Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 04:41 AM EDT

PDB ID	:	6A8J
Title	:	Crystal structure of bacterial protein toxins
Authors	:	Kim, M.H.; Hwang, J.; Jang, S.Y.
Deposited on	:	2018-07-09
Resolution	:	2.71 Å(reported)

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

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

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

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

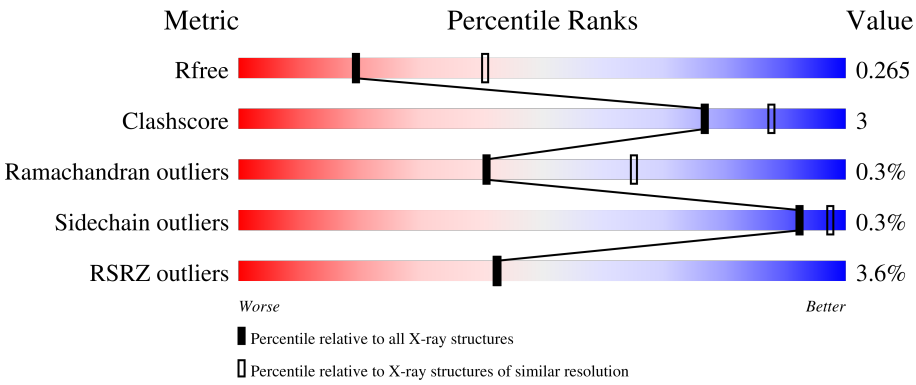
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.71 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	478	4% 92% 7% •
1	B	478	3% 91% 8% •
1	C	478	3% 91% 8% •
1	D	478	4% 90% 8% • •

2 Entry composition (i)

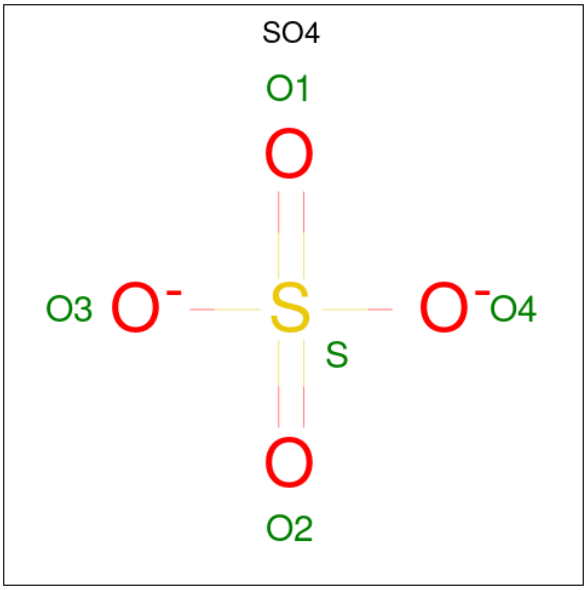
There are 4 unique types of molecules in this entry. The entry contains 14890 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RTX toxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	473	3657	2290	633	721	13	0	0	0
1	B	472	3655	2288	635	719	13	0	0	0
1	C	470	3636	2278	630	715	13	0	0	0
1	D	470	3636	2278	630	715	13	0	0	0

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



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

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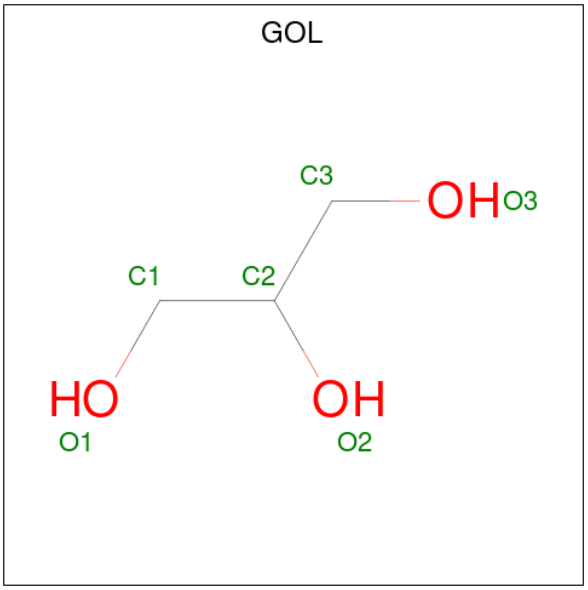
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

