Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 07:46 AM EDT

PDB ID	:	2OQH
Title	:	Crystal structure of an isomerase from Streptomyces coelicolor A3(2)
Authors	:	Agarwal, R.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2007-01-31
Resolution	:	1.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

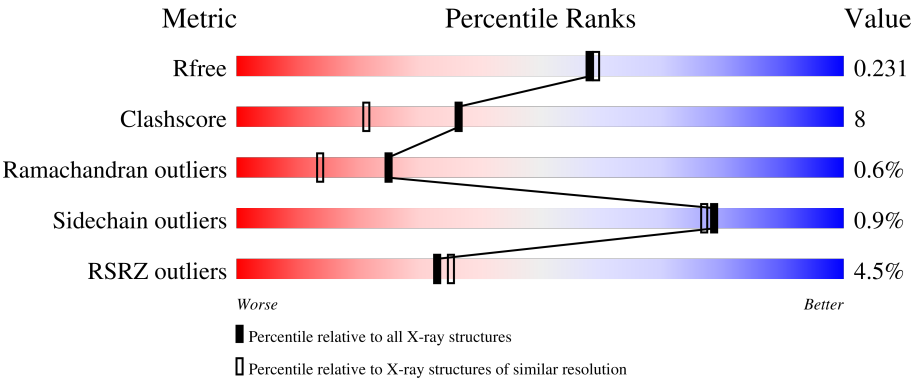
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	385	5% 76% 17% 6%
1	B	385	4% 81% 16%
1	C	385	3% 81% 15%
1	D	385	4% 82% 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11989 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 isomerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	Se	0	0	0
			2691	1705	469	501	6	10			
1	B	374	Total	C	N	O	S	Se	0	0	0
			2802	1771	487	528	6	10			
1	C	368	Total	C	N	O	S	Se	0	0	0
			2753	1743	478	516	6	10			
1	D	371	Total	C	N	O	S	Se	0	0	0
			2778	1755	484	523	6	10			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	cloning artifact	UNP Q9F3A5
A	2	SER	-	cloning artifact	UNP Q9F3A5
A	3	LEU	-	cloning artifact	UNP Q9F3A5
A	51	MSE	MET	modified residue	UNP Q9F3A5
A	63	MSE	MET	modified residue	UNP Q9F3A5
A	84	MSE	MET	modified residue	UNP Q9F3A5
A	108	MSE	MET	modified residue	UNP Q9F3A5
A	151	MSE	MET	modified residue	UNP Q9F3A5
A	232	MSE	MET	modified residue	UNP Q9F3A5
A	247	MSE	MET	modified residue	UNP Q9F3A5
A	259	MSE	MET	modified residue	UNP Q9F3A5
A	294	MSE	MET	modified residue	UNP Q9F3A5
A	326	MSE	MET	modified residue	UNP Q9F3A5
A	378	GLU	-	cloning artifact	UNP Q9F3A5
A	379	GLY	-	cloning artifact	UNP Q9F3A5
A	380	HIS	-	cloning artifact	UNP Q9F3A5
A	381	HIS	-	cloning artifact	UNP Q9F3A5
A	382	HIS	-	cloning artifact	UNP Q9F3A5
A	383	HIS	-	cloning artifact	UNP Q9F3A5
A	384	HIS	-	cloning artifact	UNP Q9F3A5
A	385	HIS	-	cloning artifact	UNP Q9F3A5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MSE	-	cloning artifact	UNP Q9F3A5
B	2	SER	-	cloning artifact	UNP Q9F3A5
B	3	LEU	-	cloning artifact	UNP Q9F3A5
B	51	MSE	MET	modified residue	UNP Q9F3A5
B	63	MSE	MET	modified residue	UNP Q9F3A5
B	84	MSE	MET	modified residue	UNP Q9F3A5
B	108	MSE	MET	modified residue	UNP Q9F3A5
B	151	MSE	MET	modified residue	UNP Q9F3A5
B	232	MSE	MET	modified residue	UNP Q9F3A5
B	247	MSE	MET	modified residue	UNP Q9F3A5
B	259	MSE	MET	modified residue	UNP Q9F3A5
B	294	MSE	MET	modified residue	UNP Q9F3A5
B	326	MSE	MET	modified residue	UNP Q9F3A5
B	378	GLU	-	cloning artifact	UNP Q9F3A5
B	379	GLY	-	cloning artifact	UNP Q9F3A5
B	380	HIS	-	cloning artifact	UNP Q9F3A5
B	381	HIS	-	cloning artifact	UNP Q9F3A5
B	382	HIS	-	cloning artifact	UNP Q9F3A5
B	383	HIS	-	cloning artifact	UNP Q9F3A5
B	384	HIS	-	cloning artifact	UNP Q9F3A5
B	385	HIS	-	cloning artifact	UNP Q9F3A5
C	1	MSE	-	cloning artifact	UNP Q9F3A5
C	2	SER	-	cloning artifact	UNP Q9F3A5
C	3	LEU	-	cloning artifact	UNP Q9F3A5
C	51	MSE	MET	modified residue	UNP Q9F3A5
C	63	MSE	MET	modified residue	UNP Q9F3A5
C	84	MSE	MET	modified residue	UNP Q9F3A5
C	108	MSE	MET	modified residue	UNP Q9F3A5
C	151	MSE	MET	modified residue	UNP Q9F3A5
C	232	MSE	MET	modified residue	UNP Q9F3A5
C	247	MSE	MET	modified residue	UNP Q9F3A5
C	259	MSE	MET	modified residue	UNP Q9F3A5
C	294	MSE	MET	modified residue	UNP Q9F3A5
C	326	MSE	MET	modified residue	UNP Q9F3A5
C	378	GLU	-	cloning artifact	UNP Q9F3A5
C	379	GLY	-	cloning artifact	UNP Q9F3A5
C	380	HIS	-	cloning artifact	UNP Q9F3A5
C	381	HIS	-	cloning artifact	UNP Q9F3A5
C	382	HIS	-	cloning artifact	UNP Q9F3A5
C	383	HIS	-	cloning artifact	UNP Q9F3A5
C	384	HIS	-	cloning artifact	UNP Q9F3A5
C	385	HIS	-	cloning artifact	UNP Q9F3A5

