Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:09 PM GMT

PDB ID	:	3WAW
Title	:	Crystal Structure of Autotaxin in Complex with 2BoA
Authors	:	Nishimasu, H.; Ishitani, R.; Nureki, O.
Deposited on	:	2013-05-09
Resolution	:	1.95 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:

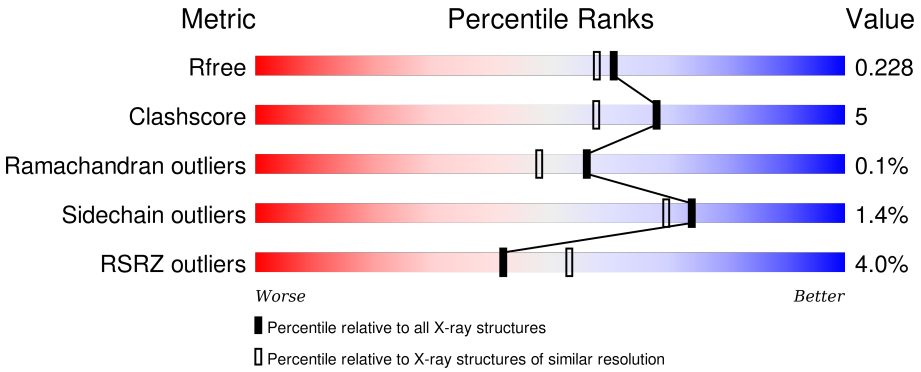
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	831	4% 84% 9% 6%

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
10	EDO	A	921	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	EDO	A	924	-	-	-	X
10	EDO	A	926	-	-	-	X
10	EDO	A	927	-	-	-	X
10	EDO	A	928	-	-	-	X
10	EDO	A	929	-	-	-	X
10	EDO	A	931	-	-	-	X
11	DWW	A	937	-	-	X	-
3	MAN	A	907	-	-	-	X
9	SCN	A	919	-	-	-	X
9	SCN	A	920	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 6867 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 Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	779	Total	C	N	O	S	0	0	0
			6249	3972	1069	1160	48			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	SEE REMARK 999	UNP Q9R1E6
A	?	-	VAL	SEE REMARK 999	UNP Q9R1E6
A	?	-	GLU	SEE REMARK 999	UNP Q9R1E6
A	?	-	PRO	SEE REMARK 999	UNP Q9R1E6
A	859	SER	-	EXPRESSION TAG	UNP Q9R1E6
A	860	ARG	-	EXPRESSION TAG	UNP Q9R1E6
A	861	GLU	-	EXPRESSION TAG	UNP Q9R1E6
A	862	ASN	-	EXPRESSION TAG	UNP Q9R1E6
A	863	LEU	-	EXPRESSION TAG	UNP Q9R1E6
A	864	TYR	-	EXPRESSION TAG	UNP Q9R1E6
A	865	PHE	-	EXPRESSION TAG	UNP Q9R1E6
A	866	GLN	-	EXPRESSION TAG	UNP Q9R1E6

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

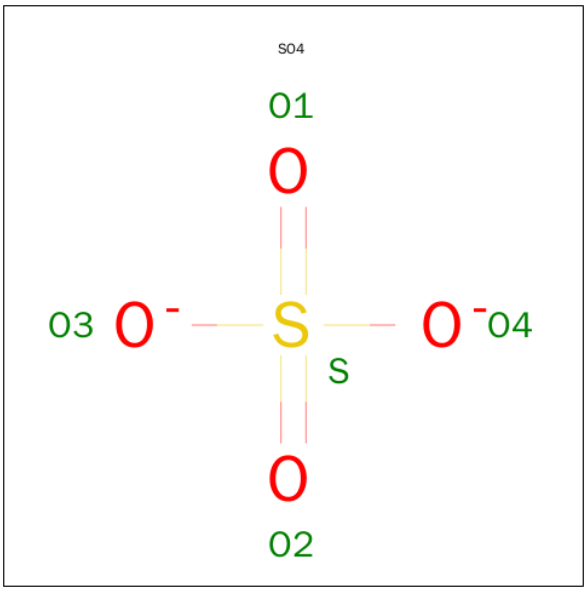
- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

