Full wwPDB X-ray Structure Validation Report (i)

Oct 12, 2021 – 02:25 PM EDT

PDB ID	:	1ZVM
Title	:	Crystal structure of human CD38: cyclic-ADP-ribosyl synthetase/NAD+ glycohydrolase
Authors	:	Shi, W.; Yang, T.; Almo, S.C.; Schramm, V.L.; Sauve, A.
Deposited on	:	2005-06-02
Resolution	:	2.20 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 following versions of software and data (see references (i)) were used in the production of this report:

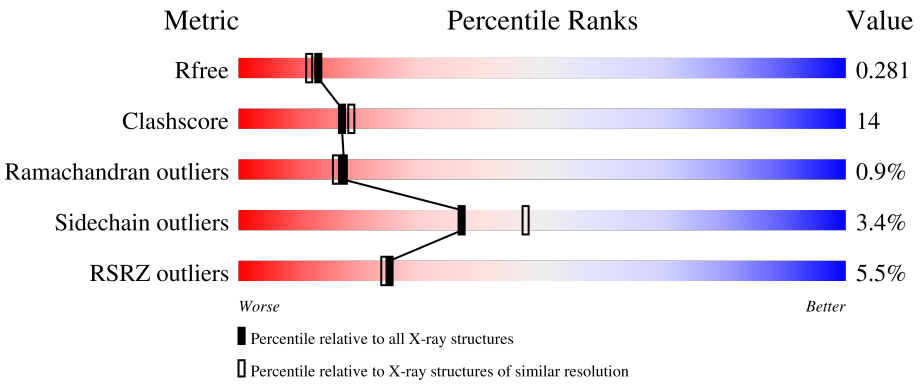
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	256	2%, 71%, 25%, • •
1	B	256	9%, 66%, 30%, • •
1	C	256	%, 74%, 22%, • •
1	D	256	9%, 69%, 28%, • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8369 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.

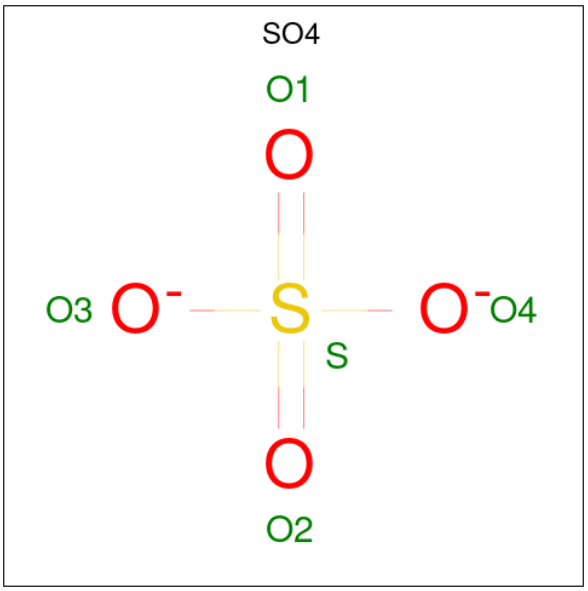
- Molecule 1 is a protein called ADP-ribosyl cyclase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	252	2025	1279	350	380	16	0	0	0
1	B	252	2025	1279	350	380	16	0	0	0
1	C	253	2031	1282	351	382	16	0	0	0
1	D	252	2025	1279	350	380	16	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ASP	ASN	engineered mutation	UNP P28907
A	164	ALA	ASN	engineered mutation	UNP P28907
A	209	ASP	ASN	engineered mutation	UNP P28907
A	219	ASP	ASN	engineered mutation	UNP P28907
B	100	ASP	ASN	engineered mutation	UNP P28907
B	164	ALA	ASN	engineered mutation	UNP P28907
B	209	ASP	ASN	engineered mutation	UNP P28907
B	219	ASP	ASN	engineered mutation	UNP P28907
C	100	ASP	ASN	engineered mutation	UNP P28907
C	164	ALA	ASN	engineered mutation	UNP P28907
C	209	ASP	ASN	engineered mutation	UNP P28907
C	219	ASP	ASN	engineered mutation	UNP P28907
D	100	ASP	ASN	engineered mutation	UNP P28907
D	164	ALA	ASN	engineered mutation	UNP P28907
D	209	ASP	ASN	engineered mutation	UNP P28907
D	219	ASP	ASN	engineered mutation	UNP P28907

- 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	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	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

