1:A:306:GLN:HB2	1:C:306:GLN:HE21	1.61	0.65
1:C:214:GLY:O	1:C:218:ILE:HG12	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ALA:HB3	1:A:337:TRP:HE1	1.60	0.65
1:B:293:ALA:HA	1:B:298:GLU:HB3	1.79	0.64
1:A:29:VAL:HG21	1:A:238:ASN:HB2	1.78	0.64
1:A:314:ASP:OD1	1:A:340:HIS:CD2	2.51	0.64
1:B:298:GLU:CG	5:B:536:HOH:O	2.43	0.63
1:D:135:GLU:HG3	1:D:141:LYS:H	1.63	0.63
1:A:134:ALA:H	1:A:354:HIS:HD2	1.47	0.63
1:B:427:ILE:HB	1:B:428:PRO:HD3	1.81	0.62
1:A:265:ILE:HG23	1:A:266:GLY:H	1.65	0.62
1:B:56:ALA:HB2	1:B:116:ALA:HB2	1.80	0.62
1:B:237:PRO:HG2	1:B:263:PRO:HA	1.83	0.61
1:A:178:ILE:HG23	1:A:192:LEU:HD23	1.82	0.61
1:D:263:PRO:HD2	1:D:276:MSE:SE	2.50	0.61
1:A:281:ARG:HH11	1:A:281:ARG:CG	2.12	0.61
1:D:273:ARG:HA	1:D:292:ILE:HD12	1.83	0.60
1:A:276:MSE:HG3	1:A:292:ILE:HD13	1.83	0.60
1:D:237:PRO:HG2	1:D:263:PRO:HA	1.83	0.60
1:C:314:ASP:HB2	1:C:340:HIS:HB3	1.83	0.60
1:A:339:CYS:O	1:A:367:ASP:HB2	2.02	0.60
1:C:263:PRO:HD2	1:C:276:MSE:SE	2.51	0.60
1:D:186:THR:HG23	1:D:220:THR:HA	1.85	0.58
1:B:304:MSE:HE2	1:B:304:MSE:HA	1.86	0.58
1:D:29:VAL:HG22	1:D:210:GLY:HA3	1.84	0.58
1:C:167:GLN:HE21	1:C:167:GLN:HA	1.69	0.58
1:A:265:ILE:HG23	1:A:266:GLY:N	2.19	0.58
1:B:24:SER:HB2	1:B:26:LEU:HD13	1.86	0.57
1:D:33:HIS:HE1	1:D:423:ARG:CZ	2.17	0.57
1:C:396:LYS:HB3	1:C:400:GLY:HA2	1.86	0.57
1:B:39:ARG:HD2	1:B:344:HIS:HA	1.87	0.56
1:A:340:HIS:CD2	1:A:340:HIS:C	2.77	0.56
1:D:15:LYS:HB2	1:D:43:ILE:HB	1.87	0.56
1:C:289:THR:CG2	1:C:308:VAL:HG11	2.36	0.56
1:B:41:ILE:CD1	1:B:55:GLU:HG3	2.36	0.55
1:B:281:ARG:HD3	5:D:468:HOH:O	2.06	0.55
1:C:427:ILE:HB	1:C:428:PRO:HD3	1.88	0.55
1:D:29:VAL:CG2	1:D:238:ASN:HB2	2.36	0.55
1:A:108:GLU:O	1:A:111:VAL:HG12	2.07	0.55
1:B:265:ILE:HG23	1:B:266:GLY:N	2.22	0.55
1:A:70:ILE:HB	1:A:71:PRO:HD3	1.90	0.54
1:A:106:THR:HG22	1:A:110:ARG:HB2	1.88	0.54
1:C:261:GLU:HA	1:C:288:ALA:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:409:LEU:O	1:C:413:GLU:HG2	2.08	0.54
1:A:265:ILE:CG2	1:A:266:GLY:N	2.71	0.53
1:A:178:ILE:CG2	1:A:192:LEU:HD23	2.38	0.53
1:B:276:MSE:HG3	1:B:292:ILE:HD13	1.90	0.52
1:A:261:GLU:HB3	1:A:288:ALA:HB3	1.91	0.52
1:C:39:ARG:HD2	1:C:344:HIS:HA	1.92	0.52
