Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:07 PM GMT

PDB ID	:	4NU7
Title	:	2.05 Angstrom Crystal Structure of Ribulose-phosphate 3-epimerase from Toxoplasma gondii.
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Deposited on	:	2013-12-03
Resolution	:	2.05 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:

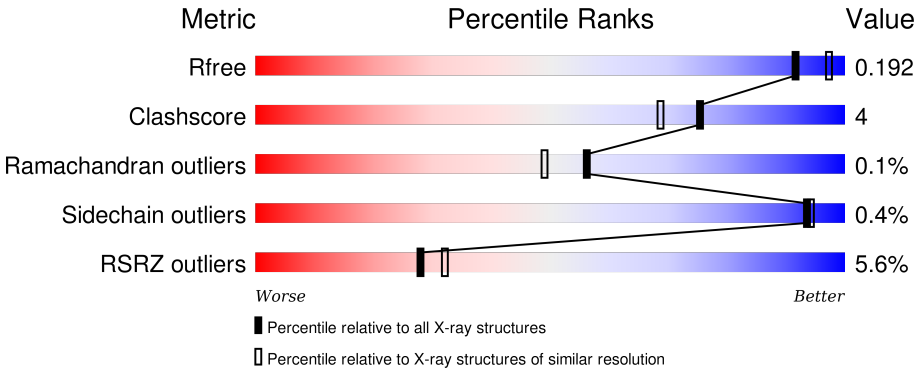
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.05 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	246	4% 83% 9% 9%
1	B	246	5% 85% 6% 9%
1	C	246	6% 85% 7% 8%
1	D	246	6% 85% 7% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7648 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 Ribulose-phosphate 3-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	14	0
			1798	1134	314	338	12			
1	B	225	Total	C	N	O	S	0	5	0
			1725	1096	295	322	12			
1	C	227	Total	C	N	O	S	0	9	0
			1772	1128	303	329	12			
1	D	226	Total	C	N	O	S	0	7	0
			1754	1110	307	325	12			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	231	GLY	-	EXPRESSION TAG	UNP B9PPN9
A	232	GLU	-	EXPRESSION TAG	UNP B9PPN9
A	233	ASN	-	EXPRESSION TAG	UNP B9PPN9
A	234	LEU	-	EXPRESSION TAG	UNP B9PPN9
A	235	TYR	-	EXPRESSION TAG	UNP B9PPN9
A	236	PHE	-	EXPRESSION TAG	UNP B9PPN9
A	237	GLN	-	EXPRESSION TAG	UNP B9PPN9
A	238	SER	-	EXPRESSION TAG	UNP B9PPN9
A	239	ALA	-	EXPRESSION TAG	UNP B9PPN9
A	240	GLY	-	EXPRESSION TAG	UNP B9PPN9
A	241	HIS	-	EXPRESSION TAG	UNP B9PPN9
A	242	HIS	-	EXPRESSION TAG	UNP B9PPN9
A	243	HIS	-	EXPRESSION TAG	UNP B9PPN9
A	244	HIS	-	EXPRESSION TAG	UNP B9PPN9
A	245	HIS	-	EXPRESSION TAG	UNP B9PPN9
A	246	HIS	-	EXPRESSION TAG	UNP B9PPN9
B	231	GLY	-	EXPRESSION TAG	UNP B9PPN9
B	232	GLU	-	EXPRESSION TAG	UNP B9PPN9
B	233	ASN	-	EXPRESSION TAG	UNP B9PPN9
B	234	LEU	-	EXPRESSION TAG	UNP B9PPN9
B	235	TYR	-	EXPRESSION TAG	UNP B9PPN9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	236	PHE	-	EXPRESSION TAG	UNP B9PPN9
B	237	GLN	-	EXPRESSION TAG	UNP B9PPN9
B	238	SER	-	EXPRESSION TAG	UNP B9PPN9
B	239	ALA	-	EXPRESSION TAG	UNP B9PPN9
B	240	GLY	-	EXPRESSION TAG	UNP B9PPN9
B	241	HIS	-	EXPRESSION TAG	UNP B9PPN9
B	242	HIS	-	EXPRESSION TAG	UNP B9PPN9
B	243	HIS	-	EXPRESSION TAG	UNP B9PPN9
B	244	HIS	-	EXPRESSION TAG	UNP B9PPN9
B	245	HIS	-	EXPRESSION TAG	UNP B9PPN9
B	246	HIS	-	EXPRESSION TAG	UNP B9PPN9
C	231	GLY	-	EXPRESSION TAG	UNP B9PPN9
C	232	GLU	-	EXPRESSION TAG	UNP B9PPN9
C	233	ASN	-	EXPRESSION TAG	UNP B9PPN9
C	234	LEU	-	EXPRESSION TAG	UNP B9PPN9
C	235	TYR	-	EXPRESSION TAG	UNP B9PPN9
C	236	PHE	-	EXPRESSION TAG	UNP B9PPN9
C	237	GLN	-	EXPRESSION TAG	UNP B9PPN9
C	238	SER	-	EXPRESSION TAG	UNP B9PPN9
C	239	ALA	-	EXPRESSION TAG	UNP B9PPN9
C	240	GLY	-	EXPRESSION TAG	UNP B9PPN9
C	241	HIS	-	EXPRESSION TAG	UNP B9PPN9
C	242	HIS	-	EXPRESSION TAG	UNP B9PPN9
C	243	HIS	-	EXPRESSION TAG	UNP B9PPN9
C	244	HIS	-	EXPRESSION TAG	UNP B9PPN9
C	245	HIS	-	EXPRESSION TAG	UNP B9PPN9
C	246	HIS	-	EXPRESSION TAG	UNP B9PPN9
D	231	GLY	-	EXPRESSION TAG	UNP B9PPN9
D	232	GLU	-	EXPRESSION TAG	UNP B9PPN9
D	233	ASN	-	EXPRESSION TAG	UNP B9PPN9
D	234	LEU	-	EXPRESSION TAG	UNP B9PPN9
D	235	TYR	-	EXPRESSION TAG	UNP B9PPN9
D	236	PHE	-	EXPRESSION TAG	UNP B9PPN9
D	237	GLN	-	EXPRESSION TAG	UNP B9PPN9
D	238	SER	-	EXPRESSION TAG	UNP B9PPN9
D	239	ALA	-	EXPRESSION TAG	UNP B9PPN9
D	240	GLY	-	EXPRESSION TAG	UNP B9PPN9
D	241	HIS	-	EXPRESSION TAG	UNP B9PPN9
D	242	HIS	-	EXPRESSION TAG	UNP B9PPN9
D	243	HIS	-	EXPRESSION TAG	UNP B9PPN9
D	244	HIS	-	EXPRESSION TAG	UNP B9PPN9
D	245	HIS	-	EXPRESSION TAG	UNP B9PPN9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	246	HIS	-	EXPRESSION TAG	UNP B9PPN9

