Full wwPDB X-ray Structure Validation Report (i)

Nov 23, 2023 – 04:04 PM EST

PDB ID	:	8HM3
Title	:	Complex of PPIase-BfUbb
Authors	:	Xu, J.H.; Chen, Z.; Gao, X.
Deposited on	:	2022-12-02
Resolution	:	2.26 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 (1)) were used in the production of this report:

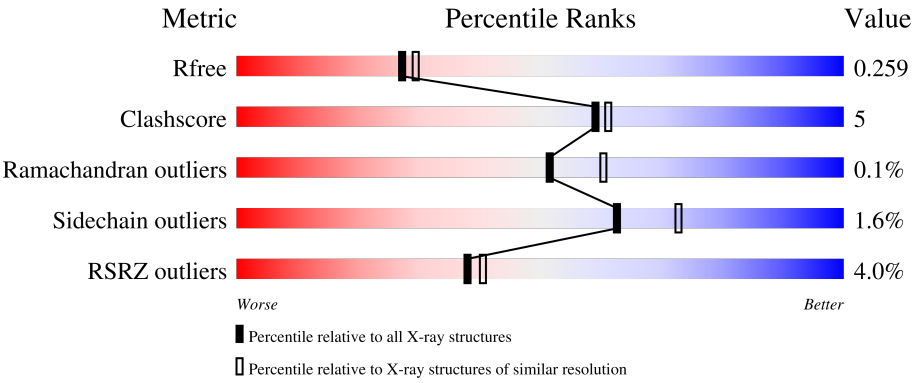
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.26 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	76	76% 24%
1	C	76	32% 71% 22%
2	B	427	% 92% 7%
2	D	427	3% 90% 9%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8797 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 ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	76	Total	C	N	O	S	0	0	0
			614	387	104	119	4			
1	C	74	Total	C	N	O	S	0	0	0
			597	377	101	116	3			

- Molecule 2 is a protein called Peptidylprolyl isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3467	2180	609	664	14			
2	D	427	Total	C	N	O	S	0	0	0
			3467	2180	609	664	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	31	MET	-	initiating methionine	UNP R6ZJY1
B	450	TRP	-	expression tag	UNP R6ZJY1
B	451	SER	-	expression tag	UNP R6ZJY1
B	452	HIS	-	expression tag	UNP R6ZJY1
B	453	PRO	-	expression tag	UNP R6ZJY1
B	454	GLN	-	expression tag	UNP R6ZJY1
B	455	PHE	-	expression tag	UNP R6ZJY1
B	456	GLU	-	expression tag	UNP R6ZJY1
B	457	LYS	-	expression tag	UNP R6ZJY1
D	31	MET	-	initiating methionine	UNP R6ZJY1
D	450	TRP	-	expression tag	UNP R6ZJY1
D	451	SER	-	expression tag	UNP R6ZJY1
D	452	HIS	-	expression tag	UNP R6ZJY1
D	453	PRO	-	expression tag	UNP R6ZJY1
D	454	GLN	-	expression tag	UNP R6ZJY1
D	455	PHE	-	expression tag	UNP R6ZJY1

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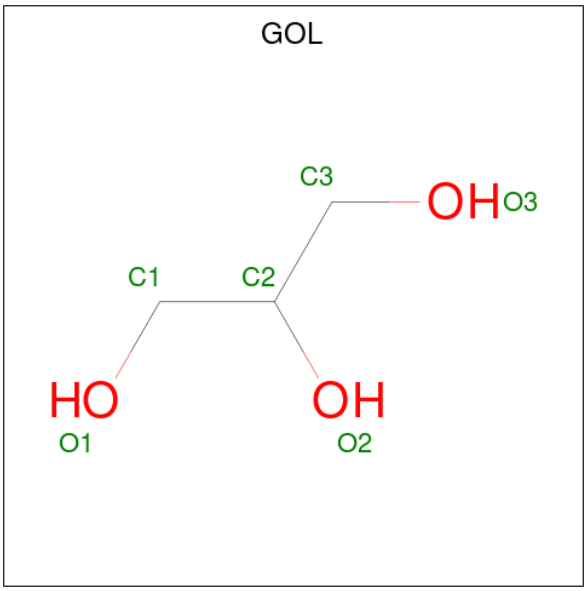
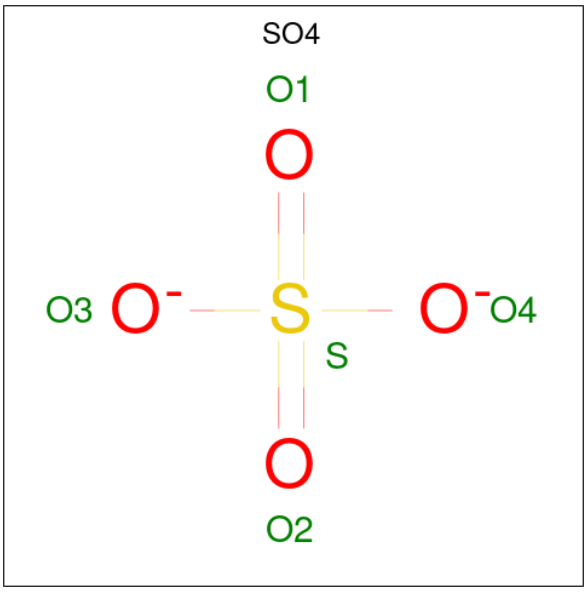
Chain	Residue	Modelled	Actual	Comment	Reference
D	456	GLU	-	expression tag	UNP R6ZJY1
D	457	LYS	-	expression tag	UNP R6ZJY1