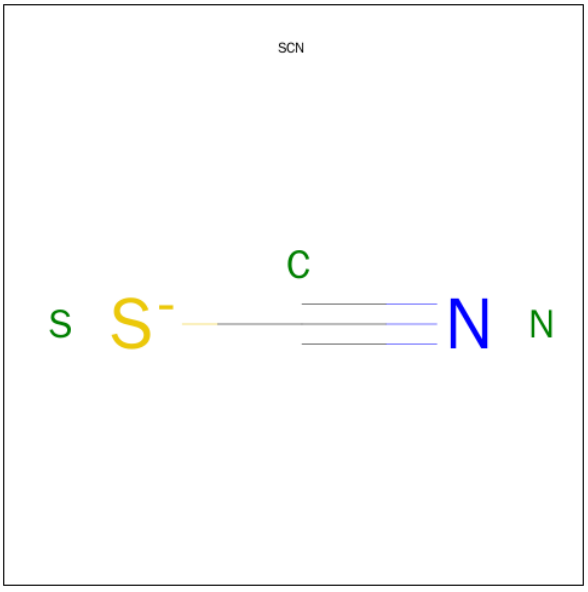
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	K	0	0
			1	1		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



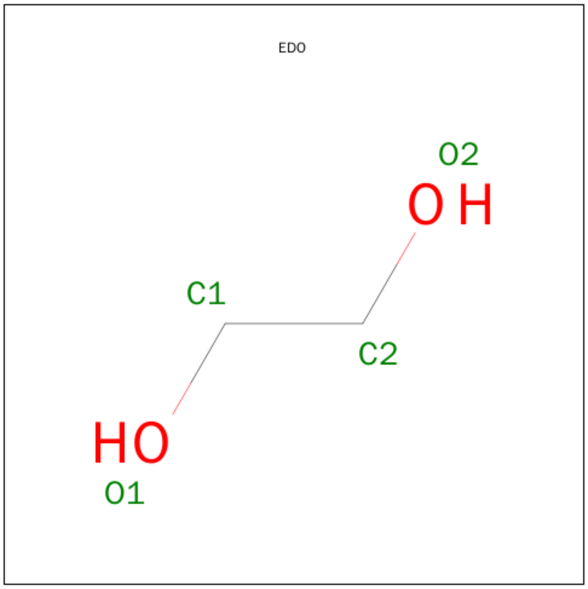
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O S 5 4 1	0	0

- Molecule 9 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C N S 3 1 1 1	0	0
9	A	1	Total C N S 3 1 1 1	0	0
9	A	1	Total C N S 3 1 1 1	0	0

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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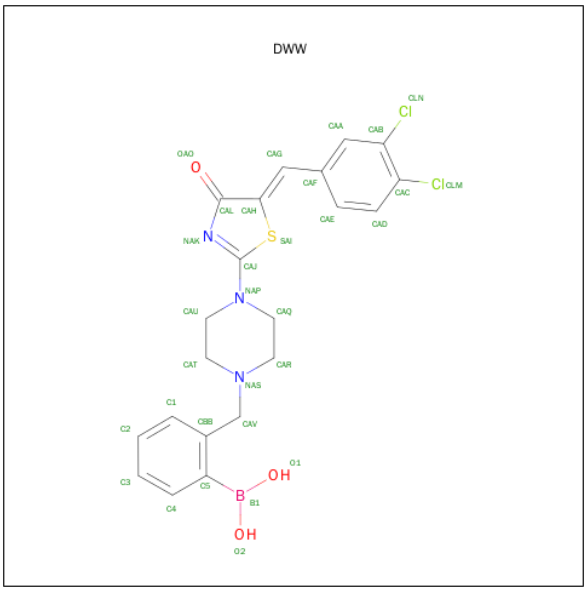
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0

- Molecule 11 is [2-({4-[(5Z)-5-(3,4-DICHLOROBENZYLIDENE)-4-OXO-4,5-DIHYDRO-1,3-THIAZOL-2-YL]PIPERAZIN-1-YL}METHYL)PHENYL]BORONIC ACID (three-letter code: DWW) (formula: $C_{21}H_{20}BCl_2N_3O_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C Cl N O S 23 16 2 3 1 1	0	0

- Molecule 12 is water.

