wwPDB X-ray Structure Validation Summary Report (i)

Oct 4, 2023 – 04:25 AM EDT

PDB ID	:	6OXB
Title	:	First bromo-adjacent homology (BAH) domain of human Polybromo-1 (PBRM1)
Authors	:	Petojevic, T.; Holliday, M.J.; Fairbrother, W.J.; Cochran, A.G.
Deposited on	:	2019-05-13
Resolution	:	1.86 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

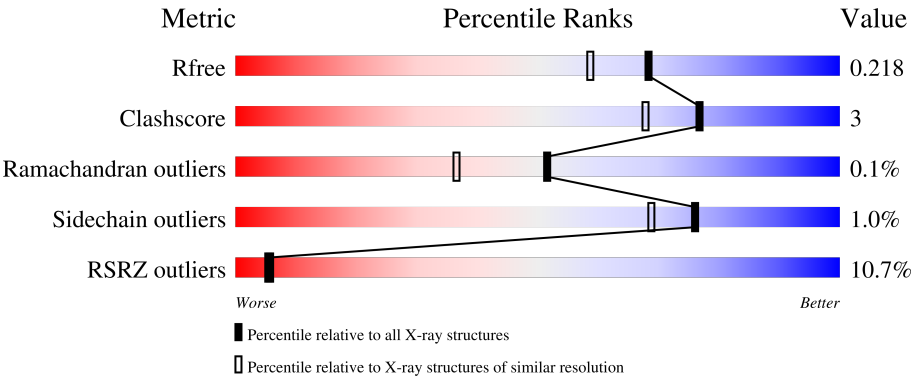
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.86 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	177	8% 82% 7% 11%
1	B	177	8% 77% 11% • 11%
1	C	177	11% 84% 6% 10%
1	D	177	7% 82% 7% 11%
1	E	177	10% 79% 10% 11%

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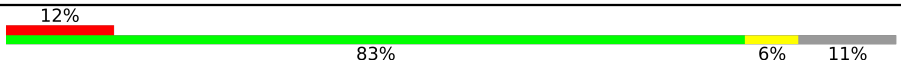
Mol	Chain	Length	Quality of chain
1	F	177	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8790 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 Protein polybromo-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	158	Total	C	N	O	S	0	0	0
			1320	862	219	230	9			
1	A	158	Total	C	N	O	S	0	0	0
			1322	864	219	230	9			
1	C	159	Total	C	N	O	S	0	0	0
			1333	873	220	231	9			
1	D	157	Total	C	N	O	S	0	0	0
			1315	859	218	229	9			
1	E	157	Total	C	N	O	S	0	0	0
			1314	858	218	229	9			
1	F	158	Total	C	N	O	S	0	0	0
			1322	864	219	230	9			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	932	GLY	-	expression tag	UNP Q86U86
B	933	SER	-	expression tag	UNP Q86U86
B	1106	GLY	-	expression tag	UNP Q86U86
B	1107	ASN	-	expression tag	UNP Q86U86
B	1108	SER	-	expression tag	UNP Q86U86
A	932	GLY	-	expression tag	UNP Q86U86
A	933	SER	-	expression tag	UNP Q86U86
A	1106	GLY	-	expression tag	UNP Q86U86
A	1107	ASN	-	expression tag	UNP Q86U86
A	1108	SER	-	expression tag	UNP Q86U86
C	932	GLY	-	expression tag	UNP Q86U86
C	933	SER	-	expression tag	UNP Q86U86
C	1106	GLY	-	expression tag	UNP Q86U86
C	1107	ASN	-	expression tag	UNP Q86U86
C	1108	SER	-	expression tag	UNP Q86U86
D	932	GLY	-	expression tag	UNP Q86U86
D	933	SER	-	expression tag	UNP Q86U86