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



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

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



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total Mg 1 1	0	0

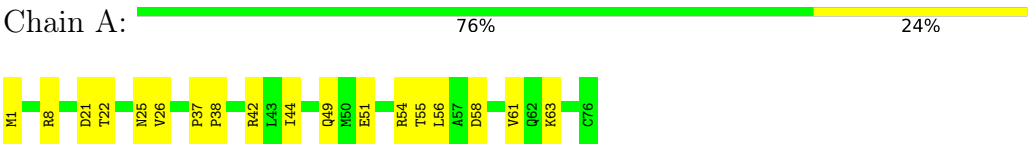
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	17	Total O 17 17	0	0
6	B	339	Total O 339 339	0	0
6	C	16	Total O 16 16	0	0
6	D	244	Total O 244 244	0	0

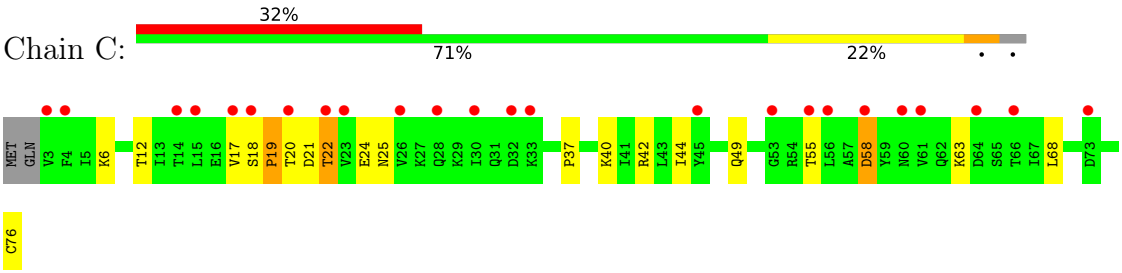
3 Residue-property plots (i)

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.