1:A:68:GLU:O	1:A:71:PRO:HD2	2.09	0.52
1:B:48:SER:HG	1:B:50:HIS:HD1	1.56	0.52
1:A:56:ALA:HB2	1:A:116:ALA:HB2	1.92	0.52
1:D:250:CYS:HA	1:D:253:LEU:HD12	1.92	0.52
1:A:55:GLU:H	1:A:351:MSE:SE	2.43	0.52
1:C:313:ALA:HB3	1:C:337:TRP:HE1	1.74	0.52
1:A:109:LEU:HD21	5:A:555:HOH:O	2.10	0.51
1:C:289:THR:HG22	1:C:308:VAL:HG11	1.92	0.51
1:D:80:ILE:HG22	1:D:83:LYS:HB3	1.92	0.51
1:C:429:MSE:HE1	1:C:445:MSE:SE	2.60	0.51
1:D:144:ASP:N	1:D:144:ASP:OD2	2.44	0.51
1:B:6:GLN:OE1	1:B:6:GLN:HA	2.10	0.51
1:B:85:VAL:HG21	1:B:118:GLU:HG3	1.92	0.51
1:C:265:ILE:HG23	1:C:266:GLY:N	2.25	0.51
1:D:147:THR:HA	1:D:390:LYS:HG3	1.94	0.50
1:C:186:THR:HG23	1:C:220:THR:HA	1.93	0.50
1:C:35:PRO:HG3	1:C:163:LEU:HB3	1.93	0.50
1:D:225:LYS:HG2	1:D:233:ILE:HD13	1.94	0.50
1:B:273:ARG:NH1	1:B:298:GLU:HG3	2.27	0.50
1:C:15:LYS:HB2	1:C:43:ILE:HB	1.94	0.50
1:A:57:PRO:HD2	1:A:112:ASN:HB3	1.93	0.49
1:D:39:ARG:HD2	1:D:344:HIS:HA	1.93	0.49
1:A:64:ASN:HA	1:A:67:THR:OG1	2.11	0.49
1:A:179:ARG:HG3	1:A:180:ARG:HG2	1.94	0.49
1:A:423:ARG:HG3	1:A:423:ARG:O	2.12	0.49
1:D:346:ASP:N	1:D:346:ASP:OD2	2.43	0.49
1:C:339:CYS:HB2	1:C:366:LEU:HD22	1.95	0.49
1:C:77:PRO:HD2	1:C:80:ILE:HD11	1.94	0.49
1:D:135:GLU:HA	1:D:140:GLY:HA2	1.95	0.48
1:A:135:GLU:HG2	5:A:522:HOH:O	2.13	0.48
1:C:78:ILE:HG22	1:C:125:MSE:HE2	1.95	0.48
1:B:14:MSE:HG2	1:B:70:ILE:HG12	1.94	0.48
1:B:32:ALA:HB3	1:B:428:PRO:HB2	1.96	0.48
1:B:304:MSE:HG3	5:B:559:HOH:O	2.14	0.48
1:B:289:THR:CG2	1:B:308:VAL:HG11	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:GLY:HA3	1:D:398:GLY:HA2	1.96	0.48
1:D:276:MSE:HG3	1:D:292:ILE:HD13	1.95	0.48
1:B:39:ARG:HD3	1:B:55:GLU:OE2	2.14	0.48
1:A:208:LYS:HE3	2:A:500:SO4:O4	2.14	0.48
1:B:112:ASN:HA	1:B:316:HIS:O	2.14	0.47
1:C:368:THR:HG22	1:C:370:TRP:H	1.78	0.47
1:A:239:GLY:N	1:A:262:ASP:O	2.47	0.47
1:C:55:GLU:H	1:C:351:MSE:SE	2.48	0.47
1:C:387:LYS:NZ	5:C:482:HOH:O	2.48	0.47
1:B:169:VAL:HG13	1:B:171:GLY:HA3	1.97	0.47
1:D:33:HIS:HE1	1:D:423:ARG:NH2	2.13	0.47
1:D:193:ALA:O	1:D:197:LYS:HB2	2.14	0.47
1:D:148:VAL:HG12	1:D:366:LEU:HB2	1.96	0.47
1:D:189:VAL:HA	1:D:192:LEU:HD12	1.97	0.47
1:D:289:THR:CG2	1:D:308:VAL:HG11	2.46	0.46
1:B:263:PRO:HD2	1:B:276:MSE:SE	2.66	0.46
