Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:47 AM GMT

PDB ID	:	3G2F
Title	:	Crystal structure of the kinase domain of bone morphogenetic protein receptor type II (BMPR2) at 2.35 A resolution
Authors	:	Chaikuad, A.; Thangaratnarajah, C.; Roos, A.K.; Filippakopoulos, P.; Salah, E.; Phillips, C.; Keates, T.; Fedorov, O.; Chalk, R.; Petrie, K.; Pike, A.C.W.; Von Delft, F.; Arrowsmith, C.H.; Edwards, A.M.; Weigelt, J.; Bountra, C.; Knapp, S.; Bullock, A.; Structural Genomics Consortium (SGC)
Deposited on	:	2009-01-31
Resolution	:	2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

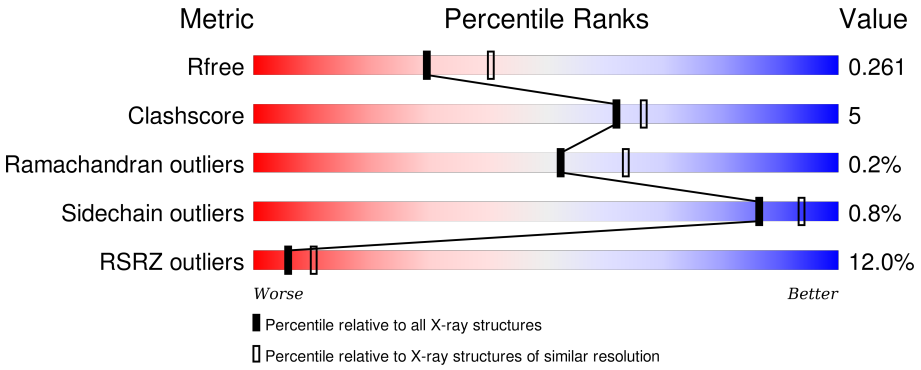
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	336	3% 79% 12% 9%
1	B	336	18% 77% 13% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	A	3	-	-	-	X
5	EDO	A	4	-	-	-	X
5	EDO	A	5	-	-	-	X
5	EDO	B	6	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5138 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.

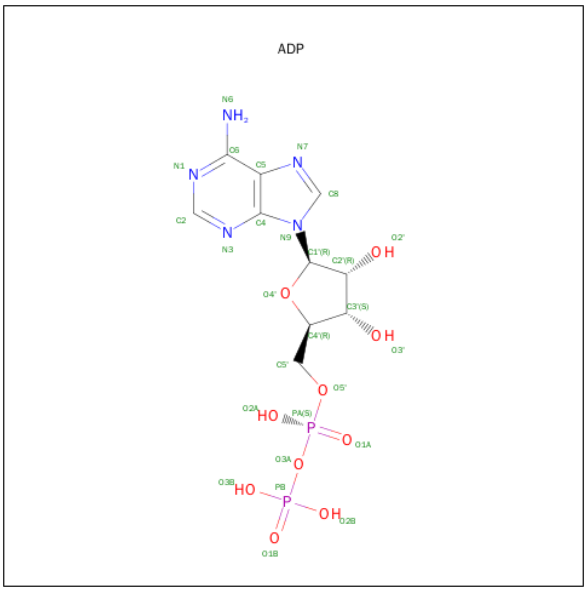
- Molecule 1 is a protein called Bone morphogenetic protein receptor type-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	305	Total	As	C	N	O	S	0	2	0
			2480	3	1564	433	461	19			
1	B	303	Total	As	C	N	O	S	0	1	0
			2454	2	1543	430	460	19			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	518	ALA	-	EXPRESSION TAG	UNP Q13873
A	519	HIS	-	EXPRESSION TAG	UNP Q13873
A	520	HIS	-	EXPRESSION TAG	UNP Q13873
A	521	HIS	-	EXPRESSION TAG	UNP Q13873
A	522	HIS	-	EXPRESSION TAG	UNP Q13873
A	523	HIS	-	EXPRESSION TAG	UNP Q13873
A	524	HIS	-	EXPRESSION TAG	UNP Q13873
B	518	ALA	-	EXPRESSION TAG	UNP Q13873
B	519	HIS	-	EXPRESSION TAG	UNP Q13873
B	520	HIS	-	EXPRESSION TAG	UNP Q13873
B	521	HIS	-	EXPRESSION TAG	UNP Q13873
B	522	HIS	-	EXPRESSION TAG	UNP Q13873
B	523	HIS	-	EXPRESSION TAG	UNP Q13873
B	524	HIS	-	EXPRESSION TAG	UNP Q13873