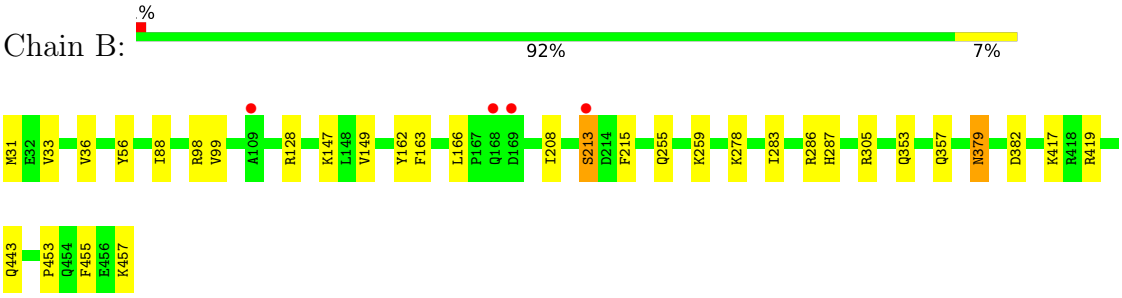
• Molecule 1: Putative ubiquitin



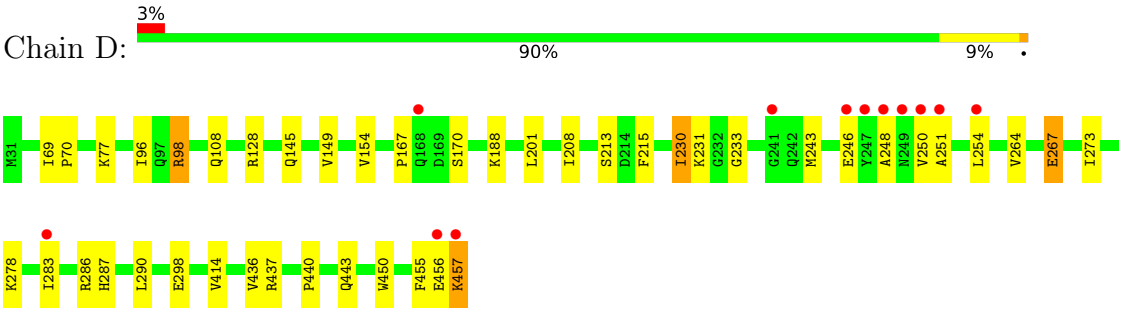
• Molecule 1: Putative ubiquitin



• Molecule 2: Peptidylprolyl isomerase



• Molecule 2: Peptidylprolyl isomerase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.86Å 100.92Å 106.18Å 90.00° 100.46° 90.00°	Depositor
Resolution (Å)	30.74 – 2.26 52.21 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.74-2.26) 99.4 (52.21-2.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.213 , 0.260 0.212 , 0.259	Depositor DCC
R_{free} test set	2970 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	39.4	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8797	wwPDB-VP
Average B, all atoms (Å^2)	54.0	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GOL, 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	0.46	0/623	0.66	0/840
1	C	0.34	0/606	0.65	0/818
2	B	0.40	0/3525	0.61	0/4749
2	D	0.40	0/3525	0.62	0/4749
All	All	0.40	0/8279	0.62	0/11156

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	614	0	619	13	0
1	C	597	0	599	15	0
2	B	3467	0	3475	21	0
2	D	3467	0	3475	30	0
3	A	6	0	8	0	0
3	B	18	0	24	0	0
3	D	6	0	8	0	0
4	B	5	0	0	0	0
5	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	17	0	0	1	0
6	B	339	0	0	3	0
6	C	16	0	0	1	0
6	D	244	0	0	1	0
All	All	8797	0	8208	77	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 5.