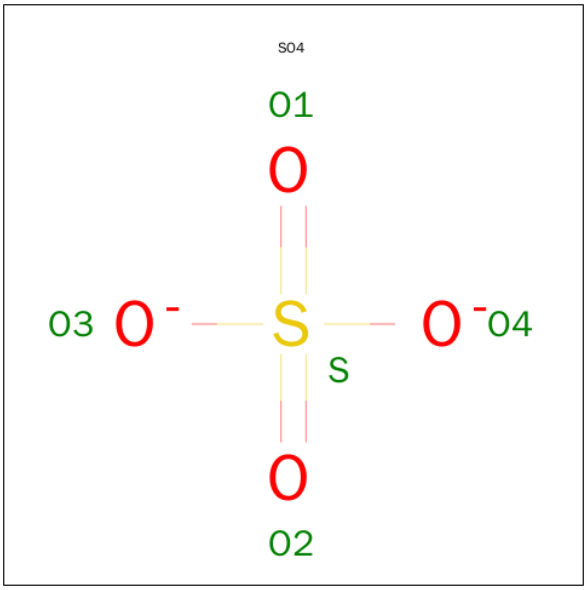
- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Cl 2 2	0	0
2	A	2	Total Cl 2 2	0	1
2	C	1	Total Cl 1 1	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