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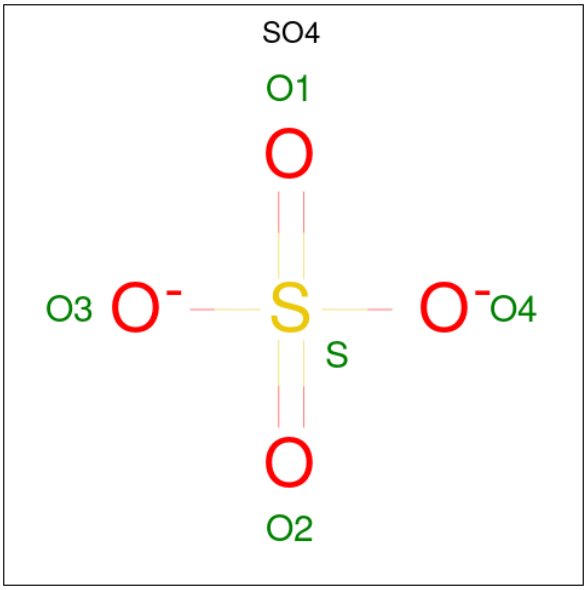
Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MSE	-	cloning artifact	UNP Q9F3A5
D	2	SER	-	cloning artifact	UNP Q9F3A5
D	3	LEU	-	cloning artifact	UNP Q9F3A5
D	51	MSE	MET	modified residue	UNP Q9F3A5
D	63	MSE	MET	modified residue	UNP Q9F3A5
D	84	MSE	MET	modified residue	UNP Q9F3A5
D	108	MSE	MET	modified residue	UNP Q9F3A5
D	151	MSE	MET	modified residue	UNP Q9F3A5
D	232	MSE	MET	modified residue	UNP Q9F3A5
D	247	MSE	MET	modified residue	UNP Q9F3A5
D	259	MSE	MET	modified residue	UNP Q9F3A5
D	294	MSE	MET	modified residue	UNP Q9F3A5
D	326	MSE	MET	modified residue	UNP Q9F3A5
D	378	GLU	-	cloning artifact	UNP Q9F3A5
D	379	GLY	-	cloning artifact	UNP Q9F3A5
D	380	HIS	-	cloning artifact	UNP Q9F3A5
D	381	HIS	-	cloning artifact	UNP Q9F3A5
D	382	HIS	-	cloning artifact	UNP Q9F3A5
D	383	HIS	-	cloning artifact	UNP Q9F3A5
D	384	HIS	-	cloning artifact	UNP Q9F3A5
D	385	HIS	-	cloning artifact	UNP Q9F3A5

- 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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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 water.