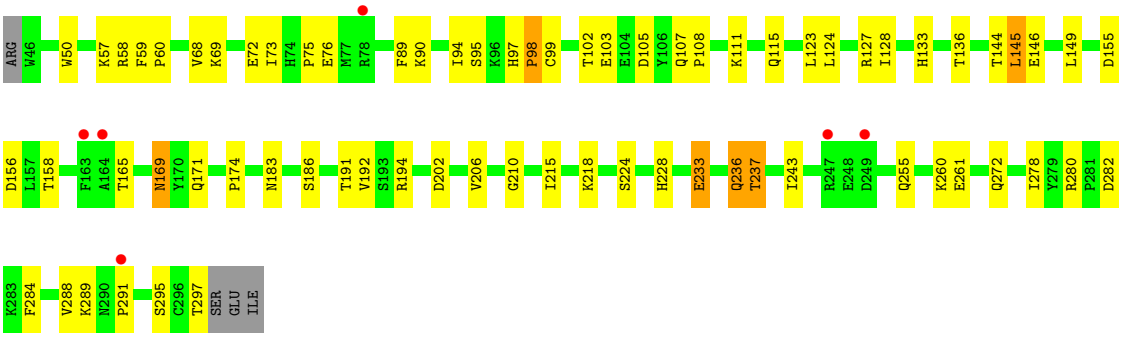
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	82	Total O 82 82	0	0
3	B	55	Total O 55 55	0	0
3	C	55	Total O 55 55	0	0
3	D	31	Total O 31 31	0	0

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.

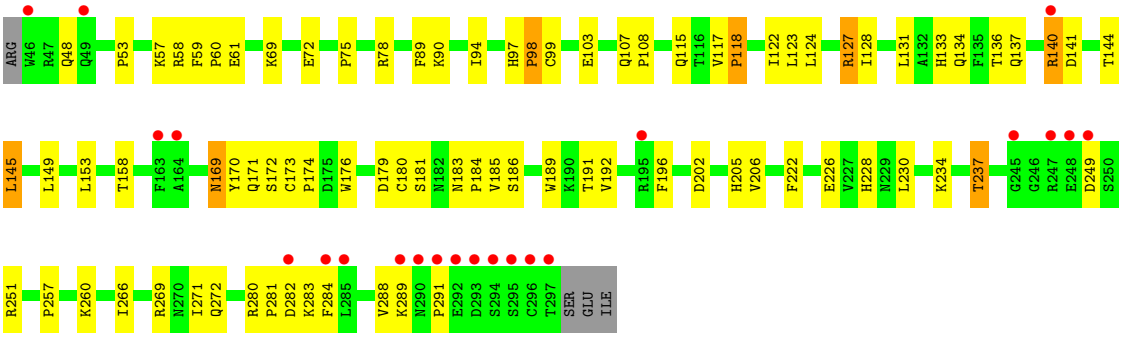
• Molecule 1: ADP-ribosyl cyclase 1

Chain A:



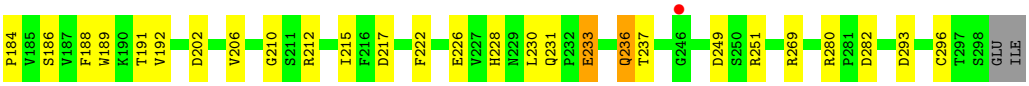
• Molecule 1: ADP-ribosyl cyclase 1

Chain B:



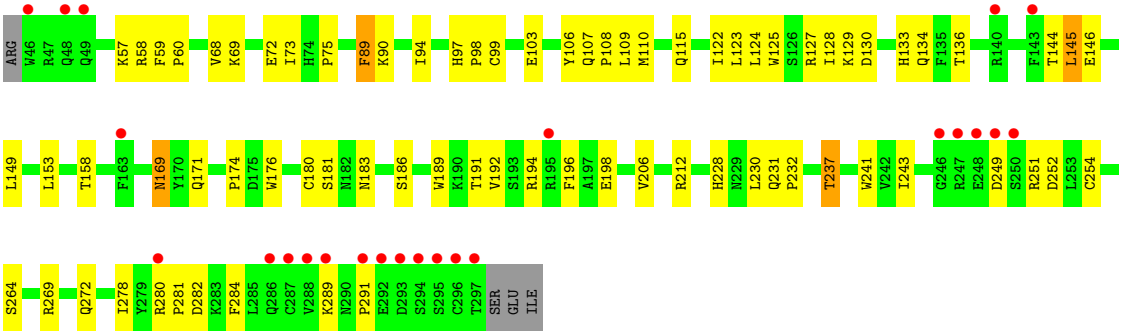
• Molecule 1: ADP-ribosyl cyclase 1

Chain C:



• Molecule 1: ADP-ribosyl cyclase 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	114.44Å 115.70Å 98.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.20 24.97 – 2.20	Depositor EDS
% Data completeness (in resolution range)	86.8 (25.00-2.20) 90.1 (24.97-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 2.19Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.228 , 0.270 0.240 , 0.281	Depositor DCC
R_{free} test set	6309 reflections (10.12%)	wwPDB-VP
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 26.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.216 for k,h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8369	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.39	0/2076	0.64	0/2816
1	B	0.37	0/2076	0.59	0/2816
1	C	0.37	0/2082	0.63	0/2824
1	D	0.36	0/2076	0.59	0/2816
All	All	0.37	0/8310	0.61	0/11272

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 (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	2025	0	1941	51	0
1	B	2025	0	1941	67	0
1	C	2031	0	1946	56	0
1	D	2025	0	1941	54	0
2	A	10	0	0	1	0
2	B	10	0	0	1	0
2	C	10	0	0	1	0
2	D	10	0	0	1	0
3	A	82	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	55	0	0	4	0
3	C	55	0	0	3	0
3	D	31	0	0	2	0
All	All	8369	0	7769	223	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 14.

All (223) 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:115:GLN:HE22	1:C:149:LEU:H	1.08	0.91
1:A:115:GLN:HE22	1:A:149:LEU:H	1.19	0.84
1:D:115:GLN:HE22	1:D:149:LEU:H	1.26	0.82
1:D:90:LYS:O	1:D:94:ILE:HG12	1.79	0.82
1:B:127:ARG:HD2	2:B:303:SO4:O3	1.81	0.80
1:A:295:SER:HA	1:C:233:GLU:HG3	1.64	0.79
1:C:90:LYS:HG2	1:C:94:ILE:HD13	1.65	0.78
1:B:136:THR:HG21	1:B:144:THR:HG23	1.67	0.75
1:C:169:ASN:HD21	1:C:171:GLN:HB3	1.52	0.75
1:B:183:ASN:ND2	1:B:186:SER:H	1.86	0.74
1:D:230:LEU:O	1:D:269:ARG:NH1	2.21	0.74
1:D:145:LEU:HD11	1:D:192:VAL:HG13	1.69	0.73
1:D:127:ARG:HD2	2:D:307:SO4:O3	1.88	0.73
1:C:145:LEU:HD21	1:C:192:VAL:HG22	1.70	0.73
1:C:280:ARG:HB3	1:C:280:ARG:NH1	2.05	0.71
1:B:183:ASN:HD21	1:B:186:SER:H	1.38	0.71
1:A:183:ASN:ND2	1:A:186:SER:H	1.89	0.70
1:B:189:TRP:HA	1:B:192:VAL:HG12	1.74	0.70
1:D:90:LYS:HG2	1:D:94:ILE:HD13	1.74	0.69
1:D:69:LYS:O	1:D:72:GLU:HG2	1.90	0.69
1:B:115:GLN:HE22	1:B:149:LEU:H	1.38	0.69
1:B:230:LEU:O	1:B:269:ARG:NH1	2.25	0.68
1:B:145:LEU:HD21	1:B:192:VAL:HG22	1.74	0.68
1:C:115:GLN:NE2	1:C:149:LEU:H	1.89	0.68
1:B:169:ASN:C	1:B:169:ASN:HD22	1.95	0.67
1:A:103:GLU:HG2	1:A:191:THR:OG1	1.95	0.67
1:B:90:LYS:O	1:B:94:ILE:HG12	1.95	0.66
1:D:228:HIS:HD2	3:D:590:HOH:O	1.78	0.66
1:B:107:GLN:HB3	1:B:108:PRO:HD3	1.77	0.66
1:A:237:THR:HB	1:A:272:GLN:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:LEU:HD11	1:B:192:VAL:HG13	1.78	0.65
1:D:237:THR:HB	1:D:272:GLN:HB2	1.79	0.64
1:C:107:GLN:HE22	1:C:111:LYS:NZ	1.95	0.64
