Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 11:21 AM JST

PDB ID	:	5X2N
Title	:	Crystal structure of the medaka fish taste receptor T1r2a-T1r3 ligand binding domains in complex with L-alanine
Authors	:	Nuemket, N.; Yasui, N.; Atsumi, N.; Yamashita, A.
Deposited on	:	2017-02-02
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

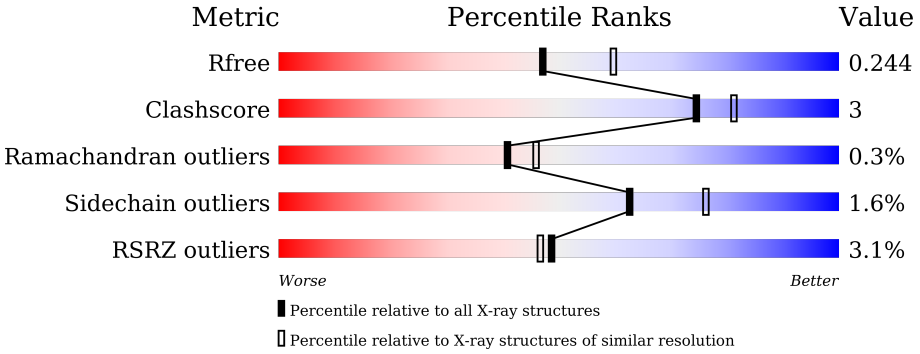
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	461	2%, 88%, 5%, 7%
1	C	461	3%, 88%, 6%, 6%
2	B	478	%, 88%, 8%, •
2	D	478	10%, 75%, 18%, 7%
3	H	225	90%, 9%, •
3	J	225	2%, 87%, 9%, • •

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Mol	Chain	Length	Quality of chain
4	K	217	88% 12%
4	L	217	91% 8%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 21672 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 Taste receptor, type 1, member 2a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	429	3395	2194	564	620	17	0	2	0
1	C	433	3434	2214	571	631	18	0	2	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	475	SER	-	expression tag	UNP A0A173M0G2
A	476	GLY	-	expression tag	UNP A0A173M0G2
A	477	ILE	-	expression tag	UNP A0A173M0G2
A	478	GLU	-	expression tag	UNP A0A173M0G2
A	479	GLY	-	expression tag	UNP A0A173M0G2
A	480	ARG	-	expression tag	UNP A0A173M0G2
C	475	SER	-	expression tag	UNP A0A173M0G2
C	476	GLY	-	expression tag	UNP A0A173M0G2
C	477	ILE	-	expression tag	UNP A0A173M0G2
C	478	GLU	-	expression tag	UNP A0A173M0G2
C	479	GLY	-	expression tag	UNP A0A173M0G2
C	480	ARG	-	expression tag	UNP A0A173M0G2

- Molecule 2 is a protein called Taste receptor, type 1, member 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	459	3592	2307	577	693	15	0	0	0
2	D	446	3481	2241	560	665	15	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	492	SER	-	expression tag	UNP A0A173M094
B	493	GLY	-	expression tag	UNP A0A173M094
B	494	ILE	-	expression tag	UNP A0A173M094
B	495	GLU	-	expression tag	UNP A0A173M094
B	496	GLY	-	expression tag	UNP A0A173M094
B	497	ARG	-	expression tag	UNP A0A173M094
D	492	SER	-	expression tag	UNP A0A173M094
D	493	GLY	-	expression tag	UNP A0A173M094
D	494	ILE	-	expression tag	UNP A0A173M094
D	495	GLU	-	expression tag	UNP A0A173M094
D	496	GLY	-	expression tag	UNP A0A173M094
D	497	ARG	-	expression tag	UNP A0A173M094

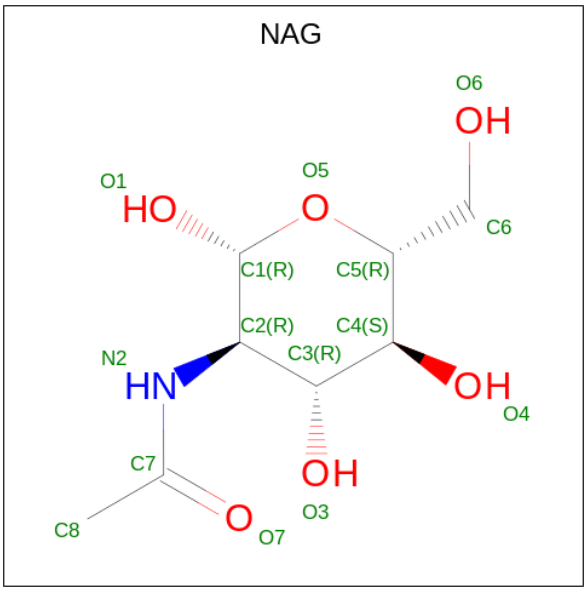
- Molecule 3 is a protein called Fab16A Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	223	1682	1067	277	330	8	0	0	0
			Total	C	N	O	S			
3	J	219	1653	1050	272	323	8	0	0	0