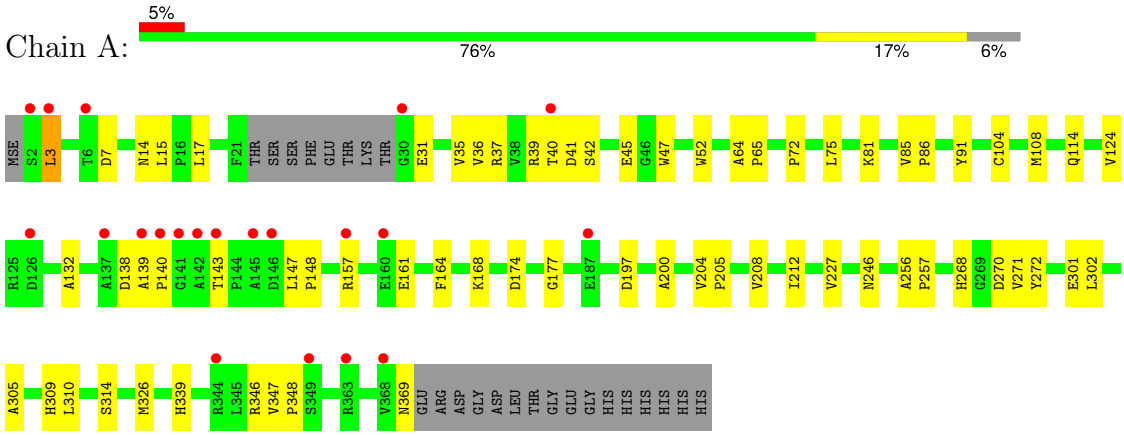
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	215	Total O 215 215	0	0
3	B	235	Total O 235 235	0	0
3	C	240	Total O 240 240	0	0
3	D	255	Total O 255 255	0	0

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.

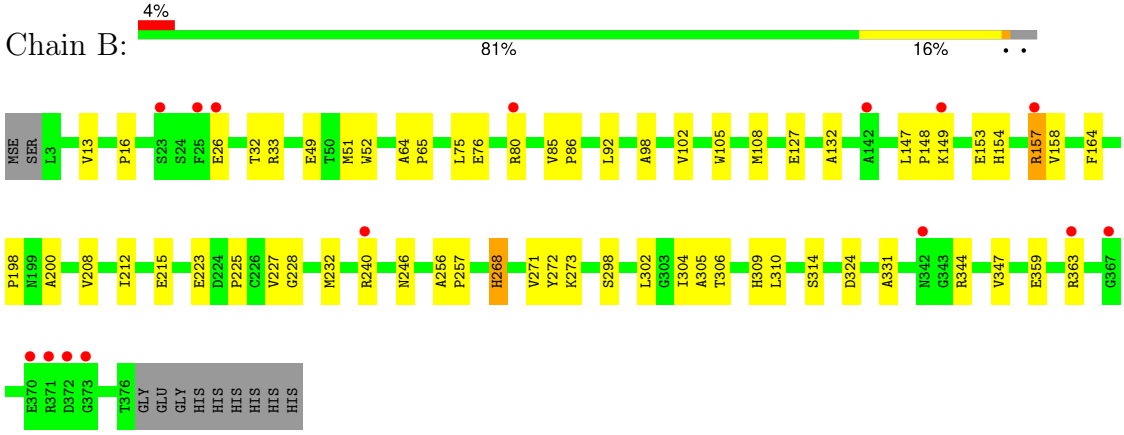
• Molecule 1: Putative isomerase

Chain A:



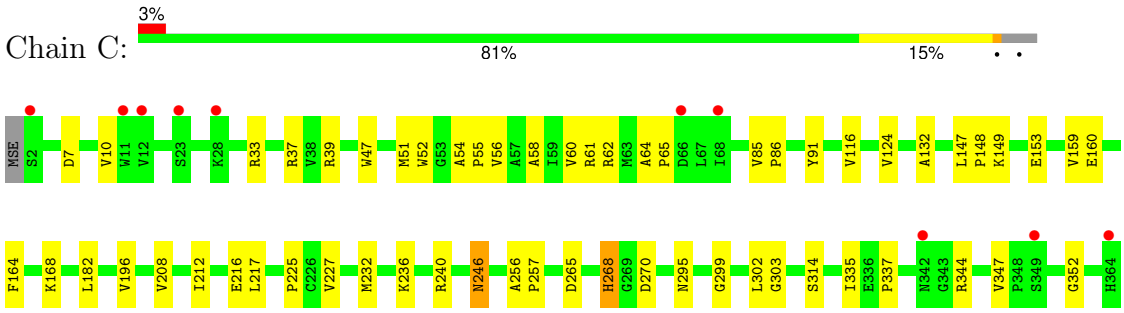
• Molecule 1: Putative isomerase

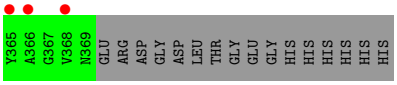
Chain B:



• Molecule 1: Putative isomerase

Chain C:





• Molecule 1: Putative isomerase

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α, β, γ	120.34Å 120.34Å 126.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.45 – 1.98 36.45 – 1.98	Depositor EDS
% Data completeness (in resolution range)	97.0 (36.45-1.98) 97.1 (36.45-1.98)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.09 (at 1.98Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.231 0.205 , 0.231	Depositor DCC
R_{free} test set	3682 reflections (2.94%)	wwPDB-VP
Wilson B-factor (Å^2)	16.9	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 50.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.011 for -h,-l,-k 0.000 for -h,l,k 0.000 for l,-k,h 0.008 for -l,-k,-h 0.032 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11989	wwPDB-VP
Average B, all atoms (Å^2)	18.0	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 36.85 % 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 4.6883e-04. 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

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	0.34	0/2738	0.62	0/3717
1	B	0.34	0/2851	0.62	0/3871
1	C	0.34	0/2802	0.64	0/3805
1	D	0.35	0/2825	0.64	0/3834
All	All	0.34	0/11216	0.63	0/15227

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
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	272	TYR	Sidechain
1	B	272	TYR	Sidechain

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	2691	0	2681	43	0
1	B	2802	0	2784	47	0
1	C	2753	0	2741	44	0
1	D	2778	0	2762	39	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	215	0	0	11	0
3	B	235	0	0	4	0
3	C	240	0	0	14	0
3	D	255	0	0	7	0
All	All	11989	0	10968	173	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 (173) 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:B:75:LEU:HD11	1:B:108:MSE:HE1	1.45	0.98
1:B:49:GLU:HG2	1:B:304:ILE:HB	1.45	0.96
1:D:246:ASN:HB3	3:D:755:HOH:O	1.77	0.82
1:A:75:LEU:HD11	1:A:108:MSE:HE1	1.59	0.82
1:B:105:TRP:HA	1:B:108:MSE:HE3	1.62	0.81
1:C:335:ILE:HG13	3:C:740:HOH:O	1.80	0.80
1:A:35:VAL:HG12	3:A:640:HOH:O	1.83	0.78
1:D:271:VAL:H	1:D:309:HIS:HE1	1.30	0.77
1:D:149:LYS:HE2	3:D:737:HOH:O	1.83	0.77
1:B:80:ARG:HG2	1:B:80:ARG:HH11	1.51	0.76
1:A:348:PRO:HD2	3:A:706:HOH:O	1.87	0.74
1:A:15:LEU:HD22	1:A:302:LEU:HD13	1.69	0.73
1:B:157:ARG:HH11	1:B:157:ARG:HB3	1.54	0.73