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

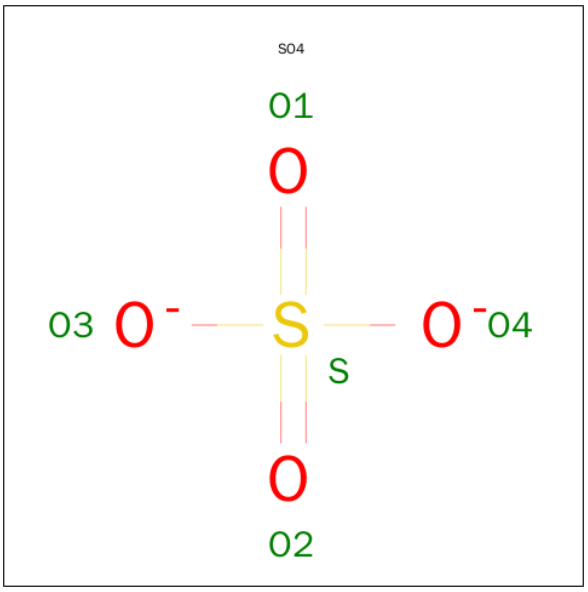


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

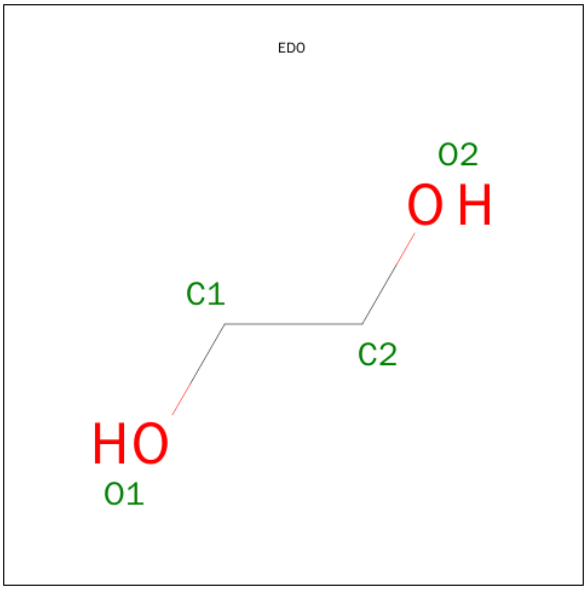
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

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



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

- Molecule 6 is water.

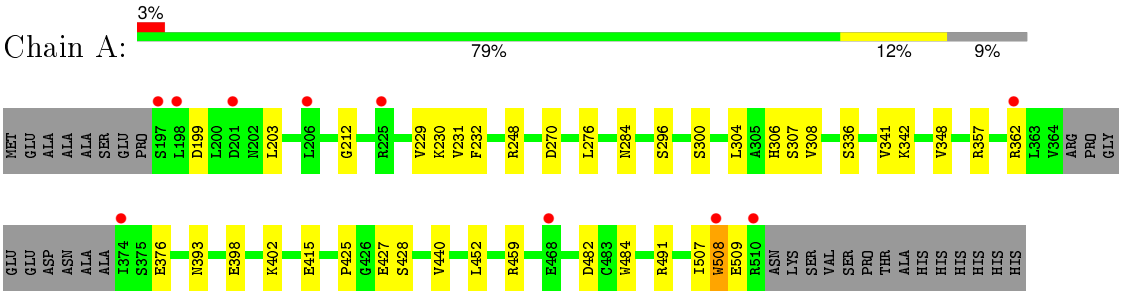
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	107	Total O 107 107	0	0
6	B	15	Total O 15 15	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