1:B:300:CYS:O	1:B:304:MSE:HG2	2.15	0.46
1:A:261:GLU:CB	1:A:288:ALA:HB3	2.45	0.46
1:A:387:LYS:HD3	1:A:388:ASP:OD1	2.16	0.46
1:C:132:PRO:HA	1:C:398:GLY:O	2.16	0.46
1:D:203:LYS:O	1:D:231:ALA:HA	2.16	0.46
1:A:242:SER:HA	1:A:267:GLU:OE2	2.16	0.46
1:A:212:PHE:HB3	1:A:213:GLU:OE1	2.15	0.46
1:A:289:THR:CG2	1:A:308:VAL:HG11	2.45	0.45
1:B:13:ASP:HB3	1:B:45:THR:OG1	2.16	0.45
1:A:147:THR:HA	1:A:390:LYS:HG3	1.98	0.45
1:C:350:ALA:HB3	1:C:401:ILE:HD11	1.99	0.45
1:D:314:ASP:HB2	1:D:340:HIS:CB	2.39	0.45
1:A:29:VAL:HG23	1:A:238:ASN:HD22	1.81	0.45
1:B:289:THR:HG22	1:B:308:VAL:HG11	1.98	0.45
1:A:106:THR:O	1:A:110:ARG:HB2	2.17	0.45
1:A:69:ALA:O	1:A:73:VAL:HG23	2.17	0.45
1:B:172:LYS:HG2	1:B:173:HIS:N	2.26	0.45
1:A:342:ASN:O	1:A:344:HIS:HD2	2.00	0.45
1:A:234:THR:HG21	1:A:259:TYR:CE1	2.52	0.45
1:A:133:VAL:HG23	1:A:398:GLY:C	2.37	0.44
1:C:109:LEU:O	1:C:112:ASN:HB2	2.17	0.44
1:B:306:GLN:HG3	1:D:306:GLN:HG3	1.99	0.44
1:B:41:ILE:HD13	1:B:55:GLU:HG3	2.00	0.44
1:B:81:LEU:HD11	1:B:122:LEU:HD23	1.98	0.44
1:A:78:ILE:HG22	1:A:125:MSE:HE2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:LEU:HD12	1:D:33:HIS:HD2	1.82	0.44
1:C:186:THR:O	1:C:190:ILE:HD12	2.17	0.44
1:C:273:ARG:HA	1:C:292:ILE:HD12	2.00	0.44
1:C:351:MSE:O	1:C:355:VAL:HG23	2.17	0.44
1:D:286:PRO:HA	1:D:309:ASP:OD1	2.16	0.44
1:D:178:ILE:HG23	1:D:192:LEU:HD23	2.00	0.44
1:D:88:MSE:SE	1:D:117:LEU:HD22	2.68	0.44
1:D:234:THR:HG21	1:D:259:TYR:CE1	2.53	0.43
1:C:218:ILE:HG23	1:C:253:LEU:HD11	2.00	0.43
1:B:70:ILE:HB	1:B:71:PRO:HD3	2.00	0.43
1:A:204:ASP:OD1	1:A:232:ARG:HB2	2.17	0.43
1:A:305:LEU:O	1:A:306:GLN:HB2	2.19	0.43
1:D:429:MSE:HG2	1:D:436:TRP:CD2	2.54	0.43
1:C:88:MSE:SE	1:C:117:LEU:HD22	2.68	0.43
1:A:423:ARG:NH1	5:A:577:HOH:O	2.49	0.43
1:B:78:ILE:HD11	1:B:125:MSE:N	2.34	0.43
1:B:344:HIS:HB2	1:B:348:SER:HB2	2.00	0.43
1:C:32:ALA:HB3	1:C:428:PRO:HB2	2.00	0.43
1:B:127:GLN:HA	1:B:397:PRO:HB2	2.00	0.43
1:C:234:THR:HG21	1:C:259:TYR:CE1	2.54	0.43
1:C:11:ILE:HG21	1:C:73:VAL:HG12	2.01	0.42
1:B:278:GLU:O	1:B:282:ARG:HG3	2.19	0.42
1:C:265:ILE:CG2	1:C:266:GLY:N	2.81	0.42
1:D:138:GLY:HA3	1:D:139:PRO:HD3	1.87	0.42
1:B:378:TYR:CD1	1:B:383:PRO:HG3	2.55	0.42