1:A:75:LEU:CD1	1:A:108:MSE:HE1	2.20	0.71
1:B:314:SER:HB2	1:B:347:VAL:HG21	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:PRO:HG2	1:B:225:PRO:HA	1.73	0.70
1:A:72:PRO:O	1:A:108:MSE:HE2	1.91	0.69
1:A:271:VAL:H	1:A:309:HIS:HE1	1.41	0.68
1:B:271:VAL:H	1:B:309:HIS:HE1	1.41	0.68
1:D:256:ALA:HB3	1:D:257:PRO:HD3	1.76	0.67
1:A:168:LYS:HE2	1:A:197:ASP:HB2	1.76	0.67
1:B:359:GLU:O	1:B:363:ARG:HG2	1.96	0.66
1:C:33:ARG:NH1	1:C:51:MSE:HG2	2.11	0.65
1:B:85:VAL:HB	1:B:86:PRO:HD3	1.80	0.64
1:D:363:ARG:HH11	1:D:363:ARG:HB3	1.61	0.64
1:C:225:PRO:HD2	1:C:232:MSE:SE	2.48	0.64
1:B:64:ALA:HB3	1:B:65:PRO:HD3	1.81	0.63
1:A:256:ALA:HB3	1:A:257:PRO:HD3	1.80	0.62
1:C:33:ARG:HH12	1:C:51:MSE:HG2	1.64	0.62
1:A:326:MSE:HE1	3:A:653:HOH:O	1.98	0.62
1:C:85:VAL:HB	1:C:86:PRO:HD3	1.83	0.61
1:A:7:ASP:OD2	1:A:39:ARG:HD2	2.01	0.61
1:C:227:VAL:HB	3:C:639:HOH:O	2.00	0.60
1:A:17:LEU:HD11	1:A:31:GLU:HB2	1.83	0.60
1:D:85:VAL:HB	1:D:86:PRO:HD3	1.84	0.60
1:A:246:ASN:HB3	1:A:268:HIS:HB2	1.84	0.59
1:D:105:TRP:HA	1:D:108:MSE:HE3	1.83	0.59
1:D:247:MSE:HG3	3:D:755:HOH:O	2.01	0.59
1:C:58:ALA:O	1:C:62:ARG:HG2	2.03	0.59
1:D:156:VAL:O	1:D:160:GLU:HG2	2.03	0.59
1:B:105:TRP:CA	1:B:108:MSE:HE3	2.31	0.58
1:B:26:GLU:O	1:B:26:GLU:HG3	2.04	0.57
1:B:80:ARG:HG2	1:B:80:ARG:NH1	2.17	0.57
1:C:256:ALA:HB3	1:C:257:PRO:HD3	1.86	0.57
1:D:147:LEU:HB3	1:D:148:PRO:HD3	1.86	0.57
1:B:198:PRO:CG	1:B:225:PRO:HA	2.34	0.57
1:B:32:THR:O	1:B:33:ARG:HD2	2.04	0.56
1:D:51:MSE:HE3	1:D:52:TRP:CD1	2.40	0.56
1:B:33:ARG:NH1	1:B:49:GLU:OE2	2.38	0.56
1:B:51:MSE:HE2	1:B:92:LEU:CD2	2.36	0.56
1:D:132:ALA:HB2	1:D:164:PHE:CG	2.41	0.55
1:D:75:LEU:CD1	1:D:108:MSE:HE1	2.37	0.55
1:D:236:LYS:HE2	3:D:702:HOH:O	2.06	0.54
1:D:225:PRO:HD2	1:D:232:MSE:SE	2.58	0.54
1:D:132:ALA:HB2	1:D:164:PHE:CD2	2.42	0.54
1:B:157:ARG:HH11	1:B:157:ARG:CB	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ARG:NH2	3:B:673:HOH:O	2.42	0.53
1:B:256:ALA:HB3	1:B:257:PRO:HD3	1.89	0.53
1:C:51:MSE:HB3	1:C:52:TRP:HD1	1.74	0.53
1:C:132:ALA:HB2	1:C:164:PHE:CG	2.43	0.53
1:D:50:THR:HB	1:D:99:ALA:HB2	1.91	0.53
1:C:149:LYS:O	1:C:153:GLU:HG2	2.09	0.52
1:D:157:ARG:O	1:D:161:GLU:HG3	2.09	0.52
1:B:223:GLU:OE2	1:B:246:ASN:ND2	2.43	0.52
1:A:314:SER:HB2	1:A:347:VAL:HG21	1.91	0.52
1:B:240:ARG:NH2	3:B:615:HOH:O	2.43	0.51
1:D:363:ARG:HB3	1:D:363:ARG:NH1	2.25	0.51
1:A:39:ARG:NH1	1:A:45:GLU:OE1	2.43	0.51