1:D:136:THR:HG21	1:D:144:THR:HG23	1.80	0.64
1:A:97:HIS:CE1	1:A:99:CYS:HB2	2.33	0.64
1:A:127:ARG:HD2	2:A:301:SO4:O1	1.98	0.62
1:D:212:ARG:HB3	3:D:524:HOH:O	1.98	0.62
1:C:106:TYR:O	1:C:110:MET:HG2	1.99	0.62
1:B:115:GLN:NE2	1:B:149:LEU:H	1.98	0.62
1:D:107:GLN:HB3	1:D:108:PRO:HD3	1.82	0.62
1:A:107:GLN:HE22	1:A:111:LYS:NZ	1.97	0.61
1:A:295:SER:OG	1:C:233:GLU:HG2	2.01	0.61
1:D:280:ARG:NH1	1:D:280:ARG:HB3	2.16	0.60
1:A:107:GLN:HB3	1:A:108:PRO:HD3	1.83	0.60
1:A:69:LYS:O	1:A:72:GLU:HG2	2.02	0.60
1:C:202:ASP:HA	1:C:236:GLN:CD	2.21	0.60
1:A:90:LYS:HG2	1:A:94:ILE:HD13	1.82	0.60
1:B:228:HIS:HD2	3:B:511:HOH:O	1.84	0.60
1:C:280:ARG:HB3	1:C:280:ARG:HH11	1.66	0.60
1:C:169:ASN:C	1:C:169:ASN:HD22	2.04	0.59
1:D:103:GLU:HG2	1:D:191:THR:OG1	2.03	0.59
1:D:169:ASN:C	1:D:169:ASN:HD22	2.06	0.59
1:A:183:ASN:HD21	1:A:186:SER:H	1.50	0.59
1:D:130:ASP:O	1:D:134:GLN:HG3	2.02	0.59
1:D:189:TRP:HA	1:D:192:VAL:HG12	1.83	0.59
1:C:127:ARG:HD2	2:C:305:SO4:O1	2.03	0.58
1:B:133:HIS:O	1:B:137:GLN:HG2	2.04	0.58
1:B:90:LYS:HG2	1:B:94:ILE:HD13	1.85	0.58
1:C:169:ASN:ND2	1:C:171:GLN:H	2.01	0.57
1:B:284:PHE:O	1:B:288:VAL:HG23	2.05	0.56
1:C:280:ARG:HH12	1:C:282:ASP:CG	2.08	0.56
1:D:98:PRO:HB2	1:D:174:PRO:HG3	1.87	0.56
1:A:284:PHE:O	1:A:288:VAL:HG23	2.05	0.56
1:C:188:PHE:O	1:C:192:VAL:HG12	2.05	0.56
1:B:185:VAL:HB	3:B:593:HOH:O	2.05	0.56
1:B:123:LEU:HD13	1:B:123:LEU:C	2.27	0.56
1:C:133:HIS:HE1	1:C:146:GLU:OE1	1.88	0.56
1:A:169:ASN:C	1:A:169:ASN:HD22	2.08	0.55
1:B:289:LYS:O	1:B:291:PRO:HD3	2.05	0.55
1:D:98:PRO:O	1:D:183:ASN:HA	2.05	0.55
1:A:210:GLY:HA2	1:A:215:ILE:HG12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:PRO:HG2	1:B:61:GLU:OE1	2.07	0.55
1:A:107:GLN:HE22	1:A:111:LYS:CE	2.21	0.54
1:B:69:LYS:O	1:B:72:GLU:HG2	2.07	0.54
1:C:230:LEU:O	1:C:269:ARG:NH1	2.40	0.54
1:A:169:ASN:HD22	1:A:171:GLN:H	1.55	0.54
1:D:133:HIS:HE1	1:D:146:GLU:OE1	1.90	0.54
1:A:169:ASN:HD21	1:A:171:GLN:HB3	1.73	0.54
1:B:280:ARG:HB3	1:B:280:ARG:NH1	2.22	0.54
1:D:124:LEU:O	1:D:206:VAL:HA	2.08	0.54
1:A:280:ARG:NH1	1:A:280:ARG:HB3	2.22	0.54
1:D:59:PHE:HB3	1:D:60:PRO:HD3	1.90	0.53
1:D:176:TRP:HA	1:D:180:CYS:O	2.07	0.53
1:B:169:ASN:ND2	1:B:171:GLN:H	2.06	0.53
1:C:183:ASN:ND2	1:C:186:SER:H	2.07	0.53
1:D:73:ILE:O	1:D:75:PRO:HD3	2.08	0.53
1:D:281:PRO:O	1:D:284:PHE:HB3	2.09	0.53
1:C:169:ASN:HD22	1:C:171:GLN:H	1.54	0.53
1:C:202:ASP:HA	1:C:236:GLN:NE2	2.23	0.52
1:A:124:LEU:O	1:A:206:VAL:HA	2.10	0.52
1:A:169:ASN:ND2	1:A:171:GLN:H	2.07	0.52
1:C:90:LYS:O	1:C:94:ILE:HG12	2.10	0.52
1:D:169:ASN:ND2	1:D:171:GLN:H	2.07	0.52
1:C:57:LYS:O	1:C:58:ARG:HB2	2.09	0.52
1:C:69:LYS:O	1:C:72:GLU:HG2	2.09	0.52
1:D:149:LEU:O	1:D:153:LEU:HG	2.10	0.52
1:D:169:ASN:HD22	1:D:171:GLN:H	1.57	0.52
1:D:145:LEU:HD21	1:D:192:VAL:HG22	1.92	0.52
1:D:106:TYR:O	1:D:110:MET:HG2	2.09	0.51
