



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:27 PM GMT

PDB ID : 4ZG6
Title : Structural basis for inhibition of human autotaxin by four novel compounds
Authors : Stein, A.J.; Bain, G.; Hutchinson, J.H.; Evans, J.F.
Deposited on : 2015-04-22
Resolution : 1.80 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

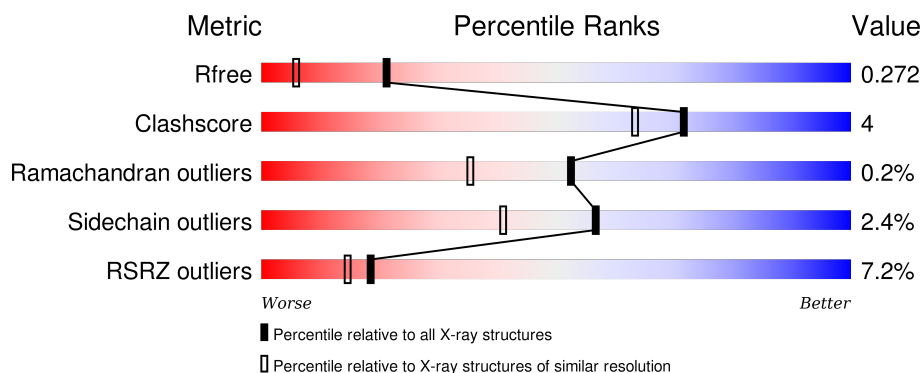
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 $\leq 5\%$. 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	855	<div> <div>7%</div> <div>78%</div> <div>9%</div> <div>12%</div> </div>
1	B	855	<div> <div>6%</div> <div>82%</div> <div>6%</div> <div>12%</div> </div>

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
7	GOL	A	909	-	-	X	-
7	GOL	B	909	-	-	X	-
9	SCN	A	916	-	-	-	X
9	SCN	A	917	-	-	-	X
9	SCN	B	912	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12830 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	754	Total	C	N	O	S	0	7	0
			6004	3826	1019	1115	44			
1	B	756	Total	C	N	O	S	0	6	0
			6014	3829	1025	1112	48			

There are 18 discrepancies between the modelled and reference sequences:

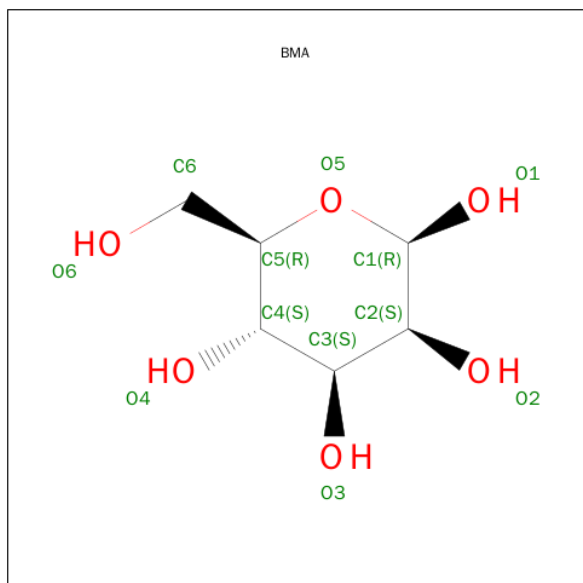
Chain	Residue	Modelled	Actual	Comment	Reference
A	411	ALA	ASN	engineered mutation	UNP Q13822
A	864	HIS	-	expression tag	UNP Q13822
A	865	HIS	-	expression tag	UNP Q13822
A	866	HIS	-	expression tag	UNP Q13822
A	867	HIS	-	expression tag	UNP Q13822
A	868	HIS	-	expression tag	UNP Q13822
A	869	HIS	-	expression tag	UNP Q13822
A	870	HIS	-	expression tag	UNP Q13822
A	871	HIS	-	expression tag	UNP Q13822
B	411	ALA	ASN	engineered mutation	UNP Q13822
B	864	HIS	-	expression tag	UNP Q13822
B	865	HIS	-	expression tag	UNP Q13822
B	866	HIS	-	expression tag	UNP Q13822
B	867	HIS	-	expression tag	UNP Q13822
B	868	HIS	-	expression tag	UNP Q13822
B	869	HIS	-	expression tag	UNP Q13822
B	870	HIS	-	expression tag	UNP Q13822
B	871	HIS	-	expression tag	UNP Q13822

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

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

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

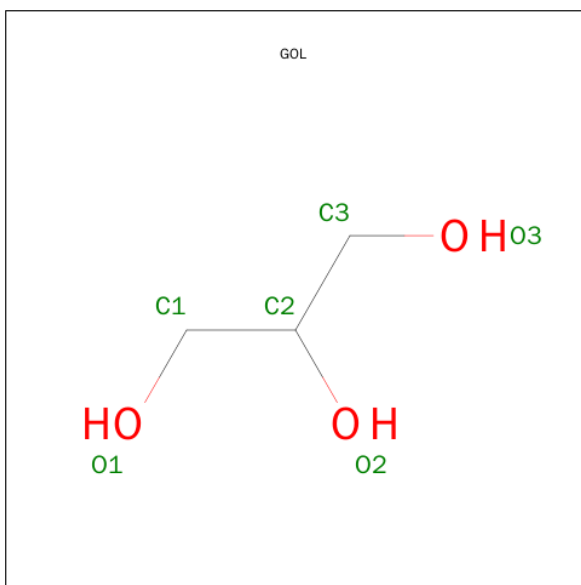
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