1:A:147:LEU:HB3	1:A:148:PRO:HD3	1.91	0.51
1:C:182:LEU:HD11	1:C:196:VAL:HB	1.93	0.51
1:D:314:SER:HB2	1:D:347:VAL:HG21	1.91	0.51
1:B:127:GLU:HB3	1:B:344:ARG:HD3	1.92	0.50
1:C:268:HIS:CD2	1:C:295:ASN:HB3	2.46	0.50
1:C:240:ARG:CD	3:C:507:HOH:O	2.59	0.50
1:B:132:ALA:HB2	1:B:164:PHE:CG	2.47	0.50
1:D:337:PRO:HG3	3:D:634:HOH:O	2.11	0.50
1:A:132:ALA:HB2	1:A:164:PHE:CG	2.47	0.49
1:C:149:LYS:HB2	3:C:615:HOH:O	2.12	0.49
1:C:314:SER:HB2	1:C:347:VAL:HG21	1.95	0.49
1:A:85:VAL:HB	1:A:86:PRO:HD3	1.95	0.49
1:D:204:VAL:HB	1:D:205:PRO:HD3	1.95	0.49
1:B:246:ASN:HB3	1:B:268:HIS:HB2	1.95	0.49
1:A:204:VAL:HB	1:A:205:PRO:HD3	1.94	0.48
1:A:301:GLU:HB3	1:A:305:ALA:HB3	1.95	0.48
1:C:147:LEU:HB3	1:C:148:PRO:HD3	1.96	0.48
1:A:64:ALA:HB3	1:A:65:PRO:HD3	1.95	0.48
1:D:124:VAL:HG22	1:D:314:SER:O	2.13	0.48
1:D:301:GLU:HB3	1:D:305:ALA:HB3	1.94	0.48
1:A:39:ARG:HG3	1:A:39:ARG:HH11	1.79	0.48
1:C:132:ALA:HB2	1:C:164:PHE:CD2	2.49	0.48
1:B:147:LEU:HB3	1:B:148:PRO:HD3	1.95	0.48
1:D:105:TRP:CA	1:D:108:MSE:HE3	2.44	0.48
1:C:52:TRP:CD1	1:C:52:TRP:N	2.80	0.47
1:C:116:VAL:HG23	1:C:352:GLY:C	2.35	0.47
1:D:340:LEU:HB2	3:D:650:HOH:O	2.14	0.47
1:B:51:MSE:HE2	1:B:92:LEU:HD23	1.96	0.47
1:B:132:ALA:HB2	1:B:164:PHE:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ASN:HB3	1:B:268:HIS:CB	2.45	0.47
1:B:273:LYS:HE2	3:B:657:HOH:O	2.14	0.47
1:C:240:ARG:HD3	3:C:507:HOH:O	2.15	0.47
1:D:271:VAL:H	1:D:309:HIS:CE1	2.21	0.47
1:A:157:ARG:O	1:A:161:GLU:HG3	2.15	0.46
1:C:337:PRO:HD2	3:C:591:HOH:O	2.15	0.46
1:A:310:LEU:HB2	3:A:706:HOH:O	2.15	0.46
1:C:64:ALA:HB3	1:C:65:PRO:HD3	1.95	0.46
1:B:16:PRO:HG2	1:B:331:ALA:HB3	1.96	0.46
1:B:49:GLU:HG3	1:B:305:ALA:HB2	1.96	0.46
1:B:98:ALA:O	1:B:102:VAL:HG23	2.15	0.46
1:C:54:ALA:N	1:C:55:PRO:HD2	2.31	0.45
1:C:168:LYS:HE2	3:C:635:HOH:O	2.16	0.45
1:C:37:ARG:HD3	1:C:47:TRP:CZ2	2.51	0.45
1:B:154:HIS:O	1:B:158:VAL:HG23	2.17	0.45
1:B:200:ALA:HB1	1:B:227:VAL:HG22	1.99	0.45
1:A:37:ARG:HD3	1:A:47:TRP:CZ2	2.51	0.45
1:D:227:VAL:HG12	1:D:228:GLY:N	2.31	0.45
1:A:114:GLN:NE2	3:A:663:HOH:O	2.50	0.45
1:A:40:THR:C	1:A:42:SER:H	2.20	0.45
1:D:154:HIS:O	1:D:158:VAL:HG23	2.17	0.45
1:C:302:LEU:HG	3:C:657:HOH:O	2.15	0.45
1:A:104:CYS:C	1:A:108:MSE:HE3	2.38	0.45
1:C:10:VAL:HB	1:C:61:ARG:HE	1.82	0.44
1:C:236:LYS:HE3	1:C:265:ASP:OD1	2.16	0.44
1:A:208:VAL:O	1:A:212:ILE:HG13	2.18	0.44
1:C:160:GLU:HG3	3:C:703:HOH:O	2.16	0.44