1:B:97:HIS:CE1	1:B:99:CYS:HB2	2.44	0.51
1:A:57:LYS:O	1:A:58:ARG:HB2	2.09	0.51
1:A:115:GLN:NE2	1:A:149:LEU:H	1.99	0.51
1:C:107:GLN:HB3	1:C:108:PRO:HD3	1.93	0.51
1:C:222:PHE:HA	1:C:226:GLU:HB2	1.92	0.51
1:A:107:GLN:HE22	1:A:111:LYS:HE2	1.77	0.50
1:C:280:ARG:HH11	1:C:280:ARG:CB	2.23	0.50
1:D:169:ASN:HD21	1:D:171:GLN:HB3	1.75	0.50
1:B:174:PRO:HA	1:B:179:ASP:OD2	2.10	0.50
1:B:169:ASN:HD22	1:B:171:GLN:H	1.60	0.50
1:C:231:GLN:HA	1:C:231:GLN:NE2	2.27	0.50
1:C:228:HIS:HD2	3:C:526:HOH:O	1.93	0.50
1:B:149:LEU:O	1:B:153:LEU:HG	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:TRP:CH2	1:C:129:LYS:HB2	2.46	0.49
1:A:233:GLU:H	1:A:233:GLU:CD	2.15	0.49
1:C:231:GLN:HA	1:C:231:GLN:HE21	1.77	0.49
1:D:183:ASN:ND2	1:D:186:SER:H	2.10	0.49
1:B:75:PRO:HA	1:B:78:ARG:HG2	1.95	0.48
1:B:124:LEU:HD22	1:B:226:GLU:OE1	2.14	0.48
1:C:145:LEU:HD13	1:C:189:TRP:HZ3	1.78	0.48
1:A:73:ILE:O	1:A:75:PRO:HD3	2.13	0.48
1:C:124:LEU:O	1:C:206:VAL:HA	2.14	0.48
1:C:98:PRO:O	1:C:183:ASN:HA	2.13	0.48
1:A:133:HIS:HE1	1:A:146:GLU:OE1	1.96	0.48
1:B:98:PRO:HB2	1:B:174:PRO:HG3	1.95	0.48
1:B:237:THR:HG22	1:B:272:GLN:HB2	1.96	0.48
1:A:280:ARG:HH12	1:A:282:ASP:CG	2.17	0.47
1:B:280:ARG:HH12	1:B:282:ASP:CG	2.17	0.47
1:B:169:ASN:C	1:B:169:ASN:ND2	2.65	0.47
1:C:97:HIS:CE1	1:C:99:CYS:HB2	2.50	0.47
1:A:218:LYS:HD2	1:A:261:GLU:OE2	2.15	0.47
1:D:97:HIS:CE1	1:D:99:CYS:HB2	2.50	0.47
1:B:176:TRP:CD1	1:B:181:SER:HA	2.49	0.46
1:B:137:GLN:O	1:B:140:ARG:HG3	2.15	0.46
1:C:169:ASN:HD22	1:C:170:TYR:N	2.13	0.46
1:C:59:PHE:HB3	1:C:60:PRO:HD3	1.97	0.46
1:B:59:PHE:N	1:B:60:PRO:HD2	2.30	0.46
1:B:206:VAL:HG21	1:B:222:PHE:CZ	2.50	0.46
1:B:131:LEU:HA	1:B:134:GLN:NE2	2.31	0.46
1:D:57:LYS:O	1:D:58:ARG:HB2	2.16	0.45
1:A:95:SER:HA	1:A:165:THR:O	2.17	0.45
1:B:169:ASN:HD21	1:B:171:GLN:HB3	1.81	0.45
1:A:50:TRP:CZ2	1:A:98:PRO:HG2	2.52	0.45
1:A:102:THR:O	1:A:105:ASP:HB2	2.15	0.45
1:B:103:GLU:HG2	1:B:191:THR:OG1	2.16	0.45
1:A:295:SER:HA	1:C:233:GLU:CG	2.40	0.45
1:D:89:PHE:HA	1:D:109:LEU:HD22	1.98	0.45
1:A:289:LYS:O	1:A:291:PRO:HD3	2.16	0.45
1:A:90:LYS:CG	1:A:94:ILE:HD13	2.46	0.45
1:D:194:ARG:O	1:D:198:GLU:HB2	2.17	0.45
1:A:136:THR:HG21	1:A:144:THR:HG23	1.98	0.45
1:D:243:ILE:HD13	1:D:278:ILE:HD12	1.99	0.45
1:A:59:PHE:N	1:A:60:PRO:CD	2.80	0.45
1:A:68:VAL:HG21	1:D:68:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:PRO:O	1:B:284:PHE:HB3	2.16	0.44
1:D:280:ARG:HH12	1:D:282:ASP:CG	2.19	0.44
1:B:122:ILE:HD12	1:B:196:PHE:CZ	2.52	0.44
1:C:212:ARG:HD3	3:C:414:HOH:O	2.18	0.44
1:A:280:ARG:HB3	1:A:280:ARG:HH11	1.82	0.44
1:B:183:ASN:ND2	3:B:593:HOH:O	2.49	0.44
1:B:57:LYS:O	1:B:58:ARG:HB2	2.18	0.44
1:C:50:TRP:CZ2	1:C:98:PRO:HG2	2.52	0.44
1:C:110:MET:CE	1:C:191:THR:HG22	2.47	0.44
1:D:125:TRP:CH2	1:D:129:LYS:HB2	2.53	0.44
1:B:169:ASN:HD22	1:B:170:TYR:N	2.15	0.44