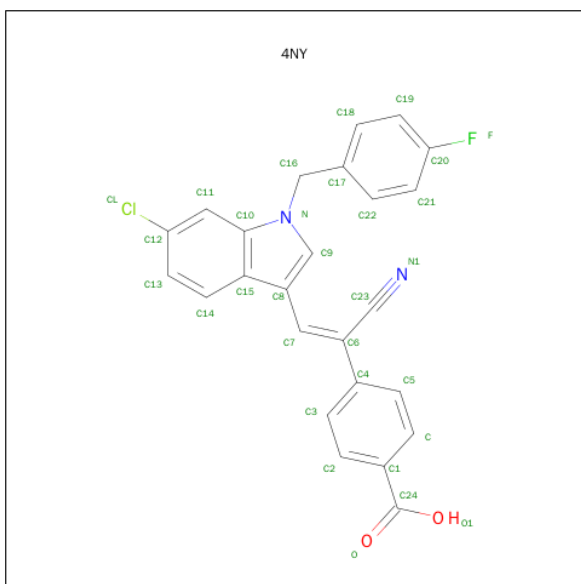
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Na	0	0
			2	2		
6	A	2	Total	Na	0	0
			2	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 8 is 4-{(Z)-2-[6-chloro-1-(4-fluorobenzyl)-1H-indol-3-yl]-1-cyanoethenyl}benzoic acid (three-letter code: 4NY) (formula: C₂₅H₁₆ClFN₂O₂).



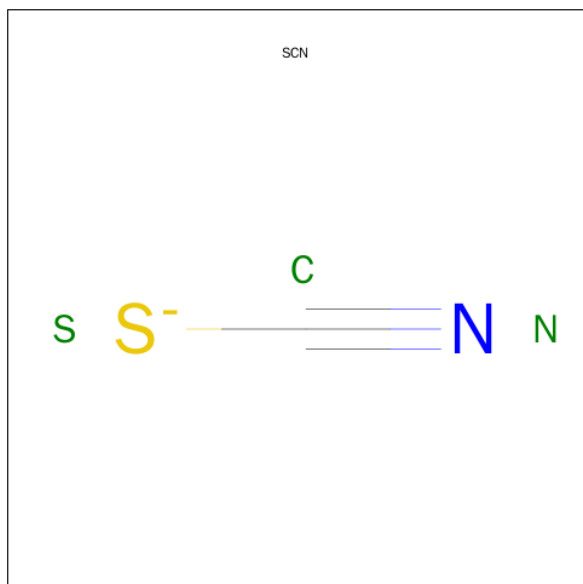
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	A	1	Total	C	Cl	F	N	O	0	0
			31	25	1	1	2	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	Cl	F	N	O	
			31	25	1	1	2	2	
								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	0	0
			3	1	1	1		
9	A	1	Total	C	N	S	0	0
			3	1	1	1		
9	A	1	Total	C	N	S	0	0
			3	1	1	1		
9	A	1	Total	C	N	S	0	0
			3	1	1	1		
9	A	1	Total	C	N	S	0	0
			3	1	1	1		
9	A	1	Total	C	N	S	0	0
			3	1	1	1		
9	B	1	Total	C	N	S	0	0
			3	1	1	1		
9	B	1	Total	C	N	S	0	0
			3	1	1	1		
9	B	1	Total	C	N	S	0	0
			3	1	1	1		