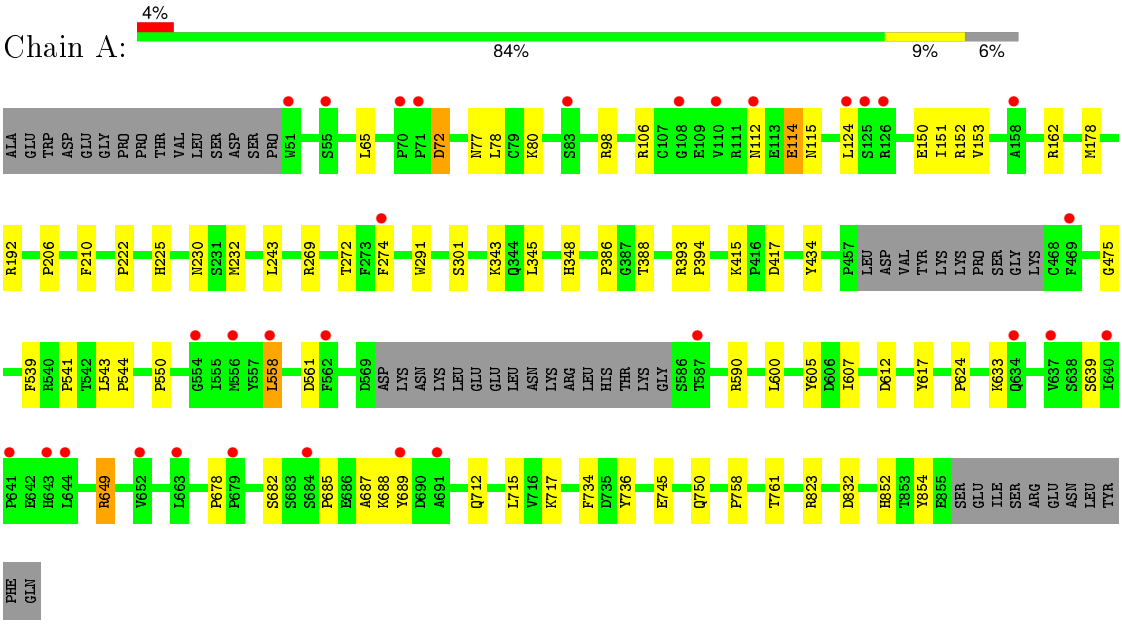
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	373	Total O 373 373	0	0

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: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.65Å 94.26Å 75.36Å 90.00° 94.73° 90.00°	Depositor
Resolution (Å)	47.13 – 1.95 47.13 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.0 (47.13-1.95) 98.0 (47.13-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.192 , 0.231 0.192 , 0.228	Depositor DCC
R_{free} test set	3081 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	29.0	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 60979 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6867	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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: ZN, BMA, NAG, NA, K, EDO, SCN, SO4, DWW, CA, MAN