All (77) 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)
2:D:243:MET:CE	2:D:248:ALA:HA	2.12	0.78
1:C:42:ARG:HD2	1:C:49:GLN:OE1	1.97	0.65
2:D:243:MET:HE3	2:D:248:ALA:HA	1.78	0.64
1:C:6:LYS:HG3	1:C:12:THR:CG2	2.28	0.64
1:C:44:ILE:HB	1:C:68:LEU:HB2	1.80	0.63
1:C:55:THR:HG22	6:C:101:HOH:O	1.99	0.63
1:C:17:VAL:HG23	1:C:18:SER:H	1.65	0.61
2:B:149:VAL:HG21	2:B:419:ARG:HA	1.82	0.60
2:B:31:MET:HE2	2:B:33:VAL:H	1.66	0.60
2:D:208:ILE:HA	2:D:213:SER:O	2.02	0.59
2:B:278:LYS:HG2	2:B:283:ILE:HG22	1.85	0.58
2:B:163:PHE:O	2:B:166:LEU:HG	2.03	0.58
2:D:98:ARG:NH2	6:D:606:HOH:O	2.37	0.58
1:C:18:SER:O	1:C:20:THR:N	2.34	0.58
2:B:215:PHE:CD1	2:B:286:ARG:HD3	2.39	0.57
2:B:36:VAL:HG21	2:B:457:LYS:HD3	1.87	0.57
2:D:246:GLU:O	2:D:250:VAL:HG22	2.06	0.56
1:C:44:ILE:HD13	1:C:49:GLN:HA	1.87	0.56
2:D:215:PHE:CD1	2:D:286:ARG:HD3	2.43	0.54
2:D:440:PRO:HG3	2:D:457:LYS:HD2	1.90	0.54
2:D:250:VAL:HG23	2:D:273:ILE:HD12	1.91	0.52
2:D:246:GLU:HB3	2:D:264:VAL:CG2	2.40	0.52
2:B:99:VAL:HG11	2:B:128:ARG:HG3	1.91	0.52
2:D:145:GLN:O	2:D:149:VAL:HG22	2.10	0.52
2:B:163:PHE:HA	2:B:166:LEU:CD2	2.39	0.51
2:D:96:ILE:HD12	2:D:128:ARG:HH21	1.74	0.51
2:D:230:ILE:HD12	2:D:231:LYS:HG3	1.92	0.51
1:A:21:ASP:OD1	1:A:25:ASN:ND2	2.42	0.50
2:B:255:GLN:HB2	2:B:259:LYS:NZ	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:230:ILE:H	2:D:230:ILE:HG13	1.44	0.48
1:C:19:PRO:HD3	1:C:63:LYS:NZ	2.29	0.48
1:C:22:THR:O	1:C:24:GLU:N	2.43	0.48
2:D:201:LEU:HG	2:D:290:LEU:HD12	1.95	0.47
2:B:443:GLN:HA	2:B:455:PHE:CZ	2.49	0.47
2:D:167:PRO:HD2	2:D:170:SER:HB2	1.97	0.47
2:D:267:GLU:H	2:D:267:GLU:HG3	1.34	0.47
1:C:18:SER:OG	1:C:20:THR:HG23	2.14	0.46
1:C:37:PRO:HG2	1:C:40:LYS:HD2	1.97	0.46
1:A:56:LEU:HB3	1:A:61:VAL:HB	1.98	0.46
2:D:69:ILE:HB	2:D:70:PRO:HD3	1.97	0.46
2:D:233:GLY:O	2:D:286:ARG:HA	2.16	0.46
1:C:22:THR:HB	1:C:25:ASN:HB2	1.97	0.46
1:C:55:THR:HG23	1:C:58:ASP:HB2	1.98	0.46
2:B:162:TYR:HE2	2:B:417:LYS:HD3	1.81	0.45
1:A:37:PRO:HA	1:A:38:PRO:HD3	1.81	0.45
1:A:55:THR:HG23	1:A:58:ASP:H	1.81	0.45
2:D:250:VAL:HG21	2:D:264:VAL:HG11	1.99	0.45
2:D:436:VAL:HG11	2:D:450:TRP:HE1	1.80	0.45
2:B:88:ILE:HD11	2:B:147:LYS:HD3	1.98	0.45
1:C:42:ARG:HH21	1:C:76:CYS:HB2	1.82	0.45
2:D:251:ALA:HA	2:D:254:LEU:HD12	1.99	0.45
2:B:31:MET:HG2	6:B:739:HOH:O	2.17	0.45
1:A:1:MET:HB3	1:A:63:LYS:HE2	1.99	0.44
1:A:42:ARG:HD2	1:A:49:GLN:OE1	2.18	0.44
1:A:26:VAL:HG21	1:A:56:LEU:HD21	1.98	0.44
1:A:51:GLU:OE1	1:A:54:ARG:NE	2.44	0.44
1:A:22:THR:HG23	1:A:25:ASN:HB2	2.00	0.44
2:D:250:VAL:CG2	2:D:273:ILE:HD12	2.48	0.43
2:B:31:MET:HE3	6:B:889:HOH:O	2.18	0.43
2:D:443:GLN:HA	2:D:455:PHE:CZ	2.53	0.43
2:B:453:PRO:HG2	2:B:455:PHE:CZ	2.54	0.43
2:D:188:LYS:HB2	2:D:298:GLU:OE1	2.19	0.43
2:B:163:PHE:CD1	2:B:166:LEU:HD21	2.54	0.43
2:D:77:LYS:HA	2:D:77:LYS:HD3	1.89	0.43
2:D:437:ARG:NE	2:D:456:GLU:HB2	2.34	0.43
2:D:154:VAL:HG11	2:D:414:VAL:HG12	2.01	0.42
2:B:208:ILE:HA	2:B:213:SER:O	2.19	0.42
2:D:437:ARG:HG3	2:D:456:GLU:HB2	2.01	0.42
1:A:8:ARG:HG3	2:B:56:TYR:CE2	2.53	0.42
1:C:21:ASP:HB3	1:C:55:THR:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:278:LYS:HG3	2:D:283:ILE:HG22	2.01	0.41
2:B:305:ARG:NH2	6:B:611:HOH:O	2.53	0.41
1:A:44:ILE:HD13	2:B:56:TYR:HA	2.02	0.41
1:A:54:ARG:NH2	6:A:204:HOH:O	2.53	0.41
2:B:379:ASN:ND2	2:B:382:ASP:H	2.19	0.41
1:A:22:THR:O	1:A:26:VAL:HG23	2.20	0.41
2:D:243:MET:HE2	2:D:248:ALA:HA	1.97	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	74/76 (97%)	72 (97%)	2 (3%)	0	100 100
1	C	72/76 (95%)	65 (90%)	6 (8%)	1 (1%)	11 7
2	B	425/427 (100%)	422 (99%)	3 (1%)	0	100 100
2	D	425/427 (100%)	422 (99%)	3 (1%)	0	100 100
All	All	996/1006 (99%)	981 (98%)	14 (1%)	1 (0%)	51 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	19	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	70/70 (100%)	70 (100%)	0	100	100
1	C	68/70 (97%)	66 (97%)	2 (3%)	42	51
2	B	379/379 (100%)	373 (98%)	6 (2%)	62	73
2	D	379/379 (100%)	373 (98%)	6 (2%)	62	73
All	All	896/898 (100%)	882 (98%)	14 (2%)	62	73