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

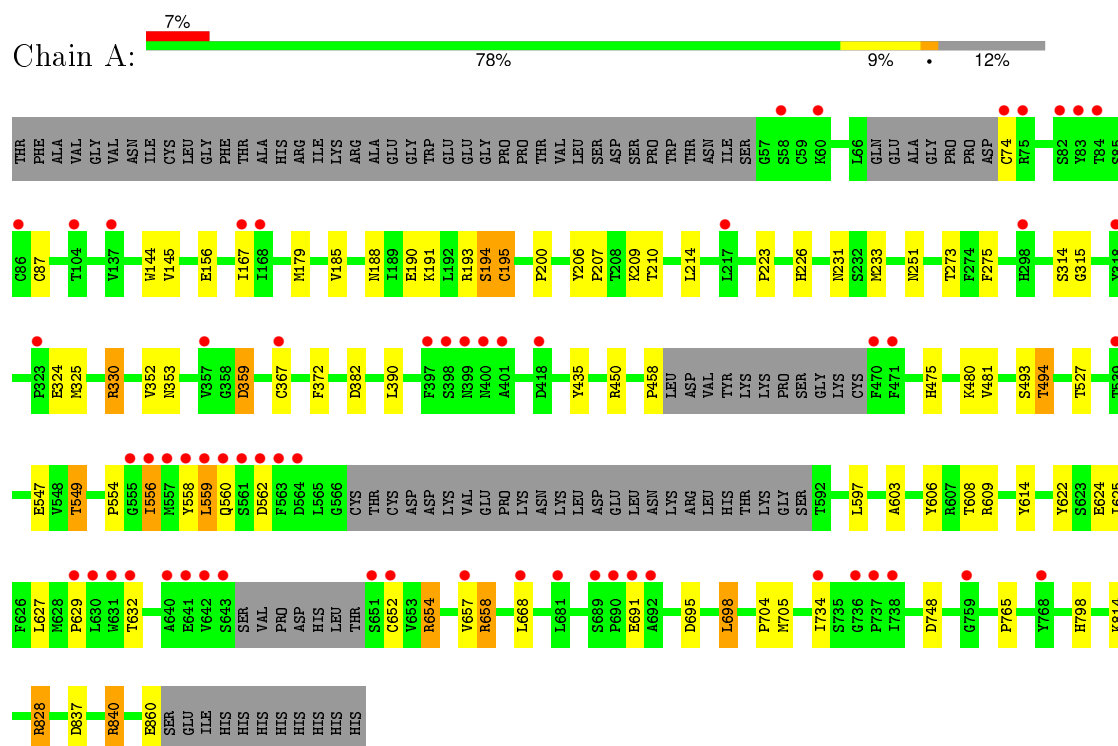
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	293	Total	O	0	0
			293	293		
10	B	321	Total	O	0	0
			321	321		

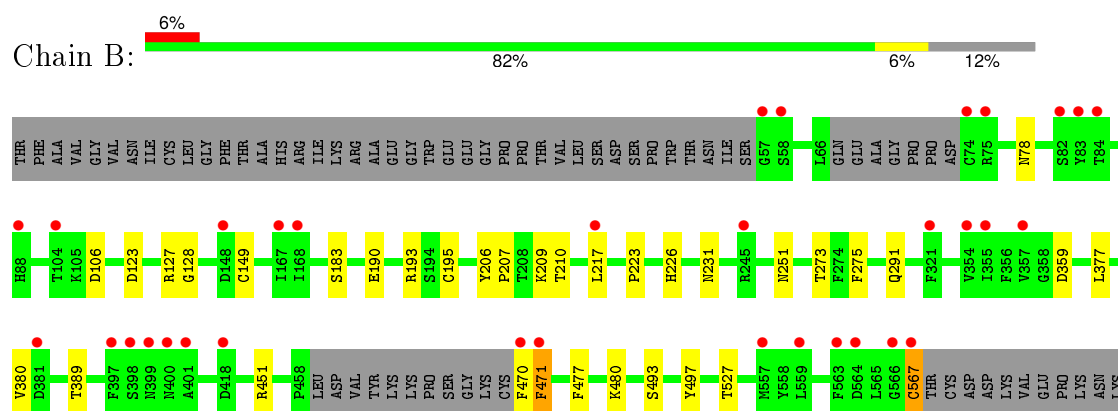
3 Residue-property plots [i](#)

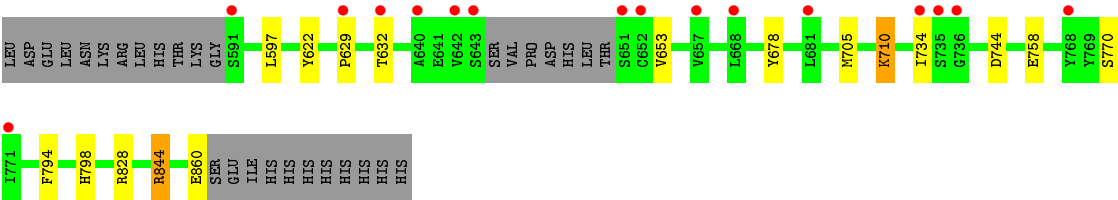
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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



- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.62Å 70.49Å 107.37Å 104.65° 99.27° 99.86°	Depositor
Resolution (Å)	34.69 – 1.80 34.69 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.0 (34.69-1.80) 86.8 (34.69-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.220 , 0.265 0.227 , 0.272	Depositor DCC
R_{free} test set	7755 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 154080 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12830	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 92.22 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.0268e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, BMA, NAG, NA, CA, 4NY, SCN

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	1/6195 (0.0%)	0.72	2/8424 (0.0%)
1	B	0.57	0/6203	0.74	3/8433 (0.0%)
All	All	0.58	1/12398 (0.0%)	0.73	5/16857 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	200	PRO	N-CD	5.55	1.55	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	ASP	CB-CG-OD1	5.75	123.48	118.30
1	B	195[A]	CYS	CA-CB-SG	5.75	124.34	114.00
1	B	195[B]	CYS	CA-CB-SG	5.75	124.34	114.00
1	B	744	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	748	ASP	CB-CG-OD2	-5.07	113.74	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6004	0	5667	64	0
1	B	6014	0	5668	32	0
2	A	28	0	24	0	0
2	B	28	0	24	0	0
3	A	11	0	10	0	0
3	B	11	0	10	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	A	6	0	7	4	0
7	B	6	0	7	5	0
8	A	31	0	15	3	0
8	B	31	0	15	5	0
9	A	21	0	0	1	0
9	B	15	0	0	2	0
10	A	293	0	0	7	0
10	B	321	0	0	7	0
All	All	12830	0	11447	102	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 4.