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	0.34	0/6431	0.52	0/8741

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	6249	0	5947	46	0
2	A	56	0	50	0	0
3	A	83	0	70	0	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	5	0	0	0	0
9	A	9	0	0	0	0
10	A	64	0	96	6	0
11	A	23	0	14	15	0
12	A	373	0	0	1	0
All	All	6867	0	6177	60	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 (60) 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)
11:A:937:DWW:NAS	11:A:937:DWW:CAU	2.08	1.16
11:A:937:DWW:NAP	11:A:937:DWW:CAT	2.07	1.15
11:A:937:DWW:NAP	11:A:937:DWW:CAR	2.13	1.11
11:A:937:DWW:NAS	11:A:937:DWW:CAQ	2.13	1.10
11:A:937:DWW:H14	11:A:937:DWW:CAR	1.47	0.99
11:A:937:DWW:H8	11:A:937:DWW:CAU	1.47	0.98
11:A:937:DWW:H9	11:A:937:DWW:CAT	1.47	0.97
11:A:937:DWW:H10	11:A:937:DWW:CAT	1.47	0.97
11:A:937:DWW:CAQ	11:A:937:DWW:H11	1.47	0.96
11:A:937:DWW:H13	11:A:937:DWW:CAR	1.47	0.96
11:A:937:DWW:CAQ	11:A:937:DWW:H12	1.47	0.96
11:A:937:DWW:CAU	11:A:937:DWW:H7	1.47	0.96
11:A:937:DWW:CAQ	11:A:937:DWW:CAR	0.84	0.84
11:A:937:DWW:CAT	11:A:937:DWW:CAU	0.83	0.83
1:A:639:SER:O	1:A:688:LYS:NZ	2.21	0.74
1:A:78:LEU:HD21	1:A:274:PHE:HB2	1.74	0.70
1:A:600:LEU:HD11	1:A:832:ASP:HB2	1.74	0.70
1:A:77:ASN:HD21	1:A:272:THR:HB	1.58	0.67
1:A:649:ARG:NH1	1:A:689:TYR:O	2.29	0.66
1:A:678:PRO:HB3	1:A:712:GLN:HB3	1.81	0.63
1:A:178:MET:HE2	1:A:192:ARG:HD3	1.80	0.62
1:A:150:GLU:OE1	1:A:152:ARG:NH1	2.34	0.61
1:A:210:PHE:HE2	1:A:243:LEU:HD23	1.66	0.60
1:A:550:PRO:HB2	1:A:607:ILE:HG12	1.86	0.57
1:A:112:ASN:HD21	1:A:114:GLU:HB3	1.69	0.57
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.40	0.56
1:A:682:SER:OG	1:A:688:LYS:HG2	2.06	0.56
1:A:758:PRO:HD3	10:A:930:EDO:H22	1.88	0.56
1:A:633:LYS:O	1:A:717:LYS:NZ	2.40	0.55
1:A:550:PRO:HB3	1:A:605:TYR:CE2	2.42	0.55
1:A:210:PHE:CE2	1:A:243:LEU:HD23	2.44	0.52
1:A:274:PHE:CE1	11:A:937:DWW:H25	2.46	0.51
1:A:852:HIS:HD2	1:A:854:TYR:CZ	2.29	0.51
1:A:151:ILE:HD12	10:A:922:EDO:H21	1.92	0.51
1:A:98:ARG:HD3	1:A:115:ASN:OD1	2.11	0.50
1:A:745:GLU:OE2	10:A:930:EDO:O1	2.26	0.50
1:A:80:LYS:NZ	12:A:1348:HOH:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:734:PHE:CD1	10:A:924:EDO:H11	2.48	0.49
1:A:612:ASP:OD2	1:A:687:ALA:HB1	2.13	0.49
1:A:685:PRO:O	1:A:689:TYR:HD1	1.96	0.48
1:A:558:LEU:HD12	1:A:561:ASP:OD2	2.14	0.48
1:A:761:THR:HA	10:A:926:EDO:H12	1.96	0.47
1:A:230:ASN:HB3	1:A:243:LEU:HG	1.95	0.47
1:A:685:PRO:HA	1:A:688:LYS:HG3	1.96	0.47
1:A:417:ASP:OD1	1:A:417:ASP:N	2.50	0.45
1:A:543:LEU:HD12	1:A:544:PRO:HD2	1.98	0.44
1:A:206:PRO:HD3	1:A:434:TYR:CE1	2.52	0.44
1:A:98:ARG:HH21	1:A:106:ARG:HG2	1.82	0.44
1:A:72:ASP:OD1	1:A:72:ASP:N	2.50	0.43
1:A:617:TYR:HA	1:A:624:PRO:HA	2.00	0.43
1:A:65:LEU:HD21	1:A:291:TRP:CE2	2.54	0.42
1:A:343:LYS:HA	1:A:348:HIS:ND1	2.35	0.42
1:A:388:THR:OG1	1:A:475:GLY:HA3	2.20	0.42
1:A:736:TYR:OH	1:A:750:GLN:HB3	2.19	0.42
1:A:162:ARG:NH2	1:A:301:SER:OG	2.52	0.42
1:A:539:PHE:O	1:A:541:PRO:HD3	2.20	0.41
1:A:393:ARG:HB2	1:A:394:PRO:HD2	2.02	0.41
1:A:715:LEU:HA	1:A:715:LEU:HD23	1.88	0.41
1:A:415:LYS:HB2	1:A:415:LYS:HE3	1.77	0.41
1:A:823:ARG:CZ	10:A:921:EDO:H11	2.50	0.41

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	773/831 (93%)	746 (96%)	26 (3%)	1 (0%)	56 48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	386	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	696/756 (92%)	686 (99%)	10 (1%)	74 70