1:C:127:ARG:NH2	1:C:217:ASP:OD1	2.51	0.44
1:D:122:ILE:HD12	1:D:196:PHE:CZ	2.53	0.44
1:D:289:LYS:O	1:D:291:PRO:HD3	2.17	0.44
1:A:297:THR:HB	1:C:269:ARG:HA	2.00	0.44
1:B:124:LEU:O	1:B:206:VAL:HA	2.18	0.44
1:B:222:PHE:HA	1:B:226:GLU:HB2	1.99	0.44
1:C:98:PRO:HB2	1:C:174:PRO:HG3	1.99	0.44
1:D:232:PRO:HB3	1:D:269:ARG:O	2.18	0.44
1:B:48:GLN:HE21	1:B:48:GLN:HB2	1.60	0.43
1:A:202:ASP:HA	1:A:236:GLN:CD	2.38	0.43
1:B:98:PRO:O	1:B:183:ASN:HA	2.18	0.43
1:B:280:ARG:HH11	1:B:280:ARG:HA	1.84	0.43
1:A:98:PRO:O	1:A:183:ASN:HA	2.19	0.43
1:B:169:ASN:HD21	1:B:172:SER:H	1.66	0.43
1:D:252:ASP:OD2	1:D:254:CYS:HB2	2.19	0.43
1:A:155:ASP:O	1:A:156:ASP:HB2	2.18	0.43
1:C:231:GLN:HB3	1:C:233:GLU:OE2	2.18	0.43
1:A:145:LEU:HD11	1:A:192:VAL:HG13	2.01	0.42
1:A:228:HIS:HD2	3:A:474:HOH:O	2.02	0.42
1:D:115:GLN:NE2	1:D:149:LEU:H	2.06	0.42
1:D:249:ASP:C	1:D:251:ARG:H	2.22	0.42
1:B:117:VAL:HG13	1:B:118:PRO:HD2	2.00	0.42
1:D:280:ARG:HA	1:D:280:ARG:HH11	1.83	0.42
1:B:123:LEU:HD23	1:B:205:HIS:HB2	2.02	0.42
1:A:255:GLN:HA	1:A:260:LYS:HE2	2.01	0.42
1:B:53:PRO:O	1:B:173:CYS:HB2	2.20	0.42
1:B:176:TRP:HA	1:B:180:CYS:O	2.20	0.42
1:B:282:ASP:OD1	1:B:283:LYS:N	2.53	0.42
1:D:241:TRP:HB3	1:D:278:ILE:CD1	2.50	0.42
1:C:206:VAL:O	1:C:206:VAL:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:GLY:HA2	1:C:215:ILE:HG12	2.02	0.42
1:A:224:SER:C	3:A:565:HOH:O	2.57	0.42
1:B:75:PRO:HG3	1:B:78:ARG:NH2	2.35	0.42
1:B:206:VAL:HG13	1:B:206:VAL:O	2.20	0.42
1:C:189:TRP:HA	1:C:192:VAL:HG12	2.01	0.42
1:C:123:LEU:HD22	1:C:124:LEU:O	2.20	0.41
1:B:169:ASN:ND2	1:B:172:SER:H	2.18	0.41
1:C:184:PRO:HD2	3:C:435:HOH:O	2.20	0.41
1:B:169:ASN:ND2	1:B:171:GLN:N	2.68	0.41
1:B:184:PRO:HD2	3:B:452:HOH:O	2.19	0.41
1:C:107:GLN:NE2	1:C:111:LYS:NZ	2.65	0.41
1:D:243:ILE:CD1	1:D:278:ILE:HD12	2.49	0.41
1:D:169:ASN:C	1:D:169:ASN:ND2	2.73	0.41
1:A:98:PRO:HB2	1:A:174:PRO:HG3	2.01	0.41
1:A:243:ILE:CD1	1:A:278:ILE:HD12	2.50	0.41
1:B:141:ASP:OD1	1:B:141:ASP:N	2.53	0.41
1:B:257:PRO:O	1:B:260:LYS:HB2	2.20	0.41
1:C:136:THR:HG21	1:C:144:THR:HG23	2.02	0.41
1:B:202:ASP:N	1:B:234:LYS:O	2.48	0.41
1:C:293:ASP:HB3	1:C:296:CYS:SG	2.60	0.41
1:D:176:TRP:CD1	1:D:181:SER:HA	2.56	0.41
1:D:145:LEU:HD23	1:D:145:LEU:HA	1.90	0.40
1:A:236:GLN:HE21	1:A:236:GLN:HB2	1.73	0.40
1:B:266:ILE:HG23	1:B:271:ILE:HB	2.03	0.40
1:C:249:ASP:C	1:C:251:ARG:H	2.24	0.40
1:D:115:GLN:HE22	1:D:149:LEU:N	2.05	0.40
1:D:231:GLN:HA	1:D:232:PRO:HD2	1.91	0.40
1:B:249:ASP:C	1:B:251:ARG:H	2.25	0.40
1:C:59:PHE:N	1:C:60:PRO:CD	2.85	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	250/256 (98%)	240 (96%)	8 (3%)	2 (1%)	19	19
1	B	250/256 (98%)	235 (94%)	11 (4%)	4 (2%)	9	7
1	C	251/256 (98%)	238 (95%)	11 (4%)	2 (1%)	19	19
1	D	250/256 (98%)	235 (94%)	14 (6%)	1 (0%)	34	37
All	All	1001/1024 (98%)	948 (95%)	44 (4%)	9 (1%)	17	16