All (102) 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:559:LEU:O	1:A:562:ASP:HB2	1.62	0.99
1:A:353:ASN:HD21	1:A:494:THR:HG23	1.28	0.97
1:A:251[B]:ASN:OD1	10:A:1002:HOH:O	1.82	0.97
1:A:494:THR:HG21	10:A:1202:HOH:O	1.72	0.88
1:A:353:ASN:HD21	1:A:494:THR:CG2	1.86	0.88
1:B:844:ARG:NH1	10:B:1002:HOH:O	2.07	0.87
1:A:353:ASN:ND2	1:A:494:THR:HG23	1.90	0.86
8:A:910:4NY:O1	10:A:1003:HOH:O	1.94	0.85
1:B:231:ASN:ND2	7:B:909:GOL:O1	2.10	0.84
1:A:556:ILE:HG23	1:A:657:VAL:HG11	1.63	0.79
1:A:559:LEU:N	1:A:562:ASP:OD2	2.14	0.79
1:B:251[B]:ASN:OD1	10:B:1001:HOH:O	2.01	0.78
1:A:231:ASN:ND2	7:A:909:GOL:O1	2.12	0.78
1:A:559:LEU:HB2	1:A:562:ASP:OD2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:LYS:HG3	9:A:915:SCN:N	2.00	0.76
9:B:912:SCN:S	10:B:1002:HOH:O	2.48	0.70
1:A:549:THR:HG23	1:A:606:TYR:O	1.91	0.69
1:B:480:LYS:O	1:B:860:GLU:HG3	1.92	0.68
1:A:556:ILE:HG23	1:A:657:VAL:CG1	2.24	0.68
1:A:549:THR:HG21	1:A:608:THR:H	1.58	0.67
1:A:475:HIS:CD2	10:A:1001:HOH:O	2.46	0.67
1:B:128:GLY:O	1:B:291:GLN:HG2	1.95	0.67
1:A:314:SER:C	1:A:325:MET:HE1	2.15	0.66
1:A:156:GLU:OE2	10:A:1004:HOH:O	2.14	0.64
1:B:149[B]:CYS:SG	1:B:497:TYR:HE1	2.22	0.63
1:A:475:HIS:HE1	7:A:909:GOL:H11	1.64	0.63
1:B:149[B]:CYS:SG	1:B:497:TYR:CE1	2.94	0.60
1:B:209:LYS:HG3	9:B:914:SCN:N	2.16	0.59
1:A:559:LEU:O	1:A:562:ASP:CB	2.44	0.59
1:B:223:PRO:HA	1:B:226:HIS:CE1	2.38	0.59
1:A:475:HIS:CE1	7:A:909:GOL:H11	2.38	0.58
1:B:210:THR:HB	7:B:909:GOL:H12	1.84	0.58
1:B:527:THR:OG1	1:B:828[A]:ARG:HD3	2.03	0.58
1:A:273:THR:HG22	1:A:275:PHE:H	1.70	0.56
1:A:223:PRO:HA	1:A:226:HIS:CE1	2.40	0.56
1:A:372:PHE:CE1	1:A:458:PRO:HA	2.40	0.55
1:B:217[B]:LEU:HD11	10:B:1040:HOH:O	2.05	0.55
1:B:567:CYS:SG	1:B:653:VAL:HB	2.46	0.55
1:B:231:ASN:HD21	7:B:909:GOL:C1	2.19	0.55
1:A:273:THR:O	10:A:1005:HOH:O	2.18	0.55
1:A:652:CYS:SG	1:A:654:ARG:HG2	2.47	0.55
1:B:217[B]:LEU:CD1	8:B:910:4NY:CL	2.91	0.54
1:B:190:GLU:OE2	1:B:193:ARG:NH1	2.41	0.53
1:A:695:ASP:HA	1:A:698:LEU:HD23	1.91	0.53
1:A:559:LEU:CB	1:A:562:ASP:OD2	2.55	0.53
1:B:210:THR:CB	7:B:909:GOL:H12	2.39	0.53
1:A:549:THR:CG2	1:A:606:TYR:O	2.56	0.52
1:B:217[B]:LEU:HD21	10:B:1040:HOH:O	2.09	0.52
1:A:554:PRO:HB2	1:A:658:ARG:HB3	1.91	0.52
8:B:910:4NY:O1	10:B:1003:HOH:O	2.19	0.51
1:A:609:ARG:NH1	1:A:624:GLU:OE1	2.35	0.51
1:A:179:MET:CE	1:A:193:ARG:HD2	2.40	0.51
1:A:558:TYR:O	1:A:657:VAL:CG1	2.59	0.50
1:A:144:TRP:O	1:A:191:LYS:NZ	2.45	0.50