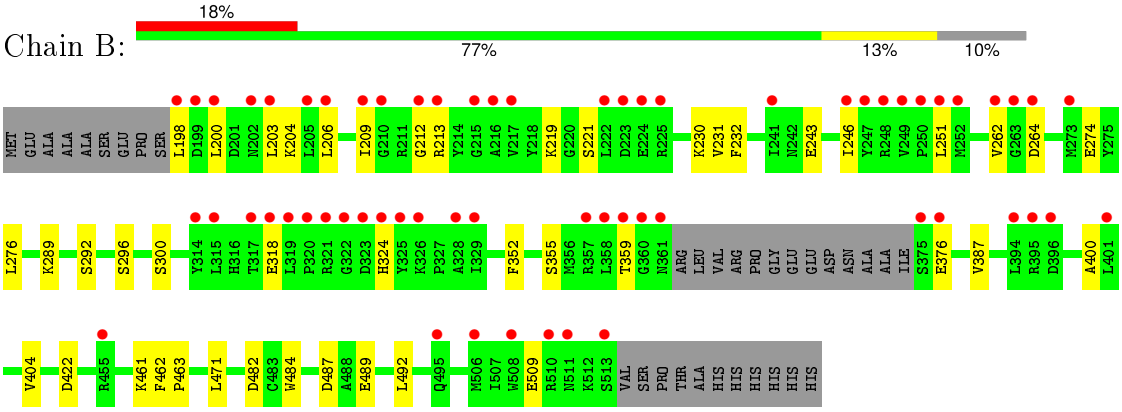
- Molecule 1: Bone morphogenetic protein receptor type-2

Chain A:



- Molecule 1: Bone morphogenetic protein receptor type-2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	94.54Å 218.79Å 44.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.35 – 2.35 47.34 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.35-2.35) 99.9 (47.34-2.35)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0055	Depositor
R, R_{free}	0.208 , 0.246 0.222 , 0.261	Depositor DCC
R_{free} test set	1975 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	42.9	Xtriage
Anisotropy	0.703	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 53.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 39339 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5138	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CAS, MG, EDO, ADP, 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	0.59	0/2510	0.66	0/3386
1	B	0.46	0/2481	0.57	0/3346
All	All	0.53	0/4991	0.62	0/6732