- Molecule 4 is a protein called Fab16A Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	L	216	1670	1035	287	342	6	0	0	0
			Total	C	N	O	S			
4	K	216	1670	1035	287	342	6	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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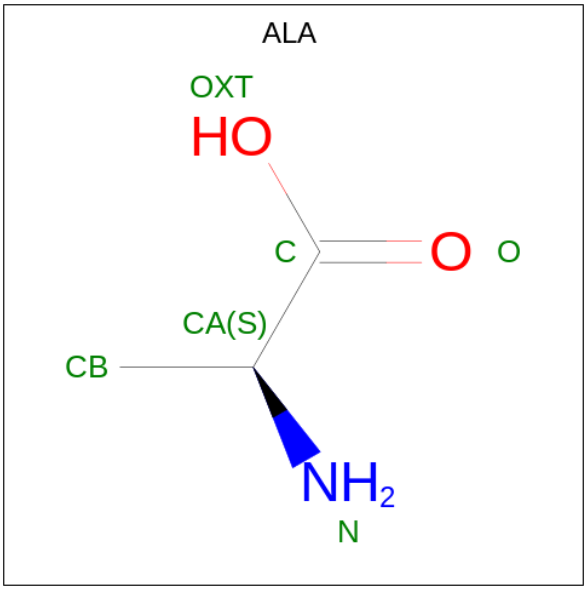
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	C	1	14	8	1	5	0	0
5	C	1	14	8	1	5	0	0
5	C	1	14	8	1	5	0	0
5	C	1	14	8	1	5	0	0
5	C	1	14	8	1	5	0	0
5	D	1	14	8	1	5	0	0
5	D	1	14	8	1	5	0	0
5	D	1	14	8	1	5	0	0
5	D	1	14	8	1	5	0	0

- Molecule 6 is ALANINE (three-letter code: ALA) (formula: $C_3H_7NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	6	3	1	2	0	0
6	B	1	6	3	1	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	C	1	6	3	1	2	0	0
6	D	1	6	3	1	2	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
7	A	1	1	1	0	0
7	C	1	1	1	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
8	B	1	1	1	0	0
8	D	1	1	1	0	0

- Molecule 9 is water.

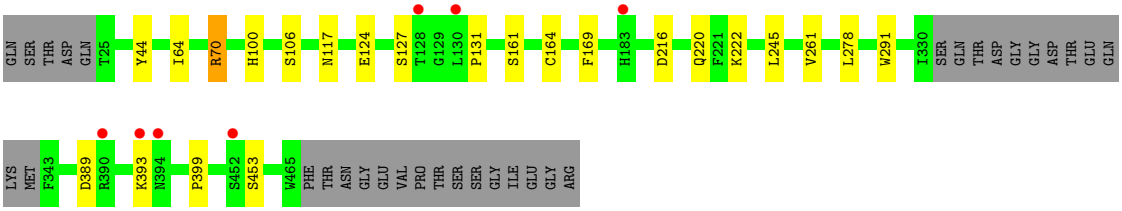
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	180	180	180	0	0
9	B	116	116	116	0	0
9	C	141	141	141	0	0
9	D	25	25	25	0	0
9	H	63	63	63	0	0
9	L	102	102	102	0	0
9	J	43	43	43	0	0
9	K	75	75	75	0	0

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.

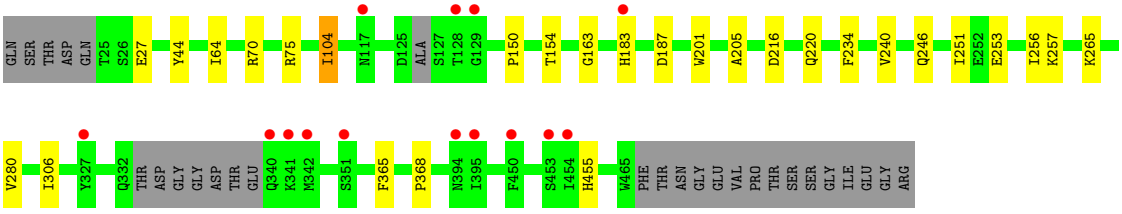
• Molecule 1: Taste receptor, type 1, member 2a

Chain A:



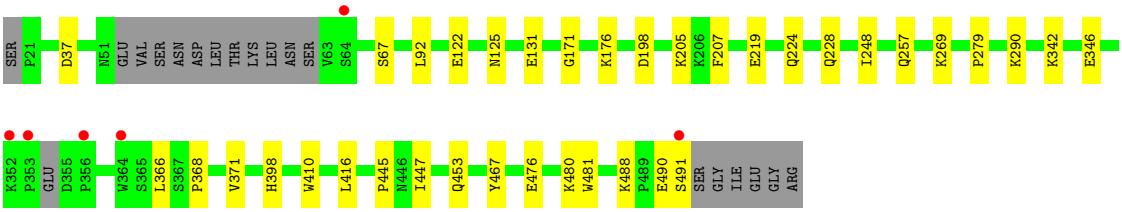
• Molecule 1: Taste receptor, type 1, member 2a