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ASP
1	A	114	GLU
1	A	124	LEU
1	A	153	VAL
1	A	232	MET
1	A	269	ARG
1	A	345	LEU
1	A	558	LEU
1	A	590	ARG
1	A	649	ARG

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

Mol	Chain	Res	Type
1	A	112	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)

11 carbohydrates 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	NAG	A	901	1,2	14,14,15	0.49	0	15,19,21	1.16	1 (6%)
2	NAG	A	902	2	14,14,15	0.53	0	15,19,21	0.85	1 (6%)
3	NAG	A	903	1,3	14,14,15	0.53	0	15,19,21	0.90	1 (6%)
3	NAG	A	904	3	14,14,15	0.62	0	15,19,21	0.72	0
3	BMA	A	905	3	11,11,12	0.64	0	14,15,17	0.92	0
3	MAN	A	906	3	11,11,12	0.64	0	14,15,17	0.97	2 (14%)
3	MAN	A	907	3	11,11,12	0.52	0	14,15,17	0.88	0
3	MAN	A	908	3	11,11,12	0.57	0	14,15,17	0.76	0
3	MAN	A	909	3	11,11,12	0.70	0	14,15,17	0.94	1 (7%)
2	NAG	A	910	1,2	14,14,15	0.46	0	15,19,21	1.00	1 (6%)
2	NAG	A	911	2	14,14,15	0.39	0	15,19,21	1.77	1 (6%)

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
2	NAG	A	901	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	902	2	-	0/6/23/26	0/1/1/1
3	NAG	A	903	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	904	3	-	0/6/23/26	0/1/1/1
3	BMA	A	905	3	-	0/2/19/22	0/1/1/1
3	MAN	A	906	3	-	0/2/19/22	0/1/1/1
3	MAN	A	907	3	-	0/2/19/22	0/1/1/1
3	MAN	A	908	3	-	0/2/19/22	0/1/1/1
3	MAN	A	909	3	-	0/2/19/22	0/1/1/1
2	NAG	A	910	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	911	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	903	NAG	O4-C4-C3	-2.25	105.27	110.34
3	A	906	MAN	O5-C5-C6	2.05	111.78	107.35
3	A	906	MAN	C1-C2-C3	2.07	112.00	109.54
2	A	902	NAG	C1-O5-C5	2.08	114.89	112.25
3	A	909	MAN	C1-C2-C3	2.43	112.42	109.54
2	A	910	NAG	C1-O5-C5	2.47	115.38	112.25
2	A	901	NAG	C1-O5-C5	3.72	116.97	112.25
2	A	911	NAG	C1-O5-C5	6.25	120.18	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 5 are monoatomic - leaving 21 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	$\#\|Z\| > 2$
8	SO4	A	917	4	4,4,4	0.42	0	6,6,6	0.40	0
9	SCN	A	918	-	2,2,2	1.86	1 (50%)	1,1,1	0.30	0
9	SCN	A	919	-	2,2,2	2.12	1 (50%)	1,1,1	0.51	0
9	SCN	A	920	-	2,2,2	1.67	1 (50%)	1,1,1	0.04	0
10	EDO	A	921	-	3,3,3	0.47	0	2,2,2	0.54	0
10	EDO	A	922	-	3,3,3	0.61	0	2,2,2	0.09	0
10	EDO	A	923	-	3,3,3	0.40	0	2,2,2	0.59	0
10	EDO	A	924	-	3,3,3	0.49	0	2,2,2	0.48	0
10	EDO	A	925	-	3,3,3	0.51	0	2,2,2	0.38	0
10	EDO	A	926	-	3,3,3	0.44	0	2,2,2	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	EDO	A	927	-	3,3,3	0.51	0	2,2,2	0.46	0
10	EDO	A	928	-	3,3,3	0.49	0	2,2,2	0.39	0
10	EDO	A	929	-	3,3,3	0.51	0	2,2,2	0.40	0
10	EDO	A	930	-	3,3,3	0.44	0	2,2,2	0.52	0
10	EDO	A	931	-	3,3,3	0.54	0	2,2,2	0.37	0
10	EDO	A	932	-	3,3,3	0.50	0	2,2,2	0.50	0
10	EDO	A	933	-	3,3,3	0.50	0	2,2,2	0.42	0
10	EDO	A	934	-	3,3,3	0.52	0	2,2,2	0.35	0
10	EDO	A	935	-	3,3,3	0.45	0	2,2,2	0.49	0
10	EDO	A	936	-	3,3,3	0.43	0	2,2,2	0.58	0
11	DWW	A	937	-	24,25,34	6.43	12 (50%)	30,35,48	3.32	11 (36%)