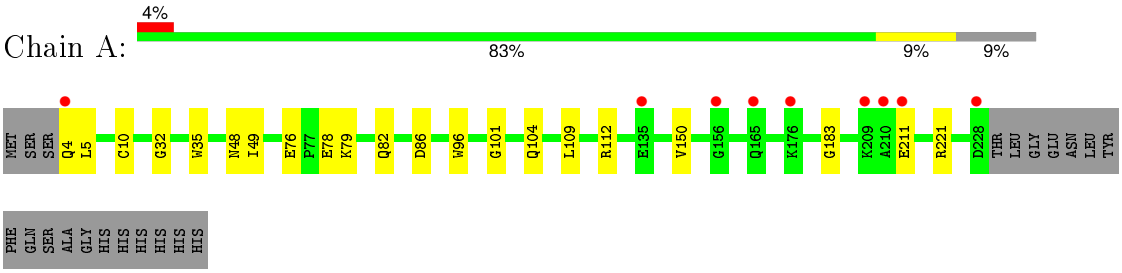
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	129	Total O 135 135	0	6
5	B	119	Total O 124 124	0	6
5	C	126	Total O 131 131	0	6
5	D	139	Total O 140 140	0	4

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.

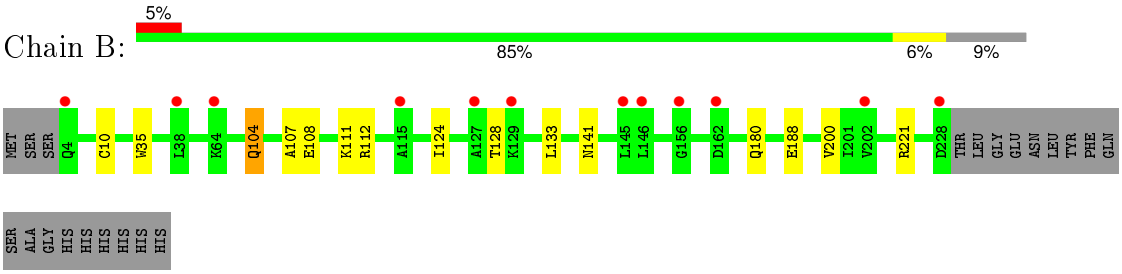
- Molecule 1: Ribulose-phosphate 3-epimerase

Chain A:



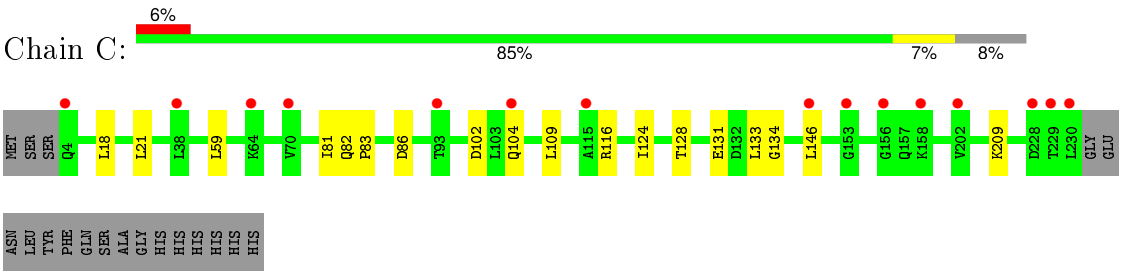
- Molecule 1: Ribulose-phosphate 3-epimerase

Chain B:



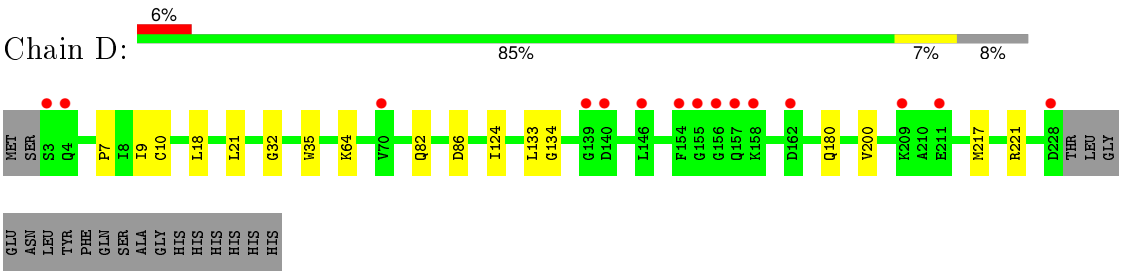
- Molecule 1: Ribulose-phosphate 3-epimerase

Chain C:



- Molecule 1: Ribulose-phosphate 3-epimerase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	138.51Å 138.51Å 349.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.88 – 2.05 29.88 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.88-2.05) 99.9 (29.88-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.63 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.8.0046	Depositor
R, R_{free}	0.149 , 0.187 0.161 , 0.192	Depositor DCC
R_{free} test set	4056 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	32.5	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 62.7	EDS
Estimated twinning fraction	0.000 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.015 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.002 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 80921 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7648	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.58% 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: ZN, 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	0.53	0/1833	0.72	0/2476
1	B	0.55	0/1759	0.72	0/2377
1	C	0.55	0/1806	0.72	0/2442
1	D	0.56	0/1788	0.72	0/2414
All	All	0.55	0/7186	0.72	0/9709

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	1798	0	1785	15	0
1	B	1725	0	1723	16	0
1	C	1772	0	1783	18	0
1	D	1754	0	1757	10	0
2	A	2	0	0	1	0
2	B	2	0	0	1	0
2	C	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	25	0	0	0	0
4	B	15	0	0	1	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
5	A	135	0	0	1	0
5	B	124	0	0	0	0
5	C	131	0	0	1	0
5	D	140	0	0	1	0
All	All	7648	0	7048	56	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 4.

All (56) 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:A:104[A]:GLN:HG2	5:A:500[A]:HOH:O	1.51	1.08
1:C:124[B]:ILE:HD11	1:C:128[B]:THR:O	1.73	0.89
1:B:104[A]:GLN:NE2	1:B:104[A]:GLN:H	1.87	0.72
1:B:221:ARG:HD2	4:B:306:SO4:O4	1.90	0.70
1:D:82:GLN:NE2	1:D:86:ASP:OD2	2.24	0.67
1:B:188:GLU:OE2	2:B:301:CL:CL	2.50	0.67
1:C:82[A]:GLN:HE22	1:C:116:ARG:NH2	1.92	0.67
1:B:104[A]:GLN:O	1:B:108:GLU:HG2	2.00	0.62
1:A:112:ARG:HD3	2:A:302[A]:CL:CL	2.39	0.60
1:C:124[B]:ILE:HG13	1:C:128[B]:THR:HB	1.85	0.59
1:A:4:GLN:HG2	1:A:5:LEU:N	2.18	0.59
1:C:18:LEU:HD23	1:C:21[B]:LEU:HD21	1.87	0.56
1:D:32:GLY:O	1:D:221[B]:ARG:NH1	2.39	0.56
1:B:107:ALA:O	1:B:111:LYS:HG2	2.06	0.55
1:B:124[A]:ILE:CG2	1:B:133:LEU:HD21	2.38	0.54
1:C:124[A]:ILE:HG23	1:C:133:LEU:HD21	1.90	0.53
1:D:64:LYS:HG2	5:D:475:HOH:O	2.08	0.53
1:B:104[B]:GLN:O	1:B:108:GLU:HG2	2.11	0.51
1:C:124[B]:ILE:CG1	1:C:128[B]:THR:HB	2.41	0.51
1:C:82[B]:GLN:NE2	1:C:86:ASP:OD2	2.44	0.50
1:A:32:GLY:O	1:A:221[A]:ARG:NH2	2.43	0.49
1:B:112:ARG:HG2	1:C:82[B]:GLN:CD	2.33	0.49
1:D:9:ILE:HG21	1:D:217:MET:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ASP:OD2	1:C:104[A]:GLN:HG3	2.13	0.48
1:A:82:GLN:NE2	1:A:86[A]:ASP:OD2	2.37	0.48
1:B:104[A]:GLN:HE21	1:B:104[A]:GLN:H	1.58	0.48
1:B:124[A]:ILE:HG21	1:B:133:LEU:HD21	1.95	0.48
1:D:124:ILE:CG2	1:D:133:LEU:HD11	2.44	0.48
1:A:10:CYS:SG	1:A:35:TRP:HB2	2.54	0.47
1:B:10:CYS:SG	1:B:35:TRP:HB2	2.55	0.46
1:A:76[A]:GLU:HG2	1:A:79:LYS:HE2	1.97	0.46
1:D:10:CYS:SG	1:D:35:TRP:HB2	2.56	0.46
1:B:111:LYS:HD3	1:B:141:ASN:OD1	2.16	0.46
1:D:133:LEU:O	1:D:134:GLY:C	2.54	0.46
1:A:4:GLN:HG2	1:A:5:LEU:H	1.79	0.45
1:D:124:ILE:HG23	1:D:133:LEU:HD11	1.98	0.45
1:C:82[A]:GLN:HE22	1:C:116:ARG:CZ	2.30	0.44
1:C:21[A]:LEU:HG	1:C:59:LEU:HD13	2.00	0.44
1:A:48[A]:ASN:CG	1:A:49:ILE:N	2.71	0.43
1:C:124[A]:ILE:CG2	1:C:133:LEU:HD21	2.48	0.43
1:C:81:ILE:HG13	1:C:109:LEU:HD11	2.01	0.43
1:C:82[B]:GLN:HB3	1:C:83:PRO:HD3	2.01	0.43
1:B:112:ARG:HG2	1:C:82[B]:GLN:NE2	2.34	0.43
1:C:146[A]:LEU:HD23	1:C:146[A]:LEU:C	2.39	0.43