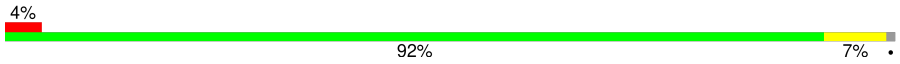
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	55	55	55	0	0
			Total	O		
4	B	61	61	61	0	0
			Total	O		
4	C	70	70	70	0	0
			Total	O		
4	D	59	59	59	0	0

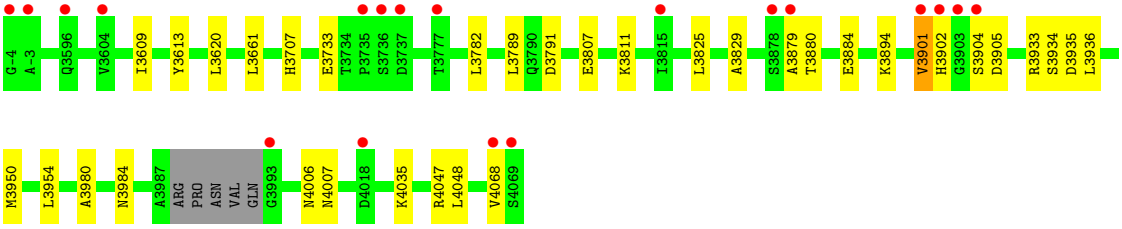
3 Residue-property plots (i)

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: RTX toxin

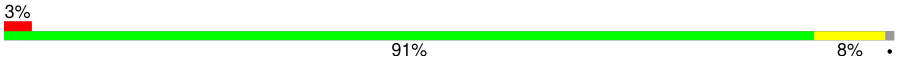
Chain A:

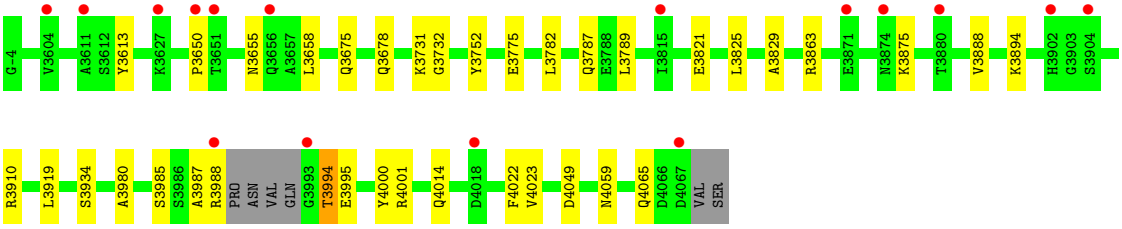




• Molecule 1: RTX toxin

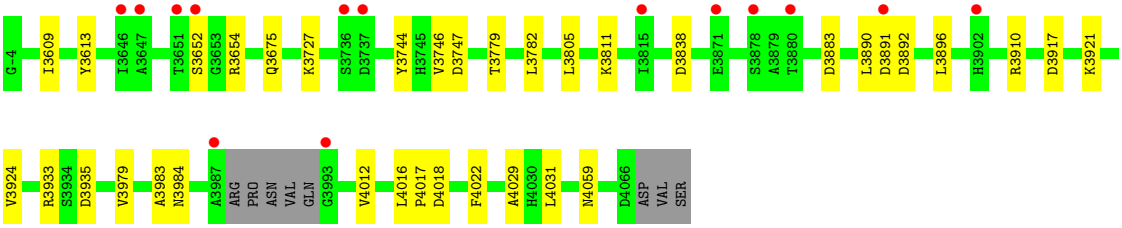
Chain B:





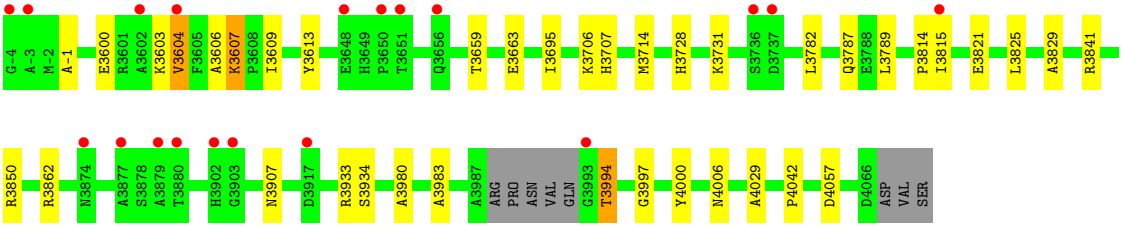
• Molecule 1: RTX toxin

Chain C:



• Molecule 1: RTX toxin

Chain D:


G-4
A-3
M-2
A-1
E3600
R3601
A3602
K3603
V3604
F3605
A3606
K3607
P3608
I3609
Y3613
E3648
H3649
P3650
T3651
Q3656
T3659
E3663
I3695
K3706
H3707
M3714
H3728
K3731
S3736
D3737
L3782
Q3787
E3788
L3789
P3814
I3815
E3821
L3825
A3829
R3841
R3850
R3862
N3874
A3877
S3878
A3879
T3880
H3902
G3903
N3907
D3917
R3933
S3934
A3980
A3983
A3987
ARG
PRO
ASN
VAL
GLN
G3993
T3994
G3997
Y4000
N4006
A4029
P4042
D4057
D4066
ASP
VAL
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	177.69Å 197.93Å 163.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.71 – 2.71 31.71 – 2.71	Depositor EDS
% Data completeness (in resolution range)	94.4 (31.71-2.71) 94.4 (31.71-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.77 (at 2.72Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.226 , 0.265 0.229 , 0.265	Depositor DCC
R_{free} test set	3708 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	36.2	Xtriage
Anisotropy	0.673	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 34.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	14890	wwPDB-VP
Average B, all atoms (Å^2)	42.0	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 22.27 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.8961e-03. 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL

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	0.20	0/3717	0.35	0/5017
1	B	0.20	0/3715	0.35	0/5013
1	C	0.20	0/3696	0.35	0/4988
1	D	0.21	0/3696	0.36	0/4988
All	All	0.20	0/14824	0.35	0/20006

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	3657	0	3602	21	0
1	B	3655	0	3601	22	0
1	C	3636	0	3584	21	0
1	D	3636	0	3584	25	0
2	A	10	0	0	0	0
2	B	20	0	0	0	0
2	C	15	0	0	0	0
2	D	10	0	0	0	0
3	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	55	0	0	1	0
4	B	61	0	0	1	0
4	C	70	0	0	0	0
4	D	59	0	0	2	0
All	All	14890	0	14379	86	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 3.