1:B:123:ASP:O	1:B:127:ARG:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217[B]:LEU:HD12	8:B:910:4NY:CL	2.49	0.50
1:B:359:ASP:HB3	8:B:910:4NY:CL	2.50	0.49
7:B:909:GOL:H31	10:B:1266:HOH:O	2.13	0.49
1:B:770:SER:HB2	1:B:794:PHE:CZ	2.48	0.49
1:A:190:GLU:O	1:A:194[A]:SER:OG	2.28	0.49
1:A:559:LEU:O	1:A:562:ASP:N	2.43	0.48
1:A:558:TYR:O	1:A:657:VAL:HG13	2.14	0.48
1:B:622:TYR:HA	1:B:629:PRO:HA	1.95	0.48
1:A:190:GLU:OE2	1:A:193:ARG:NH1	2.47	0.48
1:B:678:TYR:O	1:B:710:LYS:HE2	2.15	0.47
1:A:480:LYS:O	1:A:860:GLU:HG3	2.13	0.47
1:A:179:MET:HE2	1:A:193:ARG:HD2	1.96	0.47
1:A:622:TYR:HA	1:A:629:PRO:HA	1.97	0.47
1:A:185:VAL:O	1:A:330:ARG:CG	2.63	0.46
1:A:74:CYS:SG	1:A:87:CYS:N	2.88	0.46
1:A:191:LYS:O	1:A:195:CYS:HB2	2.17	0.45
1:A:359:ASP:HB3	8:A:910:4NY:CL	2.53	0.45
1:A:210:THR:OG1	7:A:909:GOL:H12	2.17	0.45
1:B:206:TYR:CD1	1:B:207:PRO:HA	2.52	0.45
1:B:470:PHE:O	1:B:471:PHE:HB3	2.15	0.45
1:A:559:LEU:O	1:A:560:GLN:C	2.55	0.45
1:B:377:LEU:HB2	1:B:380:VAL:HG23	1.99	0.45
1:B:273:THR:HG22	1:B:275:PHE:H	1.82	0.44
1:A:837:ASP:OD2	1:A:840:ARG:HD2	2.18	0.44
1:B:389:THR:HG22	1:B:477:PHE:CZ	2.52	0.44
1:A:167:ILE:HD12	1:A:352:VAL:HG11	1.99	0.44
1:A:608:THR:HG22	1:A:625:ILE:HG13	1.99	0.44
1:A:705:MET:HA	1:A:798:HIS:NE2	2.32	0.43
1:A:315:GLY:N	1:A:325:MET:HE1	2.34	0.43
8:B:910:4NY:C23	8:B:910:4NY:C9	2.97	0.43
1:A:704:PRO:HG2	1:A:765:PRO:HD3	2.01	0.43
1:B:632:THR:O	1:B:734:ILE:HA	2.19	0.43
1:A:206:TYR:CD1	1:A:207:PRO:HA	2.54	0.42
1:A:185:VAL:O	1:A:330:ARG:HG2	2.20	0.42
1:A:527:THR:OG1	1:A:828[A]:ARG:HD3	2.20	0.42
1:A:632:THR:O	1:A:734:ILE:HA	2.19	0.41
1:A:559:LEU:CA	1:A:562:ASP:OD2	2.68	0.41
1:A:547:GLU:HG2	1:A:603:ALA:HB1	2.01	0.41
1:A:840:ARG:HG3	10:A:1179:HOH:O	2.20	0.41
1:B:183:SER:N	1:B:190:GLU:HG3	2.36	0.41
1:A:614:TYR:O	1:A:658:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:VAL:HB	1:A:188:ASN:OD1	2.21	0.40
1:A:450:ARG:NH1	1:A:481:VAL:HG13	2.36	0.40
8:A:910:4NY:C9	8:A:910:4NY:C23	3.00	0.40
1:A:185:VAL:O	1:A:330:ARG:HG3	2.21	0.40
1:A:207:PRO:HD3	1:A:435:TYR:CE1	2.57	0.40
1:B:705:MET:HA	1:B:798:HIS:NE2	2.36	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	751/855 (88%)	721 (96%)	29 (4%)	1 (0%)	56	38
1	B	752/855 (88%)	725 (96%)	25 (3%)	2 (0%)	46	29
All	All	1503/1710 (88%)	1446 (96%)	54 (4%)	3 (0%)	52	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	556	ILE
1	B	78	ASN
1	B	471	PHE