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	2480	0	2436	27	0
1	B	2454	0	2402	26	0
2	A	27	0	12	1	0
2	B	27	0	12	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	12	0	18	4	0
5	B	4	0	6	2	0
6	A	107	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	15	0	0	2	0
All	All	5138	0	4886	53	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 (53) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:ILE:HD13	1:B:471:LEU:HD23	1.70	0.74
1:A:342:LYS:HD2	1:A:348:VAL:HG13	1.68	0.73
1:A:393:ASN:HB3	5:A:5:EDO:H21	1.71	0.73
1:B:198:LEU:HA	1:B:262:VAL:HG21	1.73	0.68
1:B:296:SER:HB3	1:B:300:SER:HB2	1.80	0.63
1:B:422:ASP:HB3	1:B:509:GLU:HG3	1.83	0.60
1:B:461:LYS:HA	5:B:6:EDO:H22	1.85	0.58
1:A:296:SER:HB3	1:A:300:SER:HB2	1.88	0.56
1:B:212:GLY:HA3	2:B:900:ADP:O2B	2.06	0.55
1:B:289:LYS:O	1:B:292:SER:HB3	2.06	0.55
1:A:357:ARG:HD3	6:A:98:HOH:O	2.07	0.54
1:A:307:SER:HB3	5:A:4:EDO:H12	1.89	0.54
1:B:230:LYS:HE2	1:B:232:PHE:CZ	2.44	0.53
1:A:306:HIS:ND1	5:A:4:EDO:H11	2.24	0.53
1:A:459:ARG:O	5:A:3:EDO:H12	2.09	0.53
5:B:6:EDO:H21	6:B:116:HOH:O	2.10	0.51
1:A:270:ASP:HB2	6:A:117:HOH:O	2.11	0.51
1:A:230:LYS:HE2	1:A:232:PHE:CZ	2.46	0.50
1:A:212:GLY:HA3	2:A:900:ADP:O2B	2.11	0.50
1:A:427:GLU:HG2	1:A:428:SER:N	2.27	0.50
1:B:482:ASP:HB3	1:B:492:LEU:HG	1.94	0.50
1:B:318:GLU:OE1	1:B:359:THR:HB	2.12	0.49
1:B:231:VAL:HG22	1:B:276:LEU:HD22	1.96	0.48
1:B:243:GLU:HG3	1:B:352:PHE:HB2	1.95	0.48
1:A:398:GLU:HG2	1:A:402:LYS:HE3	1.97	0.47
1:B:400:ALA:O	1:B:404:VAL:HG23	2.15	0.47
1:A:248:ARG:HG2	1:A:248:ARG:HH11	1.80	0.47
1:B:251:LEU:HD11	1:B:324:HIS:HB3	1.97	0.46
1:B:209:ILE:HD12	2:B:900:ADP:C2	2.51	0.46
1:A:231:VAL:HG22	1:A:276:LEU:HD22	1.98	0.46
1:B:213:ARG:O	1:B:213:ARG:HG2	2.15	0.46
1:A:199:ASP:HB3	6:A:92:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ARG:NH2	1:A:362:ARG:O	2.50	0.44
1:A:342:LYS:HD2	1:A:348:VAL:CG1	2.43	0.44
1:B:487:ASP:OD1	1:B:487:ASP:C	2.56	0.44
1:B:246:ILE:HG13	1:B:355:SER:HB2	2.00	0.44
1:B:206:LEU:HD12	1:B:219:LYS:HE3	1.99	0.43
1:B:230:LYS:HE3	2:B:900:ADP:O3A	2.18	0.43
1:B:274:GLU:HG3	6:B:36:HOH:O	2.18	0.42
1:B:204:LYS:HD2	1:B:204:LYS:HA	1.79	0.42
1:A:336:SER:OG	1:A:415:GLU:OE1	2.33	0.42
1:B:203:LEU:HA	1:B:221:SER:O	2.20	0.42
1:A:248:ARG:NH1	1:A:248:ARG:HG2	2.34	0.41
1:A:482:ASP:O	1:A:491:ARG:HA	2.19	0.41
1:A:508:TRP:O	1:A:509:GLU:HB2	2.20	0.41
1:A:304:LEU:O	1:A:308:VAL:HG12	2.20	0.41
1:A:425:PRO:HD2	6:A:120:HOH:O	2.19	0.41
1:A:440:VAL:HG13	1:A:452:LEU:HD22	2.03	0.41
1:B:462:PHE:HA	1:B:463:PRO:HD3	1.94	0.41
1:B:376:GLU:OE1	1:B:387:VAL:HG13	2.21	0.41
1:A:203:LEU:HD11	1:A:229:VAL:HG21	2.02	0.41
1:A:284:ASN:HB2	1:A:341:VAL:O	2.21	0.41
1:B:200:LEU:HD11	1:B:264:ASP:HB3	2.03	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	300/336 (89%)	285 (95%)	14 (5%)	1 (0%)	46 55
1	B	297/336 (88%)	281 (95%)	16 (5%)	0	100 100
All	All	597/672 (89%)	566 (95%)	30 (5%)	1 (0%)	52 63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	GLU

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	267/289 (92%)	265 (99%)	2 (1%)	88 95
1	B	264/289 (91%)	262 (99%)	2 (1%)	86 94
All	All	531/578 (92%)	527 (99%)	4 (1%)	86 94