Chain C:



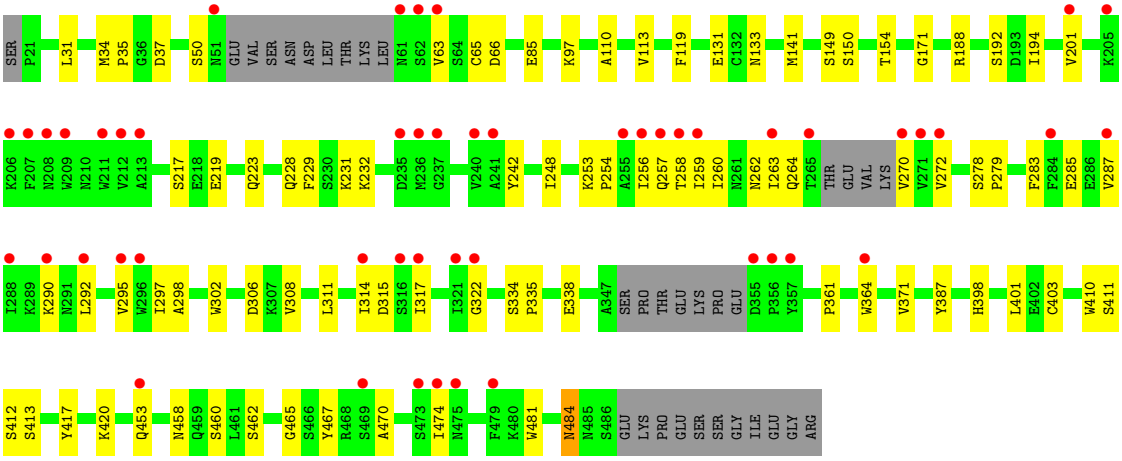
• Molecule 2: Taste receptor, type 1, member 3

Chain B:



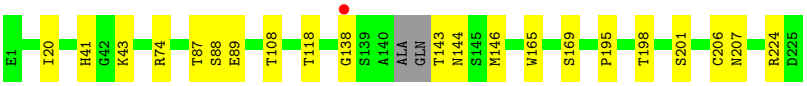
• Molecule 2: Taste receptor, type 1, member 3

Chain D:



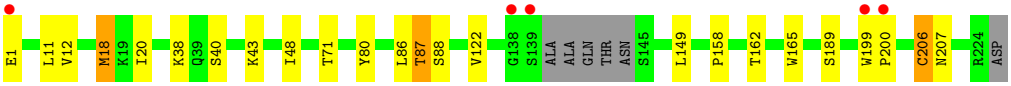
- Molecule 3: Fab16A Heavy chain

Chain H:



- Molecule 3: Fab16A Heavy chain

Chain J:

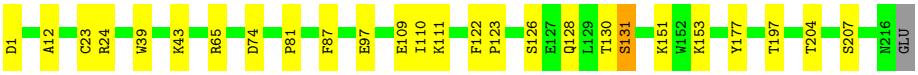


- Molecule 4: Fab16A Light chain

Chain L:

- Molecule 4: Fab16A Light chain

Chain K:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	99.37Å 117.47Å 130.06Å 90.00° 91.93° 90.00°	Depositor
Resolution (Å)	49.66 – 2.20 49.66 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.3 (49.66-2.20) 95.3 (49.66-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.195 , 0.244 0.196 , 0.244	Depositor DCC
R_{free} test set	7095 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	40.5	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 32.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	21672	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CL, NAG

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	0.47	0/3490	0.55	1/4743 (0.0%)
1	C	0.41	0/3528	0.54	1/4791 (0.0%)
2	B	0.42	0/3676	0.54	0/5002
2	D	0.35	0/3561	0.48	0/4843
3	H	0.41	0/1726	0.55	0/2358
3	J	0.37	0/1697	0.55	0/2319
4	K	0.42	0/1707	0.56	0/2320
4	L	0.50	0/1707	0.60	0/2320
All	All	0.42	0/21092	0.54	2/28696 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	70	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	C	70	ARG	NE-CZ-NH2	-5.17	117.72	120.30

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	3395	0	3316	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3434	0	3353	15	0
2	B	3592	0	3532	17	0
2	D	3481	0	3418	53	0
3	H	1682	0	1655	12	0
3	J	1653	0	1626	10	0
4	K	1670	0	1596	11	2
4	L	1670	0	1596	7	2
5	A	98	0	91	0	0
5	B	70	0	65	1	0
5	C	98	0	91	0	0
5	D	56	0	52	2	0
6	A	6	0	4	0	0
6	B	6	0	4	0	0
6	C	6	0	4	0	0
6	D	6	0	4	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
9	A	180	0	0	2	0
9	B	116	0	0	0	0
9	C	141	0	0	1	0
9	D	25	0	0	0	0
9	H	63	0	0	0	0
9	J	43	0	0	0	0
9	K	75	0	0	0	0
9	L	102	0	0	2	0
All	All	21672	0	20407	134	2

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.