1:A:14:ASN:ND2	1:A:369:ASN:HA	2.31	0.44
1:B:149:LYS:O	1:B:153:GLU:HG3	2.18	0.44
1:D:105:TRP:N	1:D:108:MSE:HE3	2.33	0.44
1:D:363:ARG:NH1	1:D:363:ARG:CB	2.81	0.44
1:C:51:MSE:HB3	1:C:52:TRP:CD1	2.52	0.44
1:D:72:PRO:O	1:D:108:MSE:HE2	2.18	0.44
3:A:654:HOH:O	1:C:55:PRO:HB3	2.18	0.43
1:B:76:GLU:O	1:B:80:ARG:HG2	2.18	0.43
1:C:216:GLU:HG3	1:C:217:LEU:HD23	2.00	0.43
1:B:298:SER:HB2	1:B:324:ASP:O	2.19	0.43
1:D:75:LEU:HD23	1:D:75:LEU:HA	1.80	0.43
1:A:36:VAL:C	3:A:640:HOH:O	2.56	0.43
1:B:227:VAL:HG12	1:B:228:GLY:N	2.33	0.43
1:B:33:ARG:HH11	1:B:33:ARG:HG3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ALA:HB1	1:A:227:VAL:HG12	2.01	0.43
1:C:51:MSE:SE	3:C:537:HOH:O	2.87	0.43
1:A:138:ASP:C	1:A:140:PRO:HD3	2.37	0.43
1:A:174:ASP:OD2	1:A:177:GLY:HA3	2.19	0.43
1:A:139:ALA:N	1:A:140:PRO:HD3	2.33	0.43
1:C:124:VAL:HG22	1:C:314:SER:O	2.18	0.43
1:D:75:LEU:HD11	1:D:108:MSE:HE1	2.00	0.43
1:C:240:ARG:HD2	3:C:507:HOH:O	2.18	0.42
1:A:124:VAL:HG22	1:A:314:SER:O	2.19	0.42
1:B:302:LEU:HD23	1:B:302:LEU:HA	1.91	0.42
1:C:7:ASP:HB2	1:C:39:ARG:HB3	2.01	0.42
1:B:13:VAL:O	1:B:32:THR:HA	2.20	0.42
1:A:81:LYS:HD3	3:A:621:HOH:O	2.20	0.42
1:D:16:PRO:HG2	1:D:331:ALA:HB3	2.01	0.42
1:A:339:HIS:HB3	1:A:346:ARG:HB3	2.01	0.42
1:B:208:VAL:O	1:B:212:ILE:HG13	2.19	0.42
1:B:215:GLU:HB3	3:B:664:HOH:O	2.18	0.42
1:A:168:LYS:HD3	3:A:625:HOH:O	2.19	0.42
1:D:284:ALA:HA	1:D:294:MSE:SE	2.70	0.42
1:C:51:MSE:HE3	1:C:299:GLY:O	2.20	0.41
1:C:208:VAL:O	1:C:212:ILE:HG13	2.20	0.41
1:C:246:ASN:ND2	3:C:553:HOH:O	2.52	0.41
1:C:302:LEU:HA	1:C:302:LEU:HD23	1.83	0.41
1:D:332:ASP:OD2	1:D:361:LYS:HE2	2.20	0.41
1:B:225:PRO:HD2	1:B:232:MSE:SE	2.71	0.41
1:C:159:VAL:HB	3:C:703:HOH:O	2.20	0.41
1:C:337:PRO:HB2	3:C:591:HOH:O	2.20	0.41
1:D:37:ARG:NH1	3:D:592:HOH:O	2.53	0.41
1:D:71:SER:HA	1:D:72:PRO:HD3	1.95	0.41
1:A:15:LEU:HD22	1:A:302:LEU:CD1	2.46	0.41
1:B:306:THR:O	1:B:310:LEU:HG	2.21	0.41
1:A:3:LEU:N	3:A:627:HOH:O	2.53	0.40
1:A:143:THR:HG23	3:A:556:HOH:O	2.19	0.40
1:A:132:ALA:HB2	1:A:164:PHE:CD2	2.56	0.40
1:C:56:VAL:O	1:C:60:VAL:HG23	2.21	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	356/385 (92%)	343 (96%)	9 (2%)	4 (1%)	14 5
1	B	372/385 (97%)	363 (98%)	8 (2%)	1 (0%)	41 29
1	C	366/385 (95%)	357 (98%)	7 (2%)	2 (0%)	29 16
1	D	367/385 (95%)	354 (96%)	11 (3%)	2 (0%)	29 16
All	All	1461/1540 (95%)	1417 (97%)	35 (2%)	9 (1%)	25 14