All (86) 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:3604:VAL:HA	1:D:3607:LYS:HE3	1.61	0.81
1:C:3652:SER:HB3	1:C:3654:ARG:H	1.52	0.74
1:D:3782:LEU:HD21	1:D:3789:LEU:HD11	1.73	0.70
1:A:4035:LYS:HZ3	1:C:3675:GLN:HB2	1.58	0.68
1:B:3782:LEU:HD21	1:B:3789:LEU:HD11	1.74	0.68
1:A:3782:LEU:HD21	1:A:3789:LEU:HD11	1.77	0.67
1:A:4035:LYS:HZ2	1:A:4068:VAL:HG13	1.62	0.65
1:B:3910:ARG:NH2	1:B:4059:ASN:OD1	2.32	0.62
1:D:3728:HIS:CE1	1:D:3731:LYS:HD2	2.34	0.62
1:D:3609:ILE:HG23	1:D:3613:TYR:HD2	1.66	0.60
1:C:3935:ASP:OD2	1:C:3984:ASN:ND2	2.27	0.59
1:A:3733:GLU:OE1	1:A:3733:GLU:N	2.30	0.59
1:C:3883:ASP:N	1:C:3883:ASP:OD1	2.38	0.57
1:A:3620:LEU:HD21	1:A:3661:LEU:HD21	1.87	0.56
1:D:3850:ARG:NH1	4:D:4207:HOH:O	2.37	0.56
1:C:3727:LYS:NZ	1:C:3838:ASP:OD1	2.34	0.55
1:A:3879:ALA:HB1	1:A:3884:GLU:HG3	1.89	0.54
1:B:3994:THR:HG22	1:B:3995:GLU:H	1.74	0.53
1:B:3919:LEU:HD13	1:B:4023:VAL:HG11	1.91	0.53
1:D:3825:LEU:HA	1:D:3829:ALA:HB2	1.91	0.53
1:B:3825:LEU:HA	1:B:3829:ALA:HB2	1.91	0.52
1:C:4016:LEU:O	1:C:4018:ASP:HA	2.10	0.51
1:D:3814:PRO:HD2	1:D:3815:ILE:HD12	1.92	0.51
1:B:3863:ARG:NH1	1:B:4049:ASP:OD2	2.43	0.51
1:D:3933:ARG:NH1	1:D:3983:ALA:O	2.43	0.51
1:A:4007:ASN:OD1	4:A:4201:HOH:O	2.19	0.51
1:A:3609:ILE:HG23	1:A:3613:TYR:HD2	1.76	0.51
1:D:3604:VAL:CA	1:D:3607:LYS:HE3	2.37	0.50
1:C:3979:VAL:HG11	1:C:4012:VAL:HG11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3988:ARG:NH2	1:C:3811:LYS:HG3	2.27	0.49
1:D:3862:ARG:NH1	4:D:4205:HOH:O	2.32	0.49
1:B:3787:GLN:NE2	1:B:3821:GLU:OE2	2.45	0.49
1:A:4035:LYS:NZ	1:C:3675:GLN:HB2	2.25	0.49
1:B:3650:PRO:O	1:B:3655:ASN:ND2	2.45	0.49
1:A:3825:LEU:HA	1:A:3829:ALA:HB2	1.93	0.49
1:D:3934:SER:HA	1:D:3980:ALA:HB3	1.95	0.48
1:C:3746:VAL:HG21	1:C:3805:LEU:HD11	1.95	0.48
1:A:3935:ASP:OD2	1:A:3984:ASN:ND2	2.41	0.48
1:B:3875:LYS:HB3	1:B:3888:VAL:HG21	1.96	0.47
1:B:3894:LYS:HD3	1:B:4014:GLN:HA	1.95	0.47
1:A:3880:THR:N	1:A:3884:GLU:OE2	2.44	0.47
1:D:3728:HIS:HE1	1:D:3731:LYS:HD2	1.77	0.47
1:D:3841:ARG:HA	1:D:4000:TYR:HE2	1.80	0.47
1:D:3600:GLU:HA	1:D:3603:LYS:HB2	1.97	0.47
1:A:3934:SER:HA	1:A:3980:ALA:HB3	1.96	0.47
1:A:3807:GLU:O	1:A:3811:LYS:HG2	2.15	0.46
1:D:3607:LYS:HZ2	1:D:3607:LYS:H	1.64	0.46
1:A:3901:VAL:HG12	1:A:3902:HIS:H	1.81	0.46
1:B:3934:SER:HA	1:B:3980:ALA:HB3	1.98	0.46
1:B:3731:LYS:HD2	1:B:3732:GLY:H	1.82	0.45
1:C:3924:VAL:HG13	1:C:4022:PHE:HA	1.97	0.45
1:C:3609:ILE:HG23	1:C:3613:TYR:HD2	1.82	0.45
1:D:3603:LYS:O	1:D:3606:ALA:N	2.49	0.45
1:B:3894:LYS:HG2	1:B:4022:PHE:HE2	1.81	0.45
1:A:3950:MET:HG3	1:A:3954:LEU:HD23	1.99	0.45
1:B:3731:LYS:HD2	1:B:3731:LYS:HA	1.69	0.45
1:D:3695:ILE:HA	1:D:3714:MET:HE2	1.99	0.44
1:B:3894:LYS:HE3	1:B:3894:LYS:HB2	1.79	0.44
1:C:3910:ARG:NH2	1:C:4059:ASN:OD1	2.45	0.44
1:C:3744:TYR:HB2	1:C:3782:LEU:HB2	1.99	0.44
1:D:4006:ASN:ND2	1:D:4042:PRO:O	2.34	0.44
1:A:3894:LYS:HD3	1:A:4048:LEU:O	2.17	0.44
1:D:3600:GLU:O	1:D:3604:VAL:HG23	2.17	0.44
1:A:3791:ASP:OD2	1:A:3933:ARG:NH1	2.48	0.43
1:C:3933:ARG:HH11	1:C:3984:ASN:HA	1.83	0.43
1:D:3787:GLN:NE2	1:D:3821:GLU:OE2	2.51	0.43
1:B:3675:GLN:HA	1:B:3678:GLN:HB2	2.01	0.43
1:B:3985:SER:HB3	1:B:4000:TYR:HE2	1.83	0.42
1:D:3706:LYS:O	1:D:3707:HIS:ND1	2.52	0.42
1:C:3890:LEU:HD21	1:C:3896:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3907:ASN:ND2	1:D:4057:ASP:OD1	2.52	0.42
1:C:3891:ASP:HA	1:C:3892:ASP:HA	1.53	0.42
1:A:3707:HIS:O	1:A:3707:HIS:ND1	2.53	0.42
1:A:4006:ASN:HB3	1:A:4047:ARG:HD3	2.01	0.42
1:A:3936:LEU:HD23	1:A:3936:LEU:HA	1.90	0.41
1:D:3659:THR:O	1:D:3663:GLU:HG3	2.20	0.41
1:B:3613:TYR:HE1	1:B:3658:LEU:HD21	1.84	0.41
1:C:3933:ARG:NH1	1:C:3983:ALA:O	2.53	0.41
1:B:3987:ALA:HB3	1:B:4001:ARG:HD2	2.03	0.41
1:C:3917:ASP:O	1:C:3921:LYS:HG3	2.21	0.41
1:C:3747:ASP:HA	1:C:3779:THR:HG22	2.02	0.41
1:D:3607:LYS:HZ3	1:D:3607:LYS:HG2	1.76	0.41
1:D:3994:THR:HG22	1:D:3997:GLY:H	1.85	0.41
1:B:4065:GLN:NE2	4:B:4213:HOH:O	2.54	0.41
1:C:4029:ALA:C	1:C:4031:LEU:H	2.24	0.41
1:B:3752:TYR:OH	1:B:3775:GLU:HG2	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	469/478 (98%)	453 (97%)	15 (3%)	1 (0%)	47 72
1	B	468/478 (98%)	451 (96%)	17 (4%)	0	100 100
1	C	466/478 (98%)	445 (96%)	20 (4%)	1 (0%)	47 72
1	D	466/478 (98%)	445 (96%)	17 (4%)	4 (1%)	17 38
All	All	1869/1912 (98%)	1794 (96%)	69 (4%)	6 (0%)	41 65