All (134) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:LEU:O	2:B:398:HIS:ND1	2.07	0.88
2:D:119:PHE:HA	2:D:141:MET:HE2	1.69	0.73
4:L:128:GLN:OE1	9:L:301:HOH:O	2.08	0.71
3:H:41:HIS:O	3:H:43:LYS:NZ	2.23	0.71
4:L:109:GLU:OE1	4:L:177:TYR:OH	2.06	0.70
3:H:138:GLY:HA2	3:H:224:ARG:HD3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:199:GLU:HG3	4:L:210:VAL:HG22	1.77	0.67
4:K:109:GLU:OE2	4:K:177:TYR:OH	2.13	0.66
2:D:465:GLY:HA3	2:D:474:ILE:HD12	1.78	0.65
1:C:201:TRP:NE1	1:C:257:LYS:HD3	2.13	0.64
2:B:257:GLN:OE1	2:B:290:LYS:NZ	2.31	0.64
2:B:122:GLU:HB3	2:B:125:ASN:HB2	1.81	0.63
2:D:131:GLU:HG3	2:D:133:ASN:H	1.63	0.63
3:H:20:ILE:HD12	3:H:118:THR:HG21	1.81	0.63
2:B:207:PHE:HE1	2:B:476:GLU:HG3	1.67	0.59
2:D:242:TYR:HE2	2:D:259:ILE:HG23	1.67	0.58
2:D:217:SER:HB2	2:D:248:ILE:HD11	1.85	0.58
3:J:88:SER:HA	3:J:122:VAL:HG13	1.86	0.58
2:D:119:PHE:HD1	2:D:141:MET:HE3	1.68	0.58
2:D:119:PHE:HA	2:D:141:MET:CE	2.34	0.57
3:H:146:MET:HG2	3:H:195:PRO:HA	1.87	0.57
1:C:154:THR:HG22	2:D:110:ALA:HA	1.85	0.57
4:K:65:ARG:HD2	4:K:81:PRO:O	2.07	0.55
1:A:453:SER:HB2	3:H:74:ARG:HE	1.71	0.55
2:D:417:TYR:HD2	2:D:420:LYS:HE2	1.72	0.54
1:C:154:THR:HG21	2:D:113:VAL:HB	1.89	0.54
1:A:216:ASP:O	1:A:220:GLN:HG2	2.08	0.54
1:C:150:PRO:O	1:C:154:THR:HG23	2.08	0.54
3:H:87:THR:HG22	3:H:89:GLU:H	1.72	0.53
2:D:298:ALA:HB3	2:D:322:GLY:HA2	1.89	0.53
2:D:229:PHE:CZ	2:D:272:VAL:HG21	2.44	0.52
2:D:287:VAL:HG13	2:D:292:LEU:HB2	1.90	0.52
2:D:401:LEU:HD13	2:D:410:TRP:HB2	1.91	0.52
2:D:188:ARG:NH2	2:D:192:SER:HB2	2.25	0.51
3:H:165:TRP:CZ3	3:H:206:CYS:HB3	2.46	0.51
1:A:44:TYR:HB2	1:A:64:ILE:HD11	1.92	0.51
2:B:342:LYS:HE2	2:B:346:GLU:HG3	1.92	0.51
2:D:272:VAL:HG22	2:D:297:ILE:HG13	1.93	0.51
3:J:12:VAL:HG11	3:J:86:LEU:HD13	1.93	0.51
2:D:201:VAL:HG11	2:D:232:LYS:HG2	1.93	0.51
2:D:260:ILE:HG21	2:D:290:LYS:HD3	1.94	0.50
2:D:37:ASP:HB3	2:D:410:TRP:CZ2	2.47	0.50
1:C:104:ILE:HG13	1:C:104:ILE:O	2.12	0.50
1:A:222:LYS:NZ	9:A:1001:HOH:O	2.30	0.49
4:K:153:LYS:HB2	4:K:197:THR:HB	1.95	0.49
2:B:366:LEU:HD21	5:B:902:NAG:H82	1.94	0.49
2:D:338:GLU:HG3	2:D:371:VAL:HG21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:314:ILE:HD12	2:D:317:ILE:HG13	1.94	0.49
2:D:315:ASP:N	2:D:315:ASP:OD1	2.45	0.49
2:D:285:GLU:HG3	2:D:311:LEU:HD13	1.95	0.49
1:A:261:VAL:HB	1:A:291:TRP:HZ2	1.78	0.49
2:D:37:ASP:N	2:D:97:LYS:O	2.41	0.49
3:J:87:THR:O	3:J:122:VAL:HG11	2.12	0.49
4:K:24:ARG:NH1	4:K:74:ASP:OD2	2.46	0.49
1:A:261:VAL:HB	1:A:291:TRP:CZ2	2.48	0.48
2:D:242:TYR:CE2	2:D:259:ILE:HG23	2.47	0.48
2:B:224:GLN:O	2:B:228:GLN:HG2	2.14	0.48
2:B:37:ASP:HB3	2:B:410:TRP:CZ2	2.48	0.48
2:B:481:TRP:CZ2	2:B:488:LYS:HG3	2.48	0.48
1:C:44:TYR:HB2	1:C:64:ILE:HD11	1.95	0.48
2:D:85:GLU:OE1	2:D:387:TYR:OH	2.25	0.47
2:D:253:LYS:O	2:D:257:GLN:HG2	2.13	0.47
2:D:334:SER:HB2	2:D:335:PRO:HD3	1.97	0.47
4:L:43:LYS:HE2	9:L:315:HOH:O	2.15	0.47
1:A:245:LEU:HA	1:A:278:LEU:HD13	1.97	0.47
3:J:71:THR:OG1	3:J:80:TYR:HB2	2.15	0.47