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

Mol	Chain	Res	Type
1	A	484	TRP
1	A	508	TRP
1	B	484	TRP
1	B	489	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

6 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CAS	A	288	1	3,6,9	0.44	0	2,6,11	1.06	0
1	CAS	A	397	1	3,6,9	0.57	0	2,6,11	1.57	1 (50%)
1	CAS	A	496	1	5,8,9	0.45	0	2,9,11	1.78	0
1	CAS	B	288	1	3,6,9	0.50	0	2,6,11	1.39	0
1	CAS	B	397	1	4,5,9	0.82	0	3,5,11	1.38	1 (33%)
1	CAS	B	496	1	5,8,9	0.62	0	2,9,11	2.51	1 (50%)

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
1	CAS	A	288	1	-	0/0/5/9	0/0/0/0
1	CAS	A	397	1	-	0/0/5/9	0/0/0/0
1	CAS	A	496	1	-	0/0/7/9	0/0/0/0
1	CAS	B	288	1	-	0/0/5/9	0/0/0/0
1	CAS	B	397	1	-	0/1/4/9	0/0/0/0
1	CAS	B	496	1	-	0/0/7/9	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	496	CAS	CA-CB-SG	-2.99	103.52	114.16
1	B	397	CAS	O-C-CA	-2.28	119.54	125.49
1	A	397	CAS	O-C-CA	-2.09	120.05	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	A	2	-	4,4,4	0.13	0	6,6,6	0.41	0
5	EDO	A	3	-	3,3,3	0.50	0	2,2,2	0.41	0
5	EDO	A	4	-	3,3,3	0.42	0	2,2,2	0.48	0
5	EDO	A	5	-	3,3,3	0.50	0	2,2,2	0.23	0
2	ADP	A	900	3	22,29,29	0.94	1 (4%)	27,45,45	2.14	3 (11%)
4	SO4	B	1	-	4,4,4	0.30	0	6,6,6	1.15	0
5	EDO	B	6	-	3,3,3	0.56	0	2,2,2	0.30	0
2	ADP	B	900	3	22,29,29	1.10	1 (4%)	27,45,45	1.95	6 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	2	-	-	0/0/0/0	0/0/0/0
5	EDO	A	3	-	-	0/1/1/1	0/0/0/0
5	EDO	A	4	-	-	0/1/1/1	0/0/0/0
5	EDO	A	5	-	-	0/1/1/1	0/0/0/0
2	ADP	A	900	3	-	0/12/32/32	0/3/3/3
4	SO4	B	1	-	-	0/0/0/0	0/0/0/0
5	EDO	B	6	-	-	0/1/1/1	0/0/0/0
2	ADP	B	900	3	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	ADP	C5-C4	2.40	1.45	1.40
2	B	900	ADP	C5-C4	2.90	1.47	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	900	ADP	N3-C2-N1	-9.69	121.47	128.89
2	B	900	ADP	N3-C2-N1	-7.49	123.16	128.89
2	B	900	ADP	C2'-C1'-N9	-3.37	109.14	114.29
2	B	900	ADP	C4-C5-N7	-3.09	106.64	109.48
2	A	900	ADP	C4-C5-N7	-2.15	107.50	109.48
2	B	900	ADP	O5'-PA-O1A	-2.11	101.43	109.62
2	B	900	ADP	O3B-PB-O2B	2.17	115.65	107.38
2	B	900	ADP	C4'-O4'-C1'	2.22	112.16	109.72
2	A	900	ADP	O3B-PB-O2B	2.59	117.24	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3	EDO	1	0
5	A	4	EDO	2	0
5	A	5	EDO	1	0
2	A	900	ADP	1	0
5	B	6	EDO	2	0
2	B	900	ADP	3	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	302/336 (89%)	0.50	10 (3%) 50 63	4, 23, 41, 76	2 (0%)