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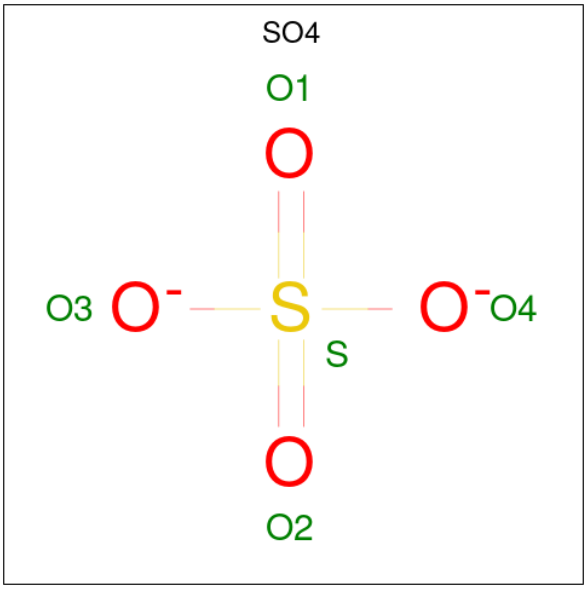
Chain	Residue	Modelled	Actual	Comment	Reference
D	1106	GLY	-	expression tag	UNP Q86U86
D	1107	ASN	-	expression tag	UNP Q86U86
D	1108	SER	-	expression tag	UNP Q86U86
E	932	GLY	-	expression tag	UNP Q86U86
E	933	SER	-	expression tag	UNP Q86U86
E	1106	GLY	-	expression tag	UNP Q86U86
E	1107	ASN	-	expression tag	UNP Q86U86
E	1108	SER	-	expression tag	UNP Q86U86
F	932	GLY	-	expression tag	UNP Q86U86
F	933	SER	-	expression tag	UNP Q86U86
F	1106	GLY	-	expression tag	UNP Q86U86
F	1107	ASN	-	expression tag	UNP Q86U86
F	1108	SER	-	expression tag	UNP Q86U86

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



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	B	1	Total O S 5 4 1	0	0

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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	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	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	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
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	F	1	Total Cl 1 1	0	0

- Molecule 4 is water.

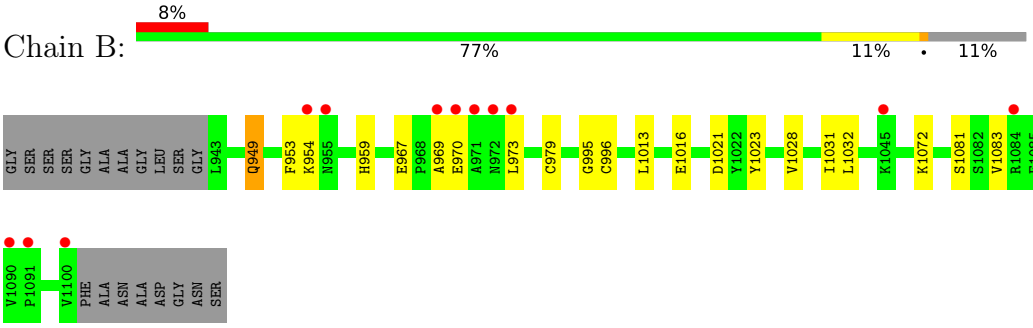
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	115	Total O 115 115	0	0
4	A	122	Total O 122 122	0	0
4	C	118	Total O 118 118	0	0
4	D	130	Total O 130 130	0	0
4	E	112	Total O 112 112	0	0
4	F	115	Total O 115 115	0	0

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.

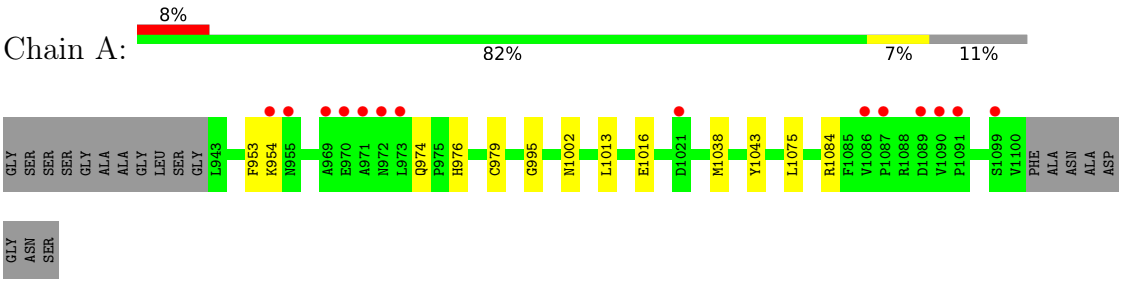
• Molecule 1: Protein polybromo-1

Chain B:



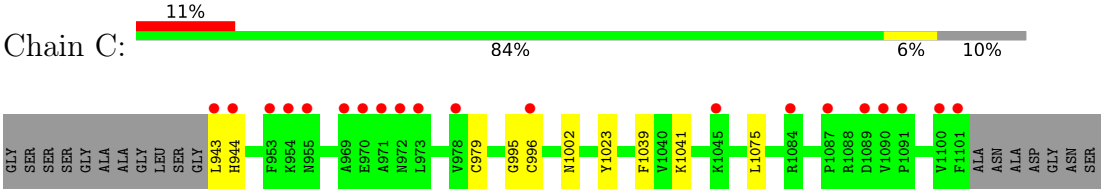
• Molecule 1: Protein polybromo-1

Chain A:



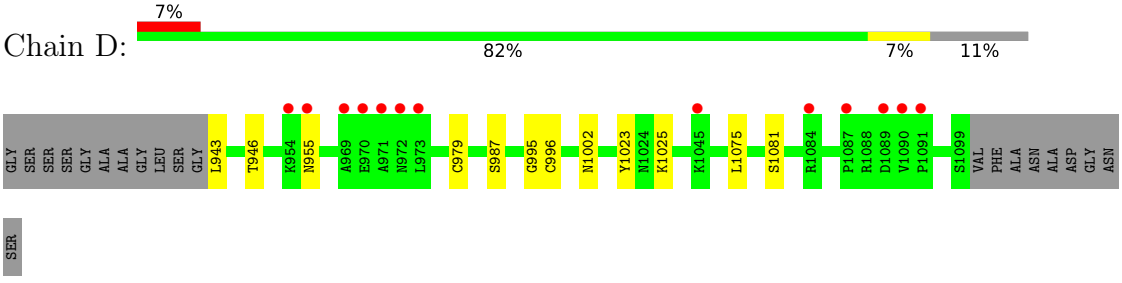
• Molecule 1: Protein polybromo-1

Chain C:



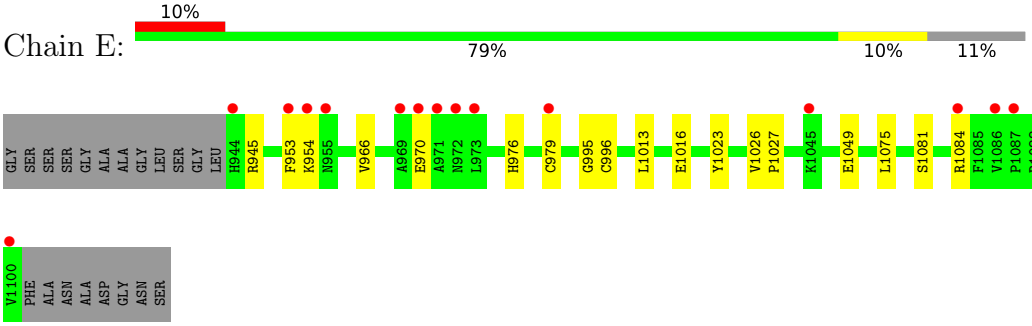
• Molecule 1: Protein polybromo-1

Chain D:



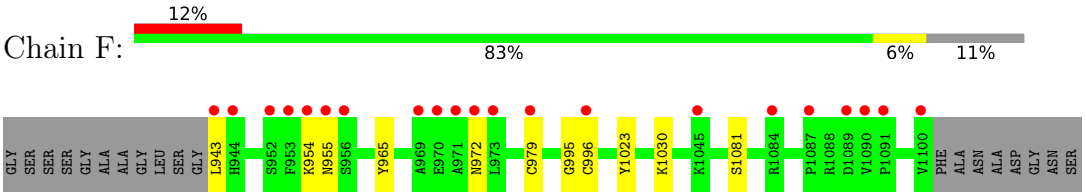
• Molecule 1: Protein polybromo-1

Chain E:



• Molecule 1: Protein polybromo-1

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	52.30Å 52.26Å 120.10Å 89.11° 88.24° 60.12°	Depositor
Resolution (Å)	30.40 – 1.86 30.40 – 1.86	Depositor EDS
% Data completeness (in resolution range)	90.3 (30.40-1.86) 90.3 (30.40-1.86)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 1.85Å)	Xtriage
Refinement program	PHENIX 1.12-2829_final	Depositor
R, R_{free}	0.179 , 0.217 0.179 , 0.218	Depositor DCC
R_{free} test set	1860 reflections (2.23%)	wwPDB-VP
Wilson B-factor (Å^2)	25.7	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 56.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.016 for h-k,h,l 0.016 for k,-h+k,l 0.055 for -k,h-k,l 0.055 for -h+k,-h,l 0.125 for -h+k,k,-l 0.084 for h,h-k,-l 0.018 for -h,-k,l 0.019 for k,h,-l 0.127 for -k,-h,-l 0.023 for h-k,-k,-l 0.024 for -h,-h+k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8790	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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: 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	0.41	0/1363	0.58	0/1845
1	B	0.43	0/1361	0.58	0/1842
1	C	0.40	0/1375	0.60	0/1861
1	D	0.42	0/1356	0.65	0/1835
1	E	0.41	0/1355	0.60	0/1834
1	F	0.40	0/1363	0.56	0/1845
All	All	0.41	0/8173	0.60	0/11062