2:D:260:ILE:O	2:D:263:ILE:HG22	2.14	0.47
2:D:481:TRP:HB3	2:D:484:ASN:O	2.15	0.46
2:B:269:LYS:HG2	2:B:490:GLU:HG3	1.98	0.46
1:A:164[A]:CYS:SG	1:A:169:PHE:CE2	3.09	0.46
2:D:270:VAL:HA	2:D:295:VAL:HB	1.98	0.46
4:K:87:PHE:HB3	4:K:110:ILE:HG12	1.97	0.46
2:D:298:ALA:HA	2:D:302:TRP:CZ2	2.52	0.45
2:B:248:ILE:HG22	2:B:279:PRO:HG3	1.98	0.45
2:D:228:GLN:HG2	2:D:231:LYS:HE3	1.98	0.45
2:D:398:HIS:CE1	2:D:403:CYS:HB2	2.52	0.45
1:C:205:ALA:HA	1:C:234:PHE:O	2.17	0.45
1:C:365:PHE:HA	1:C:368:PRO:HG2	1.97	0.45
1:C:27:GLU:HG2	1:C:75:ARG:CZ	2.47	0.44
4:L:19:ALA:HB3	4:L:79:ILE:HB	1.99	0.44
3:J:38:LYS:HB2	3:J:48:ILE:HD11	2.00	0.44
1:A:100:HIS:ND1	1:A:106:SER:HB2	2.33	0.44
4:K:126:SER:O	4:K:130:THR:HG23	2.17	0.44
1:A:70:ARG:NH2	9:A:1011:HOH:O	2.51	0.44
2:D:150:SER:O	2:D:154:THR:HG23	2.17	0.44
2:D:258:THR:O	2:D:262:ASN:ND2	2.50	0.44
3:H:108:THR:HA	4:L:95:THR:O	2.18	0.44
2:D:63:VAL:HG12	2:D:65:CYS:SG	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:LYS:NZ	9:C:1008:HOH:O	2.46	0.43
1:A:131:PRO:HG2	1:A:399:PRO:HG2	1.99	0.43
4:K:128:GLN:O	4:K:131:SER:OG	2.29	0.43
2:B:453:GLN:NE2	2:B:480:LYS:O	2.39	0.43
2:B:490:GLU:HB3	2:B:491:SER:H	1.62	0.43
2:D:453:GLN:HG3	2:D:462:SER:HB3	2.01	0.43
2:D:232:LYS:HE3	2:D:232:LYS:HB2	1.71	0.43
2:D:467:TYR:OH	2:D:470:ALA:HA	2.19	0.43
2:D:361:PRO:O	2:D:364:TRP:HD1	2.01	0.43
1:A:161:SER:HG	1:A:164[A]:CYS:HB2	1.83	0.42
2:D:253:LYS:HB2	2:D:254:PRO:HD3	2.00	0.42
1:C:365:PHE:C	1:C:368:PRO:HD2	2.39	0.42
2:D:283:PHE:O	2:D:287:VAL:HG23	2.19	0.42
3:H:43:LYS:HD3	3:H:43:LYS:HA	1.59	0.42
3:J:11:LEU:HB2	3:J:158:PRO:HG3	2.01	0.42
4:K:122:PHE:HA	4:K:123:PRO:HD3	1.85	0.42
2:B:205:LYS:HA	2:B:205:LYS:HD2	1.84	0.42
2:D:219:GLU:H	2:D:223:GLN:HG3	1.84	0.42
2:D:302:TRP:HB2	2:D:308:VAL:HG21	2.00	0.42
1:C:216:ASP:O	1:C:220:GLN:HG2	2.20	0.42
3:H:195:PRO:HB2	3:H:198:THR:HG23	2.02	0.42
3:J:18:MET:HE3	3:J:18:MET:HB2	1.75	0.42
2:D:253:LYS:HA	2:D:256:ILE:HD11	2.01	0.42
4:K:23:CYS:HB2	4:K:39:TRP:CH2	2.55	0.42
2:B:445:PRO:HB2	2:B:447:ILE:HG12	2.02	0.41
2:D:458:ASN:O	5:D:903:NAG:H82	2.20	0.41
3:H:143:THR:HB	3:H:144:ASN:H	1.68	0.41
4:K:12:ALA:HA	4:K:109:GLU:O	2.19	0.41
3:J:165:TRP:CZ3	3:J:206:CYS:HB3	2.56	0.41
2:D:34:MET:HA	2:D:35:PRO:HD2	1.87	0.41
2:D:460:SER:HB3	5:D:903:NAG:HN2	1.85	0.41
1:A:393:LYS:HA	1:A:393:LYS:HD2	1.79	0.41
2:D:194:ILE:O	2:D:232:LYS:NZ	2.54	0.41
1:C:251:ILE:HG23	1:C:256:ILE:HB	2.03	0.41
2:D:278:SER:HB3	2:D:279:PRO:HD3	2.02	0.41
4:L:80:ASN:HA	4:L:81:PRO:HA	1.84	0.41
2:B:198:ASP:OD2	2:B:467:TYR:OH	2.23	0.40
3:J:40:SER:O	3:J:43:LYS:N	2.49	0.40
2:B:368:PRO:O	2:B:371:VAL:HG23	2.21	0.40
1:C:183[A]:HIS:HB3	1:C:187:ASP:OD2	2.21	0.40
2:D:31:LEU:HD12	2:D:31:LEU:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:411:SER:C	2:D:413:SER:H	2.24	0.40
4:K:151:LYS:HB2	4:K:151:LYS:HE3	1.89	0.40
1:C:280:VAL:O	1:C:306:ILE:HA	2.21	0.40
3:H:87:THR:HG22	3:H:88:SER:N	2.36	0.40
3:J:199:TRP:CG	3:J:200:PRO:HA	2.57	0.40