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3904	SER
1	D	4029	ALA
1	D	3994	THR
1	D	-1	ALA
1	C	4017	PRO
1	D	3604	VAL

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	385/390 (99%)	383 (100%)	2 (0%)	88 95
1	B	384/390 (98%)	383 (100%)	1 (0%)	92 97
1	C	382/390 (98%)	382 (100%)	0	100 100
1	D	382/390 (98%)	381 (100%)	1 (0%)	92 97
All	All	1533/1560 (98%)	1529 (100%)	4 (0%)	92 97

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

Mol	Chain	Res	Type
1	A	3901	VAL
1	A	3905	ASP
1	B	3994	THR
1	D	3607	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3664	GLN
1	B	4046	HIS
1	D	3728	HIS
1	D	4046	HIS

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)

12 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	4103	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	B	4102	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	A	4102	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	C	4101	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	B	4104	-	4,4,4	0.24	0	6,6,6	0.09	0
3	GOL	B	4105	-	5,5,5	0.37	0	5,5,5	0.33	0
2	SO4	A	4101	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	B	4101	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	C	4102	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	B	4103	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	D	4101	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	D	4102	-	4,4,4	0.23	0	6,6,6	0.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	4105	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	4105	GOL	O1-C1-C2-C3
3	B	4105	GOL	O1-C1-C2-O2