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
8	SO4	A	917	4	-	0/0/0/0	0/0/0/0
9	SCN	A	918	-	-	0/0/0/0	0/0/0/0
9	SCN	A	919	-	-	0/0/0/0	0/0/0/0
9	SCN	A	920	-	-	0/0/0/0	0/0/0/0
10	EDO	A	921	-	-	0/1/1/1	0/0/0/0
10	EDO	A	922	-	-	0/1/1/1	0/0/0/0
10	EDO	A	923	-	-	0/1/1/1	0/0/0/0
10	EDO	A	924	-	-	0/1/1/1	0/0/0/0
10	EDO	A	925	-	-	0/1/1/1	0/0/0/0
10	EDO	A	926	-	-	0/1/1/1	0/0/0/0
10	EDO	A	927	-	-	0/1/1/1	0/0/0/0
10	EDO	A	928	-	-	0/1/1/1	0/0/0/0
10	EDO	A	929	-	-	0/1/1/1	0/0/0/0
10	EDO	A	930	-	-	0/1/1/1	0/0/0/0
10	EDO	A	931	-	-	0/1/1/1	0/0/0/0
10	EDO	A	932	-	-	0/1/1/1	0/0/0/0
10	EDO	A	933	-	-	0/1/1/1	0/0/0/0
10	EDO	A	934	-	-	0/1/1/1	0/0/0/0
10	EDO	A	935	-	-	0/1/1/1	0/0/0/0
10	EDO	A	936	-	-	0/1/1/1	0/0/0/0
11	DWW	A	937	-	-	0/8/32/38	0/3/3/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	937	DWW	CAU-CAT	-16.65	0.83	1.51
11	A	937	DWW	CAQ-CAR	-16.35	0.84	1.51
11	A	937	DWW	CAJ-SAI	-2.38	1.69	1.74
11	A	937	DWW	CBB-CAV	-2.20	1.36	1.49
11	A	937	DWW	CAJ-NAK	2.15	1.36	1.32
9	A	920	SCN	C-S	2.30	1.78	1.63
9	A	918	SCN	C-S	2.59	1.80	1.63
9	A	919	SCN	C-S	2.95	1.82	1.63
11	A	937	DWW	CAJ-NAP	3.96	1.45	1.34
11	A	937	DWW	CAT-NAS	5.29	1.61	1.46
11	A	937	DWW	CAR-NAS	5.53	1.62	1.46
11	A	937	DWW	OAO-CAL	8.14	1.38	1.24
11	A	937	DWW	CAU-NAP	8.17	1.61	1.47
11	A	937	DWW	CAQ-NAP	8.65	1.62	1.47
11	A	937	DWW	CAG-CAH	11.95	1.49	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	937	DWW	CAF-CAG-CAH	-8.63	119.05	130.96
11	A	937	DWW	SAI-CAJ-NAK	-5.80	107.91	116.22
11	A	937	DWW	CAQ-NAP-CAJ	-4.08	111.55	121.89
11	A	937	DWW	CAT-NAS-CAV	2.17	115.90	110.83
11	A	937	DWW	NAP-CAJ-NAK	2.50	126.45	123.06
11	A	937	DWW	CAR-CAQ-NAP	2.59	116.38	110.49
11	A	937	DWW	CAQ-CAR-NAS	3.23	116.42	110.63
11	A	937	DWW	SAI-CAJ-NAP	4.48	125.62	120.73
11	A	937	DWW	CAJ-SAI-CAH	4.94	96.57	90.77
11	A	937	DWW	CAU-NAP-CAJ	5.58	136.06	121.89
11	A	937	DWW	CAR-NAS-CAV	9.11	132.12	110.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	921	EDO	1	0
10	A	922	EDO	1	0
10	A	924	EDO	1	0
10	A	926	EDO	1	0
10	A	930	EDO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	937	DWW	15	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	779/831 (93%)	0.15	31 (3%) 42 53	17, 36, 65, 77	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	TRP	5.3
1	A	644	LEU	4.9
1	A	640	ILE	4.7
1	A	637	VAL	4.2
1	A	554	GLY	4.1
1	A	652	VAL	4.0
1	A	71	PRO	3.8
1	A	110	VAL	3.8
1	A	125	SER	3.8
1	A	556	MET	3.6
1	A	469	PHE	3.5
1	A	641	PRO	3.4
1	A	55	SER	3.2
1	A	679	PRO	3.0
1	A	70	PRO	3.0
1	A	634	GLN	2.7
1	A	274	PHE	2.7
1	A	689	TYR	2.7
1	A	587	THR	2.6
1	A	691	ALA	2.5
1	A	83	SER	2.5
1	A	126	ARG	2.4
1	A	158	ALA	2.4
1	A	684	SER	2.2
1	A	108	GLY	2.2
1	A	562	PHE	2.2
1	A	643	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	112	ASN	2.1
1	A	558	LEU	2.0
1	A	663	LEU	2.0
1	A	124	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)