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	52	TRP
1	A	3	LEU
1	A	41	ASP
1	A	52	TRP
1	C	270	ASP
1	A	270	ASP
1	D	270	ASP
1	D	52	TRP
1	C	303	GLY

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	278/289 (96%)	277 (100%)	1 (0%)	91 90
1	B	291/289 (101%)	289 (99%)	2 (1%)	84 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	286/289 (99%)	282 (99%)	4 (1%)	67 62
1	D	288/289 (100%)	285 (99%)	3 (1%)	76 73
All	All	1143/1156 (99%)	1133 (99%)	10 (1%)	78 77

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	TYR
1	B	157	ARG
1	B	268	HIS
1	C	91	TYR
1	C	246	ASN
1	C	268	HIS
1	C	344	ARG
1	D	91	TYR
1	D	196	VAL
1	D	268	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	A	268	HIS
1	A	297	HIS
1	A	309	HIS
1	B	309	HIS
1	C	82	GLN
1	C	154	HIS
1	C	193	ASN
1	C	246	ASN
1	C	268	HIS
1	D	246	ASN
1	D	268	HIS
1	D	309	HIS
1	D	342	ASN

5.3.3 RNA

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)

4 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	SO4	C	501	-	4,4,4	0.42	0	6,6,6	0.15	0
2	SO4	D	501	-	4,4,4	0.39	0	6,6,6	0.09	0
2	SO4	B	501	-	4,4,4	0.42	0	6,6,6	0.27	0
2	SO4	A	501	-	4,4,4	0.37	0	6,6,6	0.10	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.

No monomer is involved in short contacts.

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	350/385 (90%)	0.43	21 (6%)	21	23	8, 19, 27, 34	0
1	B	364/385 (94%)	0.36	15 (4%)	37	39	8, 18, 26, 31	0
1	C	358/385 (92%)	0.32	13 (3%)	42	45	7, 18, 26, 31	0
1	D	361/385 (93%)	0.31	16 (4%)	34	36	8, 18, 26, 32	0
All	All	1433/1540 (93%)	0.35	65 (4%)	33	35	7, 18, 27, 34	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	27	THR	5.7
1	A	2	SER	5.5
1	A	141	GLY	5.1
1	A	142	ALA	4.7
1	C	2	SER	4.7
1	D	26	GLU	4.7
1	D	140	PRO	4.5
1	D	141	GLY	4.3
1	B	371	ARG	4.0
1	A	157	ARG	4.0
1	A	140	PRO	3.9
1	D	157	ARG	3.6
1	D	142	ALA	3.5
1	C	28	LYS	3.4
1	D	2	SER	3.4
1	B	25	PHE	3.4
1	D	149	LYS	3.2
1	A	363	ARG	3.1
1	C	66	ASP	3.0
1	C	11	TRP	2.9
1	B	370	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	375	LEU	2.7
1	A	145	ALA	2.7
1	C	365	TYR	2.6
1	B	23	SER	2.6
1	A	30	GLY	2.6
1	C	342	ASN	2.5
1	B	26	GLU	2.4
1	A	143	THR	2.4
1	D	29	THR	2.4
1	D	145	ALA	2.4
1	D	144	PRO	2.4
1	C	68	ILE	2.4
1	A	146	ASP	2.3
1	B	157	ARG	2.3
1	D	349	SER	2.3
1	A	368	VAL	2.3
1	C	12	VAL	2.3
1	A	40	THR	2.3
1	B	142	ALA	2.3
1	A	344	ARG	2.2
1	B	372	ASP	2.2
1	B	367	GLY	2.2
1	A	160	GLU	2.2
1	B	363	ARG	2.2
1	A	3	LEU	2.2
1	A	6	THR	2.2
1	D	143	THR	2.2
1	A	137	ALA	2.2
1	C	366	ALA	2.2
1	C	364	HIS	2.2
1	D	160	GLU	2.2
1	B	149	LYS	2.2
1	B	342	ASN	2.2
1	C	368	VAL	2.2
1	A	349	SER	2.2
1	A	187	GLU	2.1
1	A	126	ASP	2.1
1	C	23	SER	2.1
1	D	139	ALA	2.1
1	B	373	GLY	2.1
1	A	139	ALA	2.0
1	B	240	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	349	SER	2.0
1	B	80	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	B	501	5/5	0.95	0.24	37,38,39,40	0
2	SO4	A	501	5/5	0.96	0.20	37,39,40,40	0
2	SO4	C	501	5/5	0.96	0.27	37,39,40,40	0
2	SO4	D	501	5/5	0.97	0.23	35,37,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.