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	ILE
1	B	140	ARG
1	D	128	ILE
1	B	128	ILE
1	A	98	PRO
1	C	98	PRO
1	C	128	ILE
1	B	98	PRO
1	B	118	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	227/236 (96%)	217 (96%)	10 (4%)	28	35
1	B	227/236 (96%)	221 (97%)	6 (3%)	46	58
1	C	228/236 (97%)	220 (96%)	8 (4%)	36	46
1	D	227/236 (96%)	220 (97%)	7 (3%)	40	51
All	All	909/944 (96%)	878 (97%)	31 (3%)	37	47

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	GLU
1	A	89	PHE

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Mol	Chain	Res	Type
1	A	123	LEU
1	A	145	LEU
1	A	158	THR
1	A	169	ASN
1	A	194	ARG
1	A	233	GLU
1	A	236	GLN
1	A	237	THR
1	B	89	PHE
1	B	127	ARG
1	B	145	LEU
1	B	158	THR
1	B	169	ASN
1	B	237	THR
1	C	89	PHE
1	C	123	LEU
1	C	127	ARG
1	C	145	LEU
1	C	169	ASN
1	C	233	GLU
1	C	236	GLN
1	C	237	THR
1	D	89	PHE
1	D	123	LEU
1	D	145	LEU
1	D	158	THR
1	D	169	ASN
1	D	237	THR
1	D	264	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	83	GLN
1	A	97	HIS
1	A	107	GLN
1	A	115	GLN
1	A	133	HIS
1	A	169	ASN
1	A	183	ASN
1	A	228	HIS