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	656/772 (85%)	631 (96%)	25 (4%)	40	22
1	B	657/772 (85%)	649 (99%)	8 (1%)	78	71
All	All	1313/1544 (85%)	1280 (98%)	33 (2%)	57	39

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194[A]	SER
1	A	194[B]	SER
1	A	195	CYS
1	A	214	LEU
1	A	233	MET
1	A	324	GLU
1	A	330	ARG
1	A	367	CYS
1	A	382	ASP
1	A	390	LEU
1	A	493	SER
1	A	494	THR
1	A	549	THR
1	A	559	LEU
1	A	597	LEU
1	A	627	LEU
1	A	654	ARG
1	A	658	ARG
1	A	668	LEU
1	A	691	GLU
1	A	698	LEU
1	A	814	LYS
1	A	828[A]	ARG
1	A	828[B]	ARG
1	A	840	ARG
1	B	106	ASP
1	B	451	ARG
1	B	493	SER
1	B	567	CYS
1	B	597	LEU
1	B	710	LYS
1	B	758	GLU
1	B	844	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	ASN
1	A	747	HIS
1	B	231	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 10 are monoatomic - leaving 22 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	NAG	A	901	1,2	14,14,15	1.04	1 (7%)	15,19,21	0.90	0
2	NAG	A	902	3,2	14,14,15	0.99	1 (7%)	15,19,21	1.38	3 (20%)
3	BMA	A	903	2	11,11,12	0.47	0	15,15,17	0.79	1 (6%)
7	GOL	A	909	-	5,5,5	0.55	0	5,5,5	1.39	1 (20%)
8	4NY	A	910	-	30,34,34	2.70	5 (16%)	40,48,48	1.99	8 (20%)
9	SCN	A	911	-	2,2,2	1.63	1 (50%)	1,1,1	0.40	0
9	SCN	A	912	-	2,2,2	1.54	1 (50%)	1,1,1	0.19	0
9	SCN	A	913	-	2,2,2	1.56	1 (50%)	1,1,1	0.41	0
9	SCN	A	914	-	2,2,2	1.63	1 (50%)	1,1,1	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SCN	A	915	-	2,2,2	1.72	1 (50%)	1,1,1	0.28	0
9	SCN	A	916	-	2,2,2	1.73	1 (50%)	1,1,1	0.26	0
9	SCN	A	917	-	2,2,2	1.75	1 (50%)	1,1,1	0.18	0
2	NAG	B	901	1,2	14,14,15	0.92	0	15,19,21	0.86	0
2	NAG	B	902	3,2	14,14,15	0.79	1 (7%)	15,19,21	1.55	4 (26%)
3	BMA	B	903	2	11,11,12	0.42	0	15,15,17	0.94	1 (6%)
7	GOL	B	909	-	5,5,5	0.53	0	5,5,5	1.34	1 (20%)
8	4NY	B	910	-	30,34,34	2.69	6 (20%)	40,48,48	2.13	10 (25%)
9	SCN	B	911	-	2,2,2	1.58	1 (50%)	1,1,1	0.49	0
9	SCN	B	912	-	2,2,2	1.44	0	1,1,1	0.16	0
9	SCN	B	913	-	2,2,2	1.79	1 (50%)	1,1,1	0.24	0
9	SCN	B	914	-	2,2,2	1.83	1 (50%)	1,1,1	0.20	0
9	SCN	B	915	-	2,2,2	1.66	1 (50%)	1,1,1	0.58	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
2	NAG	A	901	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	902	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	903	2	-	0/2/19/22	0/1/1/1
7	GOL	A	909	-	-	0/4/4/4	0/0/0/0
8	4NY	A	910	-	-	0/10/18/18	0/4/4/4
9	SCN	A	911	-	-	0/0/0/0	0/0/0/0
9	SCN	A	912	-	-	0/0/0/0	0/0/0/0
9	SCN	A	913	-	-	0/0/0/0	0/0/0/0
9	SCN	A	914	-	-	0/0/0/0	0/0/0/0
9	SCN	A	915	-	-	0/0/0/0	0/0/0/0
9	SCN	A	916	-	-	0/0/0/0	0/0/0/0
9	SCN	A	917	-	-	0/0/0/0	0/0/0/0
2	NAG	B	901	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	902	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	903	2	-	0/2/19/22	0/1/1/1
7	GOL	B	909	-	-	0/4/4/4	0/0/0/0
8	4NY	B	910	-	-	0/10/18/18	0/4/4/4
9	SCN	B	911	-	-	0/0/0/0	0/0/0/0
9	SCN	B	912	-	-	0/0/0/0	0/0/0/0
9	SCN	B	913	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SCN	B	914	-	-	0/0/0/0	0/0/0/0
9	SCN	B	915	-	-	0/0/0/0	0/0/0/0

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	910	4NY	C23-C6	-12.19	1.26	1.44
8	B	910	4NY	C23-C6	-12.14	1.26	1.44
2	A	902	NAG	O5-C1	-3.40	1.38	1.43
8	B	910	4NY	C10-N	-3.07	1.35	1.39
2	B	902	NAG	O5-C1	-2.65	1.39	1.43
9	B	914	SCN	C-S	-2.58	1.48	1.63
9	B	913	SCN	C-S	-2.53	1.48	1.63
9	A	917	SCN	C-S	-2.47	1.48	1.63
9	A	916	SCN	C-S	-2.45	1.49	1.63
9	A	915	SCN	C-S	-2.43	1.49	1.63
9	B	915	SCN	C-S	-2.34	1.49	1.63
9	A	914	SCN	C-S	-2.30	1.49	1.63
9	A	911	SCN	C-S	-2.29	1.50	1.63
8	A	910	4NY	C10-N	-2.28	1.36	1.39
9	B	911	SCN	C-S	-2.22	1.50	1.63
9	A	913	SCN	C-S	-2.20	1.50	1.63
9	A	912	SCN	C-S	-2.15	1.50	1.63
2	A	901	NAG	C2-N2	-2.01	1.42	1.46
8	B	910	4NY	C14-C13	2.03	1.40	1.36
8	A	910	4NY	C12-CL	2.19	1.79	1.74
8	B	910	4NY	C12-CL	2.67	1.80	1.74
8	B	910	4NY	C8-C15	2.68	1.48	1.41
8	A	910	4NY	C8-C15	2.94	1.49	1.41
8	B	910	4NY	C15-C10	4.37	1.47	1.41
8	A	910	4NY	C15-C10	4.70	1.48	1.41