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	1322	0	1307	11	0
1	B	1320	0	1300	13	0
1	C	1333	0	1316	6	0
1	D	1315	0	1298	6	0
1	E	1314	0	1296	9	0
1	F	1322	0	1307	5	0
2	A	30	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	25	0	0	1	0
2	C	25	0	0	0	0
2	D	20	0	0	1	0
2	E	25	0	0	0	0
2	F	25	0	0	0	0
3	A	1	0	0	0	0
3	F	1	0	0	0	0
4	A	122	0	0	3	1
4	B	115	0	0	2	1
4	C	118	0	0	0	0
4	D	130	0	0	2	0
4	E	112	0	0	1	0
4	F	115	0	0	1	0
All	All	8790	0	7824	48	1

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.

The worst 5 of 48 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1021:ASP:OD1	4:B:1301:HOH:O	2.08	0.72
1:F:954:LYS:HD3	1:F:955:ASN:H	1.66	0.59
1:A:974:GLN:NE2	1:A:1002:ASN:HD21	2.01	0.58
1:B:969:ALA:HB3	2:B:1205:SO4:O1	2.04	0.57
1:E:1049:GLU:HB2	1:E:1084:ARG:HG3	1.87	0.56

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1391:HOH:O	4:A:1413:HOH:O[1_455]	2.19	0.01

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	156/177 (88%)	156 (100%)	0	0	100	100
1	B	156/177 (88%)	154 (99%)	2 (1%)	0	100	100
1	C	157/177 (89%)	157 (100%)	0	0	100	100
1	D	155/177 (88%)	151 (97%)	4 (3%)	0	100	100
1	E	155/177 (88%)	152 (98%)	3 (2%)	0	100	100
1	F	156/177 (88%)	153 (98%)	2 (1%)	1 (1%)	25	12
All	All	935/1062 (88%)	923 (99%)	11 (1%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	972	ASN

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	148/158 (94%)	148 (100%)	0	100	100
1	B	147/158 (93%)	145 (99%)	2 (1%)	67	55
1	C	149/158 (94%)	149 (100%)	0	100	100
1	D	147/158 (93%)	144 (98%)	3 (2%)	55	40
1	E	147/158 (93%)	145 (99%)	2 (1%)	67	55
1	F	148/158 (94%)	146 (99%)	2 (1%)	67	55
All	All	886/948 (94%)	877 (99%)	9 (1%)	76	69

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	943	LEU
1	F	1081	SER
1	D	1075	LEU
1	D	1081	SER
1	E	1075	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1050	ASN
1	F	1050	ASN
1	A	974	GLN
1	A	976	HIS
1	A	1050	ASN

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 32 ligands modelled in this entry, 2 are monoatomic - leaving 30 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	$\#\|Z\| > 2$
2	SO4	A	1203	-	4,4,4	0.13	0	6,6,6	0.13	0
2	SO4	E	1203	-	4,4,4	0.13	0	6,6,6	0.25	0
2	SO4	A	1204	-	4,4,4	0.15	0	6,6,6	0.13	0
2	SO4	E	1202	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	B	1201	-	4,4,4	0.12	0	6,6,6	0.04	0
2	SO4	B	1204	-	4,4,4	0.13	0	6,6,6	0.10	0
2	SO4	B	1202	-	4,4,4	0.16	0	6,6,6	0.19	0
2	SO4	F	1202	-	4,4,4	0.17	0	6,6,6	0.23	0
2	SO4	F	1204	-	4,4,4	0.13	0	6,6,6	0.08	0
2	SO4	E	1201	-	4,4,4	0.17	0	6,6,6	0.20	0
2	SO4	F	1201	-	4,4,4	0.12	0	6,6,6	0.10	0
2	SO4	C	1202	-	4,4,4	0.15	0	6,6,6	0.11	0
2	SO4	C	1204	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	E	1205	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	D	1201	-	4,4,4	0.13	0	6,6,6	0.06	0
2	SO4	F	1205	-	4,4,4	0.18	0	6,6,6	0.17	0
2	SO4	B	1205	-	4,4,4	0.17	0	6,6,6	0.06	0
2	SO4	C	1205	-	4,4,4	0.13	0	6,6,6	0.17	0
2	SO4	A	1202	-	4,4,4	0.13	0	6,6,6	0.13	0
2	SO4	D	1203	-	4,4,4	0.13	0	6,6,6	0.07	0
2	SO4	B	1203	-	4,4,4	0.16	0	6,6,6	0.12	0
2	SO4	A	1201	-	4,4,4	0.15	0	6,6,6	0.09	0
2	SO4	C	1203	-	4,4,4	0.15	0	6,6,6	0.09	0
2	SO4	E	1204	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	A	1205	-	4,4,4	0.13	0	6,6,6	0.10	0
2	SO4	F	1203	-	4,4,4	0.12	0	6,6,6	0.10	0
2	SO4	C	1201	-	4,4,4	0.12	0	6,6,6	0.32	0
2	SO4	D	1202	-	4,4,4	0.17	0	6,6,6	0.23	0
2	SO4	A	1206	-	4,4,4	0.16	0	6,6,6	0.10	0
2	SO4	D	1204	-	4,4,4	0.17	0	6,6,6	0.11	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1201	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1205	SO4	1	0
2	A	1206	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	158/177 (89%)	0.58	14 (8%) 9 9	17, 32, 62, 138	0
1	B	158/177 (89%)	0.70	15 (9%) 8 7	18, 31, 68, 136	0
1	C	159/177 (89%)	0.78	20 (12%) 3 3	18, 32, 71, 98	0
1	D	157/177 (88%)	0.53	13 (8%) 11 11	17, 29, 68, 106	0
1	E	157/177 (88%)	0.77	18 (11%) 4 4	17, 32, 60, 111	0
1	F	158/177 (89%)	0.77	21 (13%) 3 3	17, 32, 64, 112	0
All	All	947/1062 (89%)	0.69	101 (10%) 6 5	17, 31, 68, 138	0