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
3	MAN	A	907	11/12	0.94	0.14	5.12	40,46,55,62	0
2	NAG	A	910	14/15	0.94	0.09	0.27	30,37,48,49	0
2	NAG	A	901	14/15	0.88	0.21	0.04	68,73,76,81	0
3	NAG	A	903	14/15	0.98	0.10	-0.54	16,24,30,31	0
3	MAN	A	908	11/12	0.92	0.09	-	31,41,45,49	0
3	MAN	A	909	11/12	0.79	0.13	-	74,76,81,82	0
3	NAG	A	904	14/15	0.96	0.09	-	28,36,45,47	0
2	NAG	A	902	14/15	0.84	0.16	-	74,81,85,86	0
3	BMA	A	905	11/12	0.90	0.09	-	50,57,65,72	0
2	NAG	A	911	14/15	0.84	0.14	-	51,60,64,65	0
3	MAN	A	906	11/12	0.91	0.09	-	46,50,53,54	0

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
10	EDO	A	924	4/4	0.90	0.20	18.03	35,36,40,41	0
10	EDO	A	929	4/4	0.86	0.16	7.98	34,39,40,46	0
10	EDO	A	928	4/4	0.95	0.15	7.26	29,34,36,37	0
10	EDO	A	926	4/4	0.90	0.23	4.05	32,36,42,46	0
10	EDO	A	921	4/4	0.95	0.15	3.06	31,34,38,41	0
9	SCN	A	920	3/3	0.93	0.14	2.87	33,33,42,49	0
9	SCN	A	919	3/3	0.98	0.16	2.68	32,32,47,66	0
10	EDO	A	931	4/4	0.93	0.12	2.42	31,37,41,43	0
10	EDO	A	927	4/4	0.94	0.12	2.13	33,33,34,38	0
10	EDO	A	930	4/4	0.92	0.16	1.67	45,46,46,54	0
11	DWW	A	937	23/31	0.86	0.16	1.38	38,48,59,72	0
10	EDO	A	933	4/4	0.92	0.12	0.95	38,41,50,52	0
10	EDO	A	925	4/4	0.94	0.13	0.93	39,40,41,44	0
9	SCN	A	918	3/3	0.89	0.12	0.87	47,47,50,50	0
10	EDO	A	922	4/4	0.89	0.13	0.56	35,36,39,42	0
10	EDO	A	923	4/4	0.88	0.14	0.06	38,38,41,53	0
4	ZN	A	913	1/1	1.00	0.12	-0.43	20,20,20,20	0
10	EDO	A	935	4/4	0.97	0.07	-1.14	29,31,33,38	0
7	K	A	916	1/1	0.93	0.06	-1.38	65,65,65,65	0
5	CA	A	914	1/1	0.99	0.07	-1.49	29,29,29,29	0
10	EDO	A	934	4/4	0.99	0.06	-1.59	25,26,26,30	0
8	SO4	A	917	5/5	0.97	0.09	-1.83	27,28,33,36	0
4	ZN	A	912	1/1	0.99	0.11	-1.87	25,25,25,25	0
6	NA	A	915	1/1	0.97	0.05	-2.71	30,30,30,30	0
10	EDO	A	936	4/4	0.95	0.11	-	31,33,34,50	0
10	EDO	A	932	4/4	0.96	0.12	-	37,41,47,54	0

6.5 Other polymers (i)

There are no such residues in this entry.