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	910	4NY	C5-C4-C6	-6.81	114.05	121.22
8	A	910	4NY	C3-C4-C6	-6.56	114.32	121.22
8	B	910	4NY	C8-C15-C10	-6.32	102.00	107.56
8	A	910	4NY	C8-C15-C10	-6.02	102.26	107.56
8	B	910	4NY	C-C1-C24	-3.11	116.33	120.43
2	A	902	NAG	O7-C7-C8	-2.84	116.83	122.07
8	B	910	4NY	C8-C7-C6	-2.70	124.55	129.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	909	GOL	C3-C2-C1	-2.69	99.72	111.06
7	A	909	GOL	O3-C3-C2	-2.63	96.66	109.97
8	A	910	4NY	C2-C1-C24	-2.48	117.16	120.43
2	B	902	NAG	O4-C4-C5	-2.41	102.87	109.23
8	A	910	4NY	C8-C7-C6	-2.34	125.20	129.47
8	A	910	4NY	C11-C10-C15	-2.29	117.24	120.48
2	B	902	NAG	O7-C7-C8	-2.22	117.99	122.07
8	B	910	4NY	C13-C14-C15	-2.20	118.25	121.15
8	A	910	4NY	C19-C20-C21	-2.20	119.67	122.87
8	B	910	4NY	C19-C20-C21	-2.17	119.71	122.87
2	A	902	NAG	O4-C4-C5	-2.16	103.55	109.23
8	B	910	4NY	C17-C16-N	-2.06	109.36	112.81
8	B	910	4NY	C11-C10-C15	-2.05	117.58	120.48
8	A	910	4NY	C13-C14-C15	-2.05	118.45	121.15
3	B	903	BMA	O3-C3-C2	-2.03	106.29	110.01
8	B	910	4NY	C18-C19-C20	2.21	120.70	118.34
3	A	903	BMA	C1-O5-C5	2.33	115.57	112.14
2	A	902	NAG	C8-C7-N2	2.40	120.70	116.10
2	B	902	NAG	O5-C5-C4	2.61	114.45	110.13
2	B	902	NAG	C1-O5-C5	3.16	116.79	112.14
8	A	910	4NY	C5-C4-C6	4.34	125.78	121.22
8	B	910	4NY	C3-C4-C6	4.36	125.81	121.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	909	GOL	4	0
8	A	910	4NY	3	0
9	A	915	SCN	1	0
7	B	909	GOL	5	0
8	B	910	4NY	5	0
9	B	912	SCN	1	0
9	B	914	SCN	1	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	754/855 (88%)	0.35	60 (7%) 15 12	20, 37, 64, 81	0
1	B	756/855 (88%)	0.22	49 (6%) 22 18	19, 35, 60, 79	0
All	All	1510/1710 (88%)	0.29	109 (7%) 18 14	19, 36, 63, 81	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	470	PHE	7.1
1	B	643	SER	6.5
1	A	559	LEU	6.4
1	A	657	VAL	6.0
1	B	567	CYS	5.9
1	A	668	LEU	5.4
1	A	471	PHE	5.2
1	A	397	PHE	4.8
1	A	651	SER	4.7
1	B	84	THR	4.7
1	B	642	VAL	4.6
1	B	397	PHE	4.5
1	A	643	SER	4.3
1	A	563	PHE	4.2
1	B	58	SER	4.0
1	A	558	TYR	4.0
1	A	641	GLU	3.9
1	A	642	VAL	3.8
1	A	84	THR	3.7
1	A	104	THR	3.7
1	A	681	LEU	3.6
1	B	470	PHE	3.6
1	A	58	SER	3.6
1	A	323	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	74	CYS	3.5
1	B	401	ALA	3.5
1	B	471	PHE	3.5
1	A	690	PRO	3.4
1	B	167	ILE	3.4
1	A	83	TYR	3.3
1	A	562	ASP	3.3
1	A	557	MET	3.3
1	A	555	GLY	3.2
1	A	367	CYS	3.2
1	B	88	HIS	3.2
1	B	321	PHE	3.2
1	A	692	ALA	3.2
1	A	82	SER	3.2
1	B	591	SER	3.2
1	A	167	ILE	3.1
1	A	734	ILE	3.1
1	B	168	ILE	3.1
1	B	74	CYS	3.1
1	A	640	ALA	3.1
1	A	401	ALA	3.0
1	A	560	GLN	3.0
1	A	561	SER	3.0
1	B	104	THR	2.9
1	B	734	ILE	2.9
1	A	318	TYR	2.9
1	B	217[A]	LEU	2.9
1	B	640	ALA	2.9
1	B	357	VAL	2.9