All (2) 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:L:189:GLU:OE1	4:K:1:ASP:N[1_545]	2.17	0.03
4:L:161:ASN:ND2	4:K:97:GLU:OE1[1_545]	2.18	0.02

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	427/461 (93%)	419 (98%)	6 (1%)	2 (0%)	29	31
1	C	429/461 (93%)	417 (97%)	11 (3%)	1 (0%)	47	55
2	B	453/478 (95%)	437 (96%)	15 (3%)	1 (0%)	47	55
2	D	438/478 (92%)	418 (95%)	17 (4%)	3 (1%)	22	22
3	H	219/225 (97%)	205 (94%)	13 (6%)	1 (0%)	29	31
3	J	215/225 (96%)	207 (96%)	8 (4%)	0	100	100
4	K	214/217 (99%)	205 (96%)	8 (4%)	1 (0%)	29	31
4	L	214/217 (99%)	209 (98%)	5 (2%)	0	100	100
All	All	2609/2762 (94%)	2517 (96%)	83 (3%)	9 (0%)	41	46

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	201	SER
4	K	131	SER
1	A	127	SER
1	A	117	ASN
2	D	412	SER
2	D	484	ASN
2	D	171	GLY
1	C	163	GLY
2	B	171	GLY

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	379/407 (93%)	377 (100%)	2 (0%)	88	94
1	C	386/407 (95%)	381 (99%)	5 (1%)	69	81
2	B	409/428 (96%)	404 (99%)	5 (1%)	71	83
2	D	392/428 (92%)	387 (99%)	5 (1%)	69	81
3	H	190/192 (99%)	188 (99%)	2 (1%)	73	85
3	J	187/192 (97%)	178 (95%)	9 (5%)	25	32
4	K	190/191 (100%)	186 (98%)	4 (2%)	53	67
4	L	190/191 (100%)	185 (97%)	5 (3%)	46	58
All	All	2323/2436 (95%)	2286 (98%)	37 (2%)	62	76

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	GLU
1	A	389	ASP
2	B	67	SER
2	B	131	GLU
2	B	176	LYS
2	B	219	GLU
2	B	416	LEU