1:A:150:VAL:HG22	1:A:183:GLY:HA3	1.99	0.43
1:A:76[B]:GLU:OE2	1:A:79:LYS:HE2	2.18	0.43
1:A:96:TRP:CE2	1:A:101:GLY:HA2	2.55	0.42
1:D:18:LEU:HD23	1:D:21:LEU:HD21	2.02	0.42
1:B:112:ARG:HD3	1:C:82[B]:GLN:OE1	2.20	0.41
1:C:131:GLU:HG3	5:C:424[A]:HOH:O	2.20	0.41
1:B:124[B]:ILE:HG13	1:B:128:THR:HB	2.02	0.41
1:B:180:GLN:HA	1:B:200:VAL:O	2.20	0.41
1:A:78:GLU:HG3	1:A:109:LEU:HD13	2.03	0.41
1:A:211:GLU:OE1	1:A:211:GLU:HA	2.22	0.40
1:D:180:GLN:HA	1:D:200:VAL:O	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	237/246 (96%)	231 (98%)	6 (2%)	0	100	100
1	B	228/246 (93%)	219 (96%)	9 (4%)	0	100	100
1	C	234/246 (95%)	227 (97%)	6 (3%)	1 (0%)	39	28
1	D	231/246 (94%)	221 (96%)	10 (4%)	0	100	100
All	All	930/984 (94%)	898 (97%)	31 (3%)	1 (0%)	56	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	134	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	189/193 (98%)	189 (100%)	0	100	100
1	B	180/193 (93%)	178 (99%)	2 (1%)	80	79
1	C	186/193 (96%)	185 (100%)	1 (0%)	92	92
1	D	183/193 (95%)	182 (100%)	1 (0%)	92	92
All	All	738/772 (96%)	734 (100%)	4 (0%)	93	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	104[A]	GLN
1	B	104[B]	GLN
1	C	209	LYS
1	D	7	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	4	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 21 ligands modelled in this entry, 9 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
4	SO4	A	304	-	4,4,4	0.20	0	6,6,6	0.49	0
4	SO4	A	305	-	4,4,4	0.44	0	6,6,6	0.17	0
4	SO4	A	306	-	4,4,4	0.21	0	6,6,6	0.27	0
4	SO4	A	307	-	4,4,4	0.33	0	6,6,6	0.10	0
4	SO4	A	308[B]	-	4,4,4	0.45	0	6,6,6	0.19	0
4	SO4	B	304	-	4,4,4	0.25	0	6,6,6	0.38	0
4	SO4	B	305	-	4,4,4	0.31	0	6,6,6	0.41	0
4	SO4	B	306	-	4,4,4	0.31	0	6,6,6	0.44	0
4	SO4	C	303	-	4,4,4	0.34	0	6,6,6	0.36	0
4	SO4	C	304[A]	-	4,4,4	0.21	0	6,6,6	0.31	0
4	SO4	D	302	-	4,4,4	0.32	0	6,6,6	0.21	0
4	SO4	D	303	-	4,4,4	0.28	0	6,6,6	0.19	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
4	SO4	A	304	-	-	0/0/0/0	0/0/0/0
4	SO4	A	305	-	-	0/0/0/0	0/0/0/0
4	SO4	A	306	-	-	0/0/0/0	0/0/0/0
4	SO4	A	307	-	-	0/0/0/0	0/0/0/0
4	SO4	A	308[B]	-	-	0/0/0/0	0/0/0/0
4	SO4	B	304	-	-	0/0/0/0	0/0/0/0
4	SO4	B	305	-	-	0/0/0/0	0/0/0/0
4	SO4	B	306	-	-	0/0/0/0	0/0/0/0
4	SO4	C	303	-	-	0/0/0/0	0/0/0/0
4	SO4	C	304[A]	-	-	0/0/0/0	0/0/0/0
4	SO4	D	302	-	-	0/0/0/0	0/0/0/0
4	SO4	D	303	-	-	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
4	B	306	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	225/246 (91%)	-0.03	9 (4%)	42	48	21, 37, 60, 83	0
1	B	225/246 (91%)	0.00	12 (5%)	30	34	24, 35, 63, 82	0
1	C	227/246 (92%)	0.10	15 (6%)	22	24	26, 37, 65, 99	0
1	D	226/246 (91%)	0.05	15 (6%)	22	24	21, 36, 68, 103	0
All	All	903/984 (91%)	0.03	51 (5%)	28	32	21, 36, 64, 103	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	SER	7.1
1	D	139	GLY	6.9
1	C	229	THR	5.9
1	D	156	GLY	5.6
1	C	4	GLN	4.8
1	B	156	GLY	4.2
1	B	4	GLN	4.0
1	B	228	ASP	3.9
1	C	146[A]	LEU	3.6
1	C	64	LYS	3.6
1	A	4	GLN	3.5
1	A	209	LYS	3.4
1	C	38	LEU	3.3
1	D	209	LYS	3.2
1	A	228	ASP	3.1
1	D	228	ASP	3.1
1	D	158	LYS	3.0
1	B	146	LEU	3.0
1	C	230	LEU	2.9
1	D	4	GLN	2.9
1	C	115	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	154	PHE	2.7
1	D	140	ASP	2.6
1	D	211	GLU	2.6
1	D	146	LEU	2.6
1	C	202	VAL	2.5
1	C	156	GLY	2.5
1	B	38	LEU	2.5
1	A	210	ALA	2.4
1	C	70	VAL	2.3
1	C	228	ASP	2.3
1	D	70	VAL	2.3
1	B	129	LYS	2.3
1	A	156	GLY	2.3
1	D	155	GLY	2.3
1	A	165	GLN	2.3
1	A	211	GLU	2.3
1	A	135	GLU	2.3
1	D	162	ASP	2.2
1	C	104[A]	GLN	2.2
1	B	115	ALA	2.2
1	C	93	THR	2.1
1	C	158	LYS	2.1
1	C	153	GLY	2.1
1	B	202	VAL	2.1
1	D	157	GLN	2.1
1	B	145	LEU	2.1
1	B	127	ALA	2.1
1	A	176	LYS	2.1
1	B	162[A]	ASP	2.1
1	B	64	LYS	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