The worst 5 of 101 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	972	ASN	12.6
1	B	971	ALA	10.6
1	E	971	ALA	10.2
1	C	972	ASN	10.2
1	A	972	ASN	9.7

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	1205	5/5	0.64	0.38	109,112,114,116	0
2	SO4	F	1203	5/5	0.74	0.22	92,93,95,98	0
2	SO4	C	1205	5/5	0.81	0.27	91,93,94,99	0
2	SO4	A	1204	5/5	0.81	0.35	64,79,86,88	0
2	SO4	A	1201	5/5	0.82	0.22	91,96,97,98	0
2	SO4	C	1203	5/5	0.82	0.24	88,90,91,94	0
2	SO4	A	1206	5/5	0.83	0.35	114,119,119,122	0
2	SO4	D	1201	5/5	0.85	0.31	87,87,91,93	0
2	SO4	E	1203	5/5	0.85	0.21	71,74,79,85	0
2	SO4	A	1205	5/5	0.85	0.13	88,88,90,92	0
2	SO4	A	1203	5/5	0.86	0.27	77,79,83,86	0
2	SO4	C	1204	5/5	0.86	0.19	92,98,100,100	0
2	SO4	E	1205	5/5	0.86	0.20	95,95,98,99	0
2	SO4	C	1202	5/5	0.86	0.17	69,73,76,84	0
2	SO4	D	1204	5/5	0.87	0.27	64,67,77,80	0
2	SO4	D	1203	5/5	0.87	0.27	88,92,93,94	0
2	SO4	F	1205	5/5	0.88	0.30	63,68,76,81	0
2	SO4	F	1204	5/5	0.89	0.23	91,92,93,98	0
3	CL	A	1207	1/1	0.89	0.08	54,54,54,54	0
2	SO4	B	1201	5/5	0.91	0.25	68,70,73,77	0
2	SO4	B	1203	5/5	0.91	0.23	72,72,76,80	0
2	SO4	E	1204	5/5	0.91	0.26	91,91,92,92	0
2	SO4	B	1204	5/5	0.91	0.16	89,91,97,98	0
2	SO4	E	1202	5/5	0.94	0.18	69,71,74,79	0
2	SO4	B	1202	5/5	0.96	0.16	49,49,58,62	0
2	SO4	F	1201	5/5	0.96	0.13	55,62,63,66	0
3	CL	F	1206	1/1	0.97	0.07	38,38,38,38	0
2	SO4	A	1202	5/5	0.98	0.14	56,57,61,66	0
2	SO4	E	1201	5/5	0.98	0.09	39,39,42,44	0
2	SO4	D	1202	5/5	0.98	0.12	40,44,47,51	0
2	SO4	C	1201	5/5	0.98	0.11	32,38,41,47	0
2	SO4	F	1202	5/5	0.99	0.13	38,40,41,43	0

6.5 Other polymers (i)

There are no such residues in this entry.