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Mol	Chain	Res	Type
1	C	104	ILE
1	C	240	VAL
1	C	246	GLN
1	C	253	GLU
1	C	455	HIS
2	D	50	SER
2	D	66	ASP
2	D	149	SER
2	D	264	GLN
2	D	306	ASP
3	H	169	SER
3	H	207	ASN
4	L	87	PHE
4	L	120	SER
4	L	126	SER
4	L	185	LEU
4	L	194	ASN
3	J	1	GLU
3	J	18	MET
3	J	20	ILE
3	J	87	THR
3	J	149	LEU
3	J	162	THR
3	J	189	SER
3	J	206	CYS
3	J	207	ASN
4	K	43	LYS
4	K	111	LYS
4	K	204	THR
4	K	207	SER

Sometimes 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)

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 31 ligands modelled in this entry, 4 are monoatomic - leaving 27 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	$\#\|Z\| > 2$
5	NAG	D	901	2	14,14,15	0.44	0	17,19,21	1.57	3 (17%)
5	NAG	C	905	1	14,14,15	0.68	0	17,19,21	1.28	3 (17%)
5	NAG	B	905	2	14,14,15	0.62	0	17,19,21	1.12	2 (11%)
5	NAG	A	904	1	14,14,15	0.70	0	17,19,21	1.03	2 (11%)
5	NAG	D	902	2	14,14,15	0.60	0	17,19,21	0.65	0
5	NAG	A	905	1	14,14,15	0.60	0	17,19,21	1.09	1 (5%)
5	NAG	B	904	2	14,14,15	0.53	0	17,19,21	1.13	2 (11%)
6	ALA	D	951	-	5,5,5	1.22	1 (20%)	6,6,6	1.33	1 (16%)
5	NAG	C	901	1	14,14,15	0.63	0	17,19,21	1.33	2 (11%)
5	NAG	C	902	1	14,14,15	0.62	0	17,19,21	0.84	0
5	NAG	D	903	2	14,14,15	0.45	0	17,19,21	1.10	1 (5%)
5	NAG	B	901	2	14,14,15	0.66	0	17,19,21	1.07	1 (5%)
5	NAG	D	904	2	14,14,15	0.53	0	17,19,21	0.71	0
6	ALA	A	951	-	5,5,5	1.38	2 (40%)	6,6,6	1.04	0
5	NAG	C	907	1	14,14,15	0.43	0	17,19,21	0.87	1 (5%)
5	NAG	A	907	1	14,14,15	0.50	0	17,19,21	1.53	2 (11%)
5	NAG	A	903	1	14,14,15	0.44	0	17,19,21	1.29	1 (5%)
6	ALA	C	951	-	5,5,5	1.44	1 (20%)	6,6,6	1.64	2 (33%)
5	NAG	C	903	1	14,14,15	0.49	0	17,19,21	1.07	2 (11%)
5	NAG	B	903	2	14,14,15	0.53	0	17,19,21	0.92	0
5	NAG	A	902	1	14,14,15	0.55	0	17,19,21	0.77	0
5	NAG	A	906	1	14,14,15	0.60	0	17,19,21	0.84	0
5	NAG	B	902	2	14,14,15	0.45	0	17,19,21	0.98	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	C	906	1	14,14,15	0.53	0	17,19,21	1.13	2 (11%)
5	NAG	C	904	1	14,14,15	0.58	0	17,19,21	0.80	0
6	ALA	B	951	-	5,5,5	1.01	0	6,6,6	1.40	2 (33%)
5	NAG	A	901	1	14,14,15	0.66	0	17,19,21	1.24	3 (17%)

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
5	NAG	D	901	2	-	2/6/23/26	0/1/1/1
5	NAG	C	905	1	-	2/6/23/26	0/1/1/1
5	NAG	B	905	2	-	0/6/23/26	0/1/1/1
5	NAG	A	904	1	-	0/6/23/26	0/1/1/1
5	NAG	D	902	2	-	0/6/23/26	0/1/1/1
5	NAG	A	905	1	-	0/6/23/26	0/1/1/1
5	NAG	B	904	2	-	0/6/23/26	0/1/1/1
6	ALA	D	951	-	-	3/4/4/4	-
5	NAG	C	901	1	-	2/6/23/26	0/1/1/1
5	NAG	C	902	1	-	2/6/23/26	0/1/1/1
5	NAG	D	903	2	-	0/6/23/26	0/1/1/1
5	NAG	B	901	2	-	1/6/23/26	0/1/1/1
5	NAG	D	904	2	-	0/6/23/26	0/1/1/1
6	ALA	A	951	-	-	3/4/4/4	-
5	NAG	C	907	1	-	0/6/23/26	0/1/1/1
5	NAG	A	907	1	-	0/6/23/26	0/1/1/1
5	NAG	A	903	1	-	1/6/23/26	0/1/1/1
6	ALA	C	951	-	-	0/4/4/4	-
5	NAG	C	903	1	-	0/6/23/26	0/1/1/1
5	NAG	B	903	2	-	0/6/23/26	0/1/1/1
5	NAG	A	902	1	-	2/6/23/26	0/1/1/1
5	NAG	A	906	1	-	2/6/23/26	0/1/1/1
5	NAG	B	902	2	-	0/6/23/26	0/1/1/1
5	NAG	C	906	1	-	0/6/23/26	0/1/1/1
5	NAG	C	904	1	-	0/6/23/26	0/1/1/1
6	ALA	B	951	-	-	0/4/4/4	-
5	NAG	A	901	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	951	ALA	OXT-C	-2.52	1.22	1.30
6	D	951	ALA	OXT-C	-2.09	1.23	1.30
6	A	951	ALA	CA-C	-2.03	1.52	1.54
6	A	951	ALA	OXT-C	-2.03	1.23	1.30