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 (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	473/478 (98%)	0.05	19 (4%)	38	37	13, 40, 78, 105	0
1	B	472/478 (98%)	0.10	16 (3%)	45	45	21, 40, 82, 99	0
1	C	470/478 (98%)	-0.08	14 (2%)	50	51	20, 36, 68, 85	0
1	D	470/478 (98%)	0.09	19 (4%)	38	37	16, 38, 79, 104	0
All	All	1885/1912 (98%)	0.04	68 (3%)	42	42	13, 38, 77, 105	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3993	GLY	9.4
1	A	-4	GLY	5.9
1	D	3815	ILE	5.6
1	B	3902	HIS	5.2
1	C	3993	GLY	5.1
1	B	3815	ILE	5.1
1	D	3993	GLY	4.9
1	B	3988	ARG	4.5
1	C	3815	ILE	4.3
1	D	3879	ALA	4.0
1	D	3917	ASP	4.0
1	D	3602	ALA	3.9
1	A	3993	GLY	3.6
1	A	3815	ILE	3.5
1	B	3604	VAL	3.4
1	A	3903	GLY	3.4
1	A	3902	HIS	3.3
1	B	4067	ASP	3.3
1	A	3878	SER	3.3
1	C	3902	HIS	3.2
1	C	3880	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	-3	ALA	3.2
1	A	3737	ASP	3.2
1	A	3736	SER	2.9
1	C	3878	SER	2.9
1	D	3880	THR	2.9
1	B	3874	ASN	2.8
1	D	3650	PRO	2.8
1	B	3650	PRO	2.8
1	D	3902	HIS	2.8
1	D	3604	VAL	2.7
1	D	3648	GLU	2.7
1	D	3656	GLN	2.7
1	D	3877	ALA	2.7
1	B	3611	ALA	2.7
1	A	4069	SER	2.7
1	D	3651	THR	2.6
1	B	3651	THR	2.5
1	C	3871	GLU	2.5
1	C	3646	ILE	2.5
1	C	3737	ASP	2.5
1	A	4018	ASP	2.5
1	C	3891	ASP	2.5
1	B	4018	ASP	2.5
1	D	3736	SER	2.5
1	C	3651	THR	2.4
1	D	-3	ALA	2.4
1	A	3596	GLN	2.4
1	B	3627	LYS	2.4
1	D	3874	ASN	2.4
1	A	3604	VAL	2.4
1	D	3903	GLY	2.4
1	B	3880	THR	2.3
1	C	3987	ALA	2.3
1	A	3735	PRO	2.3
1	B	3904	SER	2.3
1	A	3777	THR	2.3
1	A	4068	VAL	2.2
1	B	3871	GLU	2.2
1	C	3736	SER	2.2
1	A	3904	SER	2.2
1	B	3656	GLN	2.1
1	D	3737	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	-4	GLY	2.1
1	A	3901	VAL	2.1
1	C	3652	SER	2.1
1	C	3647	ALA	2.1
1	A	3879	ALA	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	B	4102	5/5	0.81	0.23	106,112,115,115	0
2	SO4	D	4102	5/5	0.87	0.37	95,99,102,103	0
2	SO4	B	4104	5/5	0.90	0.23	55,60,73,76	0
2	SO4	A	4102	5/5	0.90	0.17	99,101,102,106	0
2	SO4	D	4101	5/5	0.92	0.18	50,55,69,81	0
2	SO4	B	4101	5/5	0.92	0.21	74,78,87,92	0
2	SO4	B	4103	5/5	0.93	0.21	80,81,86,111	0
2	SO4	A	4101	5/5	0.94	0.13	61,66,67,69	0
3	GOL	B	4105	6/6	0.94	0.14	5,17,23,27	0
2	SO4	C	4103	5/5	0.95	0.12	62,64,71,72	0
2	SO4	C	4101	5/5	0.95	0.17	54,57,64,69	0
2	SO4	C	4102	5/5	0.96	0.12	31,47,49,53	0

6.5 Other polymers (i)

There are no such residues in this entry.