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Mol	Chain	Res	Type
1	A	231	GLN
1	A	236	GLN
1	B	48	GLN
1	B	83	GLN
1	B	115	GLN
1	B	134	GLN
1	B	169	ASN
1	B	183	ASN
1	B	228	HIS
1	B	231	GLN
1	B	236	GLN
1	C	48	GLN
1	C	107	GLN
1	C	115	GLN
1	C	133	HIS
1	C	169	ASN
1	C	183	ASN
1	C	228	HIS
1	C	231	GLN
1	C	236	GLN
1	D	48	GLN
1	D	83	GLN
1	D	115	GLN
1	D	133	HIS
1	D	134	GLN
1	D	169	ASN
1	D	183	ASN
1	D	228	HIS
1	D	231	GLN
1	D	236	GLN

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)

8 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	A	301	-	4,4,4	0.14	0	6,6,6	0.17	0
2	SO4	D	307	-	4,4,4	0.28	0	6,6,6	0.18	0
2	SO4	C	305	-	4,4,4	0.17	0	6,6,6	0.14	0
2	SO4	D	308	-	4,4,4	0.30	0	6,6,6	0.15	0
2	SO4	B	304	-	4,4,4	0.28	0	6,6,6	0.11	0
2	SO4	C	306	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	B	303	-	4,4,4	0.26	0	6,6,6	0.10	0
2	SO4	A	302	-	4,4,4	0.26	0	6,6,6	0.13	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.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	SO4	1	0
2	D	307	SO4	1	0
2	C	305	SO4	1	0
2	B	303	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	252/256 (98%)	-0.18	6 (2%) 59 56	14, 25, 56, 68	0
1	B	252/256 (98%)	0.22	22 (8%) 10 8	17, 33, 62, 73	0
1	C	253/256 (98%)	-0.12	3 (1%) 79 77	15, 26, 55, 68	0
1	D	252/256 (98%)	0.24	24 (9%) 8 7	23, 36, 64, 73	0
All	All	1009/1024 (98%)	0.04	55 (5%) 25 24	14, 31, 59, 73	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	295	SER	9.4
1	D	297	THR	9.2
1	B	294	SER	8.8
1	B	248	GLU	7.8
1	B	297	THR	7.7
1	D	295	SER	7.1
1	D	292	GLU	6.6
1	B	292	GLU	5.5
1	D	294	SER	5.4
1	D	248	GLU	5.3
1	D	288	VAL	5.0
1	D	293	ASP	5.0
1	B	291	PRO	4.8
1	B	296	CYS	4.6
1	D	296	CYS	4.5
1	B	293	ASP	4.5
1	D	250	SER	4.4
1	D	289	LYS	4.2
1	D	291	PRO	3.8
1	B	249	ASP	3.7
1	D	140	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	163	PHE	3.6
1	D	163	PHE	3.5
1	B	290	ASN	3.4
1	B	247	ARG	3.3
1	D	247	ARG	3.2
1	D	49	GLN	3.2
1	C	164	ALA	3.1
1	D	249	ASP	3.1
1	B	285	LEU	3.0
1	D	48	GLN	3.0
1	B	282	ASP	2.9
1	B	49	GLN	2.8
1	D	195	ARG	2.7
1	C	246	GLY	2.6
1	D	287	CYS	2.6
1	D	286	GLN	2.6
1	A	163	PHE	2.6
1	D	143	PHE	2.5
1	B	163	PHE	2.5
1	A	164	ALA	2.5
1	D	246	GLY	2.4
1	A	291	PRO	2.4
1	B	245	GLY	2.4
1	A	78	ARG	2.4
1	B	140	ARG	2.3
1	A	247	ARG	2.2
1	B	195	ARG	2.2
1	B	289	LYS	2.1
1	B	164	ALA	2.1
1	B	46	TRP	2.1
1	B	284	PHE	2.1
1	A	249	ASP	2.1
1	D	280	ARG	2.0
1	D	46	TRP	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	D	308	5/5	0.95	0.12	42,43,46,46	0
2	SO4	C	306	5/5	0.97	0.11	39,40,40,40	0
2	SO4	D	307	5/5	0.97	0.12	39,41,43,44	0
2	SO4	B	304	5/5	0.97	0.12	44,45,45,47	0
2	SO4	A	301	5/5	0.98	0.18	25,29,29,30	0
2	SO4	B	303	5/5	0.98	0.11	37,38,39,39	0
2	SO4	C	305	5/5	0.99	0.17	28,32,33,33	0
2	SO4	A	302	5/5	0.99	0.14	35,35,35,37	0

6.5 Other polymers (i)

There are no such residues in this entry.