1:B:42:VAL:CG2	1:B:66:LEU:HD13	2.50	0.42
1:C:429:MSE:HG2	1:C:436:TRP:CD2	2.55	0.42
1:A:412:HIS:O	1:A:416:LYS:HG3	2.20	0.42
1:A:429:MSE:HG2	1:A:436:TRP:CD2	2.54	0.42
1:A:186:THR:O	1:A:190:ILE:HD12	2.19	0.42
1:C:236:ASP:HB2	1:C:261:GLU:HG2	2.02	0.42
1:D:346:ASP:O	1:D:349:LEU:HB3	2.20	0.42
1:D:315:PRO:HD3	1:D:339:CYS:SG	2.60	0.42
1:C:390:LYS:HE3	1:C:390:LYS:HB2	1.92	0.42
1:D:179:ARG:NH1	1:D:371:ILE:O	2.51	0.42
1:A:145:GLU:HA	1:A:391:ILE:O	2.20	0.42
1:A:289:THR:HG22	1:A:308:VAL:CG1	2.49	0.41
1:A:288:ALA:HA	1:A:310:ILE:O	2.20	0.41
1:A:294:THR:OG1	1:A:298:GLU:OE2	2.36	0.41
1:B:29:VAL:HG13	1:B:210:GLY:HA3	2.02	0.41
1:B:78:ILE:HD11	1:B:124:LEU:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:MSE:HG2	1:D:70:ILE:HG12	2.02	0.41
1:D:234:THR:HG21	1:D:259:TYR:CZ	2.55	0.41
1:A:214:GLY:O	1:A:218:ILE:HG12	2.21	0.41
1:C:135:GLU:HA	1:C:140:GLY:HA2	2.02	0.41
1:B:61:THR:HG23	1:B:105:TRP:HB3	2.03	0.41
1:C:377:PHE:CE2	1:C:411:ALA:HB2	2.56	0.41
1:D:32:ALA:HB3	1:D:428:PRO:HB2	2.03	0.41
1:C:17:ILE:HA	1:C:18:PRO:HD2	1.97	0.40
1:A:352:PHE:CE2	1:A:368:THR:HG23	2.56	0.40
1:A:234:THR:HG21	1:A:259:TYR:CZ	2.57	0.40
1:B:110:ARG:O	1:B:114:VAL:HG23	2.22	0.40
1:C:138:GLY:HA3	1:C:139:PRO:HD3	1.90	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	426/455 (94%)	401 (94%)	24 (6%)	1 (0%)	52	64
1	B	430/455 (94%)	413 (96%)	15 (4%)	2 (0%)	34	41
1	C	423/455 (93%)	407 (96%)	15 (4%)	1 (0%)	52	64
1	D	422/455 (93%)	399 (94%)	20 (5%)	3 (1%)	26	31
All	All	1701/1820 (94%)	1620 (95%)	74 (4%)	7 (0%)	39	48

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	448	GLU
1	D	172	LYS
1	A	425	ASP

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Mol	Chain	Res	Type
1	C	81	LEU
1	B	171	GLY
1	D	80	ILE
1	D	263	PRO

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	356/361 (99%)	330 (93%)	26 (7%)	17	22
1	B	359/361 (99%)	333 (93%)	26 (7%)	18	22
1	C	354/361 (98%)	329 (93%)	25 (7%)	18	23
1	D	353/361 (98%)	328 (93%)	25 (7%)	18	23
All	All	1422/1444 (98%)	1320 (93%)	102 (7%)	18	22

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	16	VAL
1	A	67	THR
1	A	81	LEU
1	A	90	ASN
1	A	110	ARG
1	A	117	LEU
1	A	151	TYR