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	98	ARG
2	B	213	SER
2	B	287	HIS
2	B	353	GLN
2	B	357	GLN
2	B	379	ASN
1	C	22	THR
1	C	58	ASP
2	D	98	ARG
2	D	108	GLN
2	D	230	ILE
2	D	267	GLU
2	D	287	HIS
2	D	457	LYS

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

Mol	Chain	Res	Type
1	A	62	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)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	$\#\|Z\| > 2$
3	GOL	D	501	-	5,5,5	0.63	0	5,5,5	0.26	0
3	GOL	B	501	-	5,5,5	0.54	0	5,5,5	0.38	0
4	SO4	B	504	-	4,4,4	0.12	0	6,6,6	0.19	0
3	GOL	A	101	-	5,5,5	0.61	0	5,5,5	0.31	0
3	GOL	B	502	-	5,5,5	0.57	0	5,5,5	0.23	0
3	GOL	B	503	-	5,5,5	0.62	0	5,5,5	0.32	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	D	501	-	-	0/4/4/4	-
3	GOL	B	501	-	-	3/4/4/4	-
3	GOL	A	101	-	-	0/4/4/4	-
3	GOL	B	502	-	-	2/4/4/4	-
3	GOL	B	503	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	GOL	C1-C2-C3-O3
3	B	501	GOL	O1-C1-C2-C3
3	B	503	GOL	O1-C1-C2-C3
3	B	501	GOL	O1-C1-C2-O2
3	B	503	GOL	O1-C1-C2-O2
3	B	502	GOL	O2-C2-C3-O3
3	B	501	GOL	O2-C2-C3-O3

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	76/76 (100%)	0.54	0 100 100	38, 68, 91, 110	0
1	C	74/76 (97%)	1.59	24 (32%) 0 0	51, 93, 132, 146	0
2	B	427/427 (100%)	0.20	4 (0%) 84 85	24, 42, 73, 132	0
2	D	427/427 (100%)	0.34	12 (2%) 53 55	24, 52, 89, 114	0
All	All	1004/1006 (99%)	0.39	40 (3%) 38 40	24, 50, 97, 146	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	17	VAL	8.4
2	D	457	LYS	5.3
2	D	168	GLN	4.7
1	C	61	VAL	4.6
1	C	15	LEU	4.1
1	C	22	THR	3.7
2	D	249	ASN	3.7
1	C	28	GLN	3.7
1	C	58	ASP	3.6
1	C	53	GLY	3.4
1	C	32	ASP	3.2
2	D	250	VAL	3.1
2	D	247	TYR	3.1
2	D	456	GLU	3.1
2	B	109	ALA	3.0
2	D	246	GLU	2.9
1	C	73	ASP	2.9
2	D	248	ALA	2.7
1	C	4	PHE	2.6
1	C	45	TYR	2.6
1	C	33	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	20	THR	2.5
1	C	55	THR	2.5
2	B	168	GLN	2.5
2	D	283	ILE	2.4
1	C	23	VAL	2.4
2	D	241	GLY	2.4
1	C	64	ASP	2.3
1	C	56	LEU	2.3
1	C	14	THR	2.3
1	C	18	SER	2.2
1	C	66	THR	2.2
1	C	60	ASN	2.2
2	B	213	SER	2.2
1	C	3	VAL	2.2
1	C	30	ILE	2.1
1	C	26	VAL	2.1
2	B	169	ASP	2.1
2	D	251	ALA	2.1
2	D	254	LEU	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)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers (i)

There are no such residues in this entry.