1	B	300/336 (89%)	1.29	62 (20%) 1 2	4, 22, 44, 74	2 (0%)
All	All	602/672 (89%)	0.89	72 (11%) 6 10	4, 23, 43, 76	4 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	323	ASP	8.8
1	B	324	HIS	8.8
1	B	198	LEU	8.7
1	B	314	TYR	7.2
1	B	375	SER	6.6
1	B	251	LEU	6.6
1	B	360	GLY	6.3
1	B	262	VAL	6.0
1	B	357	ARG	6.0
1	A	198	LEU	5.5
1	B	321	ARG	5.5
1	B	320	PRO	5.4
1	B	319	LEU	5.0
1	A	374	ILE	4.8
1	B	225	ARG	4.7
1	B	358	LEU	4.7
1	A	508	TRP	4.5
1	B	508	TRP	4.4
1	B	248	ARG	4.3
1	B	200	LEU	4.1
1	B	510	ARG	4.0
1	B	264	ASP	4.0
1	B	203	LEU	3.8
1	B	241	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	197	SER	3.7
1	B	394	LEU	3.6
1	B	249	VAL	3.6
1	B	317	THR	3.5
1	B	359	THR	3.3
1	B	506	MET	3.2
1	B	395	ARG	3.1
1	B	202	ASN	3.0
1	B	222	LEU	3.0
1	B	199	ASP	3.0
1	B	209	ILE	3.0
1	B	252	MET	3.0
1	B	329	ILE	2.8
1	B	322	GLY	2.8
1	B	263	GLY	2.8
1	B	223	ASP	2.7
1	B	326	LYS	2.7
1	B	273	MET	2.6
1	B	513	SER	2.6
1	A	201	ASP	2.6
1	B	215	GLY	2.6
1	B	315	LEU	2.6
1	B	216	ALA	2.5
1	A	468	GLU	2.5
1	B	396	ASP	2.5
1	A	206	LEU	2.4
1	B	325	TYR	2.4
1	B	361	ASN	2.4
1	B	511	ASN	2.4
1	B	205	LEU	2.3
1	A	510	ARG	2.3
1	B	318	GLU	2.3
1	B	376	GLU	2.3
1	B	247	TYR	2.3
1	B	328	ALA	2.3
1	B	246	ILE	2.2
1	B	217	VAL	2.2
1	B	455	ARG	2.2
1	B	495	GLN	2.2
1	B	213	ARG	2.2
1	B	250	PRO	2.2
1	B	212	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	210	GLY	2.2
1	A	362	ARG	2.2
1	B	401	LEU	2.2
1	A	225	ARG	2.1
1	B	224	GLU	2.1
1	B	206	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	CAS	A	397	7/10	0.64	0.25	-	6,7,14,43	1
1	CAS	A	496	9/10	0.88	0.17	-	25,26,44,45	2
1	CAS	B	288	7/10	0.76	0.27	-	22,23,25,50	2
1	CAS	B	397	6/10	0.81	0.19	-	17,17,17,18	0
1	CAS	B	496	9/10	0.80	0.15	-	20,21,47,48	2
1	CAS	A	288	7/10	0.89	0.20	-	23,24,26,42	2

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	EDO	A	3	4/4	0.87	0.34	11.06	56,59,59,60	0
5	EDO	A	5	4/4	0.93	0.31	6.93	53,55,55,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	EDO	A	4	4/4	0.94	0.27	5.96	50,52,54,55	0
5	EDO	B	6	4/4	0.77	0.27	3.87	63,63,64,64	0
4	SO4	B	1	5/5	0.95	0.26	1.77	55,56,57,57	0
2	ADP	A	900	27/27	0.97	0.16	0.00	24,32,49,51	0
2	ADP	B	900	27/27	0.95	0.20	-0.39	37,45,61,63	0
4	SO4	A	2	5/5	0.97	0.12	-1.87	62,65,65,65	0
3	MG	A	901	1/1	0.94	0.05	-	40,40,40,40	0
3	MG	B	901	1/1	0.45	0.14	-	47,47,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.