1	A	172	LYS
1	A	178	ILE
1	A	185	ASP
1	A	197	LYS
1	A	203	LYS
1	A	225	LYS
1	A	255	ASP
1	A	261	GLU
1	A	265	ILE

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Mol	Chain	Res	Type
1	A	281	ARG
1	A	308	VAL
1	A	317	PHE
1	A	352	PHE
1	A	368	THR
1	A	387	LYS
1	A	388	ASP
1	A	390	LYS
1	A	423	ARG
1	B	6	GLN
1	B	7	SER
1	B	15	LYS
1	B	26	LEU
1	B	29	VAL
1	B	79	SER
1	B	105	TRP
1	B	106	THR
1	B	107	PHE
1	B	151	TYR
1	B	170	THR
1	B	172	LYS
1	B	197	LYS
1	B	204	ASP
1	B	216	LYS
1	B	225	LYS
1	B	255	ASP
1	B	264	CYS
1	B	265	ILE
1	B	298	GLU
1	B	312	LEU
1	B	314	ASP
1	B	325	ARG
1	B	339	CYS
1	B	396	LYS
1	B	440	ARG
1	C	28	ASN
1	C	80	ILE
1	C	83	LYS
1	C	89	HIS
1	C	106	THR
1	C	135	GLU
1	C	144	ASP

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Mol	Chain	Res	Type
1	C	151	TYR
1	C	167	GLN
1	C	172	LYS
1	C	178	ILE
1	C	185	ASP
1	C	197	LYS
1	C	216	LYS
1	C	225	LYS
1	C	238	ASN
1	C	251	LYS
1	C	265	ILE
1	C	280	ARG
1	C	307	SER
1	C	321	THR
1	C	339	CYS
1	C	368	THR
1	C	387	LYS
1	C	390	LYS
1	D	28	ASN
1	D	39	ARG
1	D	53	VAL
1	D	61	THR
1	D	81	LEU
1	D	110	ARG
1	D	131	VAL
1	D	151	TYR
1	D	172	LYS
1	D	185	ASP
1	D	197	LYS
1	D	240	CYS
1	D	261	GLU
1	D	265	ILE
1	D	304	MSE
1	D	321	THR
1	D	339	CYS
1	D	346	ASP
1	D	364	THR
1	D	368	THR
1	D	383	PRO
1	D	387	LYS
1	D	390	LYS
1	D	406	ASP

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Mol	Chain	Res	Type
1	D	442	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	HIS
1	A	328	GLN
1	A	340	HIS
1	A	342	ASN
1	A	354	HIS
1	B	290	ASN
1	C	28	ASN
1	C	173	HIS
1	C	238	ASN
1	C	306	GLN
1	D	33	HIS
1	D	89	HIS
1	D	328	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	500	-	4,4,4	0.22	0	6,6,6	0.19	0
2	SO4	B	500	-	4,4,4	0.08	0	6,6,6	0.26	0
2	SO4	C	500	-	4,4,4	0.25	0	6,6,6	0.29	0
2	SO4	D	500	-	4,4,4	0.19	0	6,6,6	0.10	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	SO4	A	500	-	-	0/0/0/0	0/0/0/0
2	SO4	B	500	-	-	0/0/0/0	0/0/0/0
2	SO4	C	500	-	-	0/0/0/0	0/0/0/0
2	SO4	D	500	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	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, 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	415/455 (91%)	-0.09	12 (2%) 55 64	13, 28, 48, 80	0