1	A	398	SER	2.8
1	B	668	LEU	2.8
1	B	651	SER	2.8
1	B	657	VAL	2.8
1	A	564	ASP	2.7
1	B	75	ARG	2.7
1	B	557	MET	2.7
1	B	355	ILE	2.7
1	B	559	LEU	2.7
1	A	759	GLY	2.6
1	A	399	ASN	2.6
1	B	148	ASP	2.6
1	A	217[A]	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	298	HIS	2.6
1	B	398	SER	2.5
1	A	689	SER	2.5
1	A	736	GLY	2.5
1	B	399	ASN	2.5
1	B	418	ASP	2.4
1	B	564	ASP	2.4
1	B	83	TYR	2.4
1	B	381	ASP	2.4
1	B	400	ASN	2.4
1	A	75	ARG	2.4
1	A	168	ILE	2.4
1	B	563	PHE	2.3
1	A	632	THR	2.3
1	B	566	GLY	2.3
1	B	629	PRO	2.3
1	B	736	GLY	2.3
1	A	630	LEU	2.3
1	B	82	SER	2.3
1	A	137	VAL	2.3
1	B	354	VAL	2.3
1	A	86	CYS	2.3
1	A	629	PRO	2.3
1	B	681	LEU	2.3
1	B	652	CYS	2.3
1	B	771	ILE	2.2
1	B	245	ARG	2.2
1	A	60	LYS	2.2
1	A	652	CYS	2.2
1	A	738	ILE	2.2
1	A	400	ASN	2.2
1	A	357	VAL	2.2
1	A	418	ASP	2.2
1	A	737	PRO	2.1
1	B	735	SER	2.1
1	B	57	GLY	2.1
1	A	691	GLU	2.1
1	A	539	THR	2.1
1	A	631	TRP	2.1
1	A	768	TYR	2.0
1	A	556	ILE	2.0
1	B	768	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	632	THR	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 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
9	SCN	A	916	3/3	0.94	0.26	6.49	50,50,52,55	0
9	SCN	A	917	3/3	0.95	0.18	3.54	54,54,56,56	0
9	SCN	B	912	3/3	0.93	0.18	2.81	42,42,46,51	0
7	GOL	B	909	6/6	0.95	0.14	1.64	29,38,39,48	0
9	SCN	B	913	3/3	0.96	0.14	1.57	52,52,55,56	0
7	GOL	A	909	6/6	0.96	0.11	0.79	29,35,36,38	0
8	4NY	A	910	31/31	0.83	0.15	-0.01	36,44,63,66	0
8	4NY	B	910	31/31	0.87	0.14	-0.22	37,46,61,66	0
9	SCN	B	915	3/3	0.97	0.09	-0.27	60,60,65,65	0
9	SCN	A	912	3/3	0.97	0.09	-0.42	43,43,44,48	0
2	NAG	B	901	14/15	0.95	0.07	-0.89	21,24,28,31	0
2	NAG	A	901	14/15	0.95	0.07	-1.00	22,24,27,31	0
5	CA	A	906	1/1	0.99	0.04	-1.08	28,28,28,28	0
5	CA	B	907	1/1	0.99	0.04	-1.16	25,25,25,25	0
6	NA	A	907	1/1	0.92	0.06	-1.25	39,39,39,39	0
9	SCN	A	914	3/3	0.98	0.06	-1.28	57,57,57,58	0
6	NA	B	908	1/1	0.94	0.05	-1.31	37,37,37,37	0
6	NA	B	906	1/1	0.97	0.05	-1.39	34,34,34,34	0
6	NA	A	908	1/1	0.98	0.03	-1.43	31,31,31,31	0
9	SCN	B	911	3/3	0.96	0.07	-1.57	37,37,42,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	ZN	B	905	1/1	1.00	0.05	-2.04	31,31,31,31	0
9	SCN	B	914	3/3	0.99	0.06	-2.44	45,45,48,51	0
4	ZN	A	905	1/1	0.99	0.03	-3.10	34,34,34,34	0
9	SCN	A	911	3/3	0.97	0.06	-3.37	40,40,41,45	0
4	ZN	A	904	1/1	0.99	0.03	-3.39	39,39,39,39	0
4	ZN	B	904	1/1	0.99	0.01	-4.02	40,40,40,40	0
9	SCN	A	915	3/3	0.98	0.07	-5.43	49,49,50,55	0
3	BMA	B	903	11/12	0.85	0.22	-	53,58,64,69	0
2	NAG	A	902	14/15	0.90	0.14	-	30,41,45,48	0
9	SCN	A	913	3/3	0.81	0.19	-	55,55,59,67	0
3	BMA	A	903	11/12	0.74	0.26	-	48,54,64,64	0
2	NAG	B	902	14/15	0.91	0.16	-	29,38,45,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.