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
4	SO4	B	305	5/5	0.97	0.15	0.69	40,43,49,52	5
4	SO4	A	308[B]	5/5	0.93	0.13	0.16	52,54,58,61	5
4	SO4	C	303	5/5	0.99	0.08	-0.77	43,46,53,56	0
4	SO4	B	304	5/5	0.99	0.09	-0.83	46,49,50,57	0
4	SO4	D	302	5/5	0.98	0.08	-0.87	57,58,65,73	0
4	SO4	A	304	5/5	0.98	0.08	-0.90	43,47,58,71	0
3	ZN	C	302	1/1	0.98	0.10	-1.70	36,36,36,36	1
3	ZN	A	303	1/1	0.99	0.07	-1.81	35,35,35,35	1
3	ZN	D	301	1/1	0.98	0.04	-2.34	37,37,37,37	1
3	ZN	B	303	1/1	0.97	0.06	-2.35	38,38,38,38	1
2	CL	B	301	1/1	0.87	0.07	-	78,78,78,78	0
2	CL	C	301	1/1	0.91	0.06	-	63,63,63,63	0
4	SO4	A	307	5/5	0.74	0.25	-	55,60,68,70	5
4	SO4	D	303	5/5	0.93	0.19	-	37,44,47,49	5
4	SO4	A	306	5/5	0.94	0.12	-	44,50,52,59	5
4	SO4	B	306	5/5	0.96	0.17	-	49,51,59,60	5
4	SO4	A	305	5/5	0.88	0.13	-	55,66,67,80	5
2	CL	B	302	1/1	0.89	0.16	-	66,66,66,66	0
2	CL	A	301	1/1	0.85	0.08	-	78,78,78,78	0
4	SO4	C	304[A]	5/5	0.91	0.20	-	48,53,60,62	5
2	CL	A	302[A]	1/1	0.91	0.09	-	46,46,46,46	1

6.5 Other polymers

There are no such residues in this entry.