1	B	418/455 (91%)	-0.06	6 (1%) 78 83	15, 30, 47, 72	0
1	C	412/455 (90%)	0.72	58 (14%) 4 6	20, 51, 102, 122	0
1	D	410/455 (90%)	1.41	120 (29%) 1 1	25, 79, 109, 124	0
All	All	1655/1820 (90%)	0.49	196 (11%) 6 10	13, 39, 100, 124	0

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	TRP	10.0
1	D	419	PRO	7.3
1	D	170	THR	7.1
1	B	105	TRP	6.1
1	D	74	VAL	5.8
1	C	7	SER	5.7
1	D	162	ASP	5.5
1	D	375	GLY	5.5
1	D	420	ASN	5.3
1	D	171	GLY	5.3
1	D	401	ILE	5.3
1	C	395	ASP	5.3
1	D	448	GLU	5.2
1	D	406	ASP	5.2
1	D	51	THR	5.2
1	C	79	SER	5.1
1	D	47	ASN	4.9
1	D	400	GLY	4.8
1	C	397	PRO	4.8
1	D	31	GLY	4.8
1	D	397	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	43	ILE	4.6
1	C	420	ASN	4.5
1	D	49	GLY	4.5
1	C	107	PHE	4.5
1	C	171	GLY	4.5
1	D	396	LYS	4.4
1	C	47	ASN	4.3
1	C	49	GLY	4.3
1	C	136	LEU	4.3
1	C	8	VAL	4.2
1	A	422	ALA	4.1
1	C	90	ASN	4.1
1	D	110	ARG	4.1
1	D	354	HIS	4.1
1	D	446	VAL	4.1
1	D	442	ARG	4.0
1	D	108	GLU	4.0
1	D	176	TYR	4.0
1	D	174	GLU	4.0
1	D	71	PRO	3.9
1	D	87	ASP	3.9
1	D	381	LYS	3.9
1	D	172	LYS	3.8
1	D	78	ILE	3.8
1	D	402	GLU	3.8
1	D	395	ASP	3.8
1	D	175	TRP	3.7
1	D	75	GLY	3.7
1	D	434	PRO	3.7
1	D	89	HIS	3.7
1	C	67	THR	3.6
1	D	15	LYS	3.6
1	C	78	ILE	3.5
1	D	173	HIS	3.5
1	D	16	VAL	3.5
1	D	388	ASP	3.4
1	D	161	THR	3.4
1	D	345	PHE	3.4
1	C	50	HIS	3.4
1	D	26	LEU	3.3
1	D	317	PHE	3.3
1	A	448	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	128	PHE	3.3
1	D	159	LYS	3.3
1	C	381	LYS	3.3
1	D	169	VAL	3.3
1	C	48	SER	3.2
1	C	388	ASP	3.2
1	D	144	ASP	3.2
1	A	419	PRO	3.2
1	D	17	ILE	3.2
1	D	132	PRO	3.1
1	A	104	ALA	3.1
1	D	392	LYS	3.1
1	A	107	PHE	3.1
1	C	417	LYS	3.1
1	C	106	THR	3.1
1	D	385	GLU	3.1
1	A	252	GLY	3.1
1	C	172	LYS	3.0
1	D	7	SER	3.0
1	D	399	LEU	3.0
1	D	64	ASN	3.0
1	D	60	ALA	3.0
1	C	170	THR	3.0
1	C	42	VAL	2.9
1	A	251	LYS	2.9
1	C	11	ILE	2.9
1	C	51	THR	2.9
1	D	387	LYS	2.9
1	D	422	ALA	2.9
1	D	177	ASP	2.9
1	C	317	PHE	2.9
1	D	409	LEU	2.9
1	D	230	ASP	2.9
1	A	90	ASN	2.8
1	D	145	GLU	2.8
1	D	342	ASN	2.8
1	C	15	LYS	2.8
1	C	86	ASN	2.8
1	C	419	PRO	2.8
1	C	406	ASP	2.8
1	D	80	ILE	2.8
1	B	449	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	122	LEU	2.7
1	D	427	ILE	2.7
1	D	416	LYS	2.7
1	D	160	ILE	2.7
1	D	20	ALA	2.7
1	C	402	GLU	2.7
1	D	53	VAL	2.7
1	D	8	VAL	2.7
1	D	84	ILE	2.7
1	B	107	PHE	2.7
1	D	37	PHE	2.7
1	C	77	PRO	2.6
1	D	235	LEU	2.6
1	D	140	GLY	2.6
1	D	252	GLY	2.6
1	C	392	LYS	2.6
1	D	163	LEU	2.6
1	D	438	PHE	2.6
1	C	54	GLY	2.6
1	D	377	PHE	2.5
1	B	6	GLN	2.5
1	C	413	GLU	2.5
1	D	86	ASN	2.5
1	B	263	PRO	2.5
1	D	378	TYR	2.5
1	D	79	SER	2.5
1	D	36	TYR	2.5
1	D	403	LEU	2.5
1	D	41	ILE	2.5
1	D	361	GLY	2.4
1	D	229	PRO	2.4
1	C	17	ILE	2.4
1	C	53	VAL	2.4
1	D	122	LEU	2.4
1	A	420	ASN	2.4
1	A	435	GLY	2.4
1	B	252	GLY	2.4
1	D	72	HIS	2.4
1	C	12	THR	2.4
1	C	13	ASP	2.4
1	C	252	GLY	2.4
1	D	198	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	44	LEU	2.3
1	D	62	ILE	2.3
1	D	67	THR	2.3
1	D	63	GLU	2.3
1	D	129	LEU	2.3
1	C	387	LYS	2.3
1	C	416	LYS	2.3
1	C	401	ILE	2.3
1	D	35	PRO	2.3
1	D	119	ALA	2.3
1	D	127	GLN	2.3
1	D	42	VAL	2.3
1	C	117	LEU	2.3
1	D	199	ARG	2.3
1	C	89	HIS	2.3
1	D	157	ASP	2.3
1	C	41	ILE	2.2
1	A	268	ASN	2.2
1	D	205	PHE	2.2
1	C	124	LEU	2.2
1	D	393	LEU	2.2
1	D	22	HIS	2.2
1	D	153	PHE	2.2
1	D	421	GLY	2.2
1	D	418	LEU	2.2
1	D	225	LYS	2.2
1	C	110	ARG	2.2
1	D	226	LYS	2.2
1	C	44	LEU	2.2
1	D	353	SER	2.2
1	C	203	LYS	2.1
1	C	230	ASP	2.1
1	C	440	ARG	2.1
1	C	362	ASN	2.1
1	D	182	LYS	2.1
1	D	413	GLU	2.1
1	D	164	PRO	2.1
1	D	248	GLN	2.1
1	D	203	LYS	2.1
1	C	385	GLU	2.1
1	C	409	LEU	2.1
1	D	191[A]	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	76	ARG	2.1
1	D	168	PRO	2.1
1	D	130	GLY	2.0
1	D	431	PHE	2.0
1	D	43	ILE	2.0
1	D	414	LEU	2.0
1	D	227	HIS	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 carbohydrates 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. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	MG	B	501	1/1	0.96	0.21	1.94	45,45,45,45	0
2	SO4	A	500	5/5	0.97	0.10	-0.57	40,41,41,48	0
2	SO4	B	500	5/5	0.98	0.10	-0.62	38,38,38,40	0
3	MG	D	501	1/1	0.96	0.10	-1.37	49,49,49,49	0
2	SO4	D	500	5/5	0.96	0.11	-1.58	75,76,78,82	0
2	SO4	C	500	5/5	0.98	0.08	-2.74	42,48,49,50	0
3	MG	A	501	1/1	0.99	0.04	-4.30	28,28,28,28	0
3	MG	C	501	1/1	0.92	0.10	-	40,40,40,40	0
4	CL	B	503	1/1	0.94	0.05	-	56,56,56,56	0

6.5 Other polymers (i)

There are no such residues in this entry.