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	907	NAG	C1-O5-C5	5.07	119.06	112.19
5	A	903	NAG	C1-O5-C5	4.18	117.86	112.19
5	D	903	NAG	C1-O5-C5	3.43	116.84	112.19
6	C	951	ALA	OXT-C-O	-3.37	116.43	124.09
5	D	901	NAG	C1-O5-C5	3.33	116.70	112.19
5	D	901	NAG	O5-C5-C6	3.31	112.39	107.20
5	B	904	NAG	C1-O5-C5	2.97	116.22	112.19
5	C	905	NAG	O5-C1-C2	2.84	115.78	111.29
5	C	903	NAG	C1-O5-C5	2.78	115.95	112.19
5	B	904	NAG	O5-C1-C2	2.74	115.62	111.29
5	D	901	NAG	C2-N2-C7	-2.64	119.15	122.90
5	B	902	NAG	C1-O5-C5	2.58	115.69	112.19
5	C	901	NAG	O4-C4-C3	-2.58	104.39	110.35
5	B	901	NAG	C1-C2-N2	-2.56	106.11	110.49
5	C	906	NAG	C2-N2-C7	-2.56	119.25	122.90
5	A	904	NAG	C1-O5-C5	2.56	115.67	112.19
5	A	905	NAG	O5-C5-C6	2.56	111.22	107.20
5	C	901	NAG	C1-O5-C5	2.51	115.59	112.19
6	B	951	ALA	OXT-C-O	-2.47	118.48	124.09
5	C	907	NAG	O5-C5-C6	2.47	111.08	107.20
6	D	951	ALA	OXT-C-O	-2.45	118.52	124.09
5	C	905	NAG	C1-C2-N2	-2.43	106.33	110.49
5	B	905	NAG	C4-C3-C2	2.39	114.52	111.02
5	A	901	NAG	C2-N2-C7	2.38	126.29	122.90
5	B	905	NAG	C1-C2-N2	-2.34	106.48	110.49
5	C	905	NAG	C2-N2-C7	-2.31	119.61	122.90
5	C	906	NAG	C1-O5-C5	2.29	115.29	112.19
5	A	901	NAG	O5-C5-C6	2.29	110.79	107.20
5	C	903	NAG	C2-N2-C7	-2.20	119.76	122.90
6	B	951	ALA	OXT-C-CA	2.14	121.79	114.06
5	A	907	NAG	C6-C5-C4	-2.13	108.02	113.00
6	C	951	ALA	OXT-C-CA	2.08	121.57	114.06
5	A	901	NAG	C6-C5-C4	-2.06	108.18	113.00
5	A	904	NAG	C1-C2-N2	-2.03	107.01	110.49

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	902	NAG	O5-C5-C6-O6
5	A	902	NAG	C4-C5-C6-O6
5	D	901	NAG	O5-C5-C6-O6
5	C	901	NAG	C8-C7-N2-C2
5	C	901	NAG	O7-C7-N2-C2
5	D	901	NAG	C4-C5-C6-O6
5	C	905	NAG	O5-C5-C6-O6
5	C	905	NAG	C4-C5-C6-O6
5	C	902	NAG	O5-C5-C6-O6
5	A	903	NAG	O5-C5-C6-O6
5	A	906	NAG	C4-C5-C6-O6
6	A	951	ALA	O-C-CA-CB
6	A	951	ALA	OXT-C-CA-CB
6	D	951	ALA	O-C-CA-CB
6	D	951	ALA	OXT-C-CA-CB
5	B	901	NAG	C4-C5-C6-O6
6	D	951	ALA	OXT-C-CA-N
6	A	951	ALA	OXT-C-CA-N
5	A	906	NAG	O5-C5-C6-O6
5	C	902	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	903	NAG	2	0
5	B	902	NAG	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	429/461 (93%)	-0.16	7 (1%) 72 70	27, 38, 66, 138	0
1	C	433/461 (93%)	-0.06	14 (3%) 47 45	28, 41, 76, 135	0
2	B	459/478 (96%)	-0.07	6 (1%) 77 75	27, 43, 68, 118	0
2	D	446/478 (93%)	0.51	50 (11%) 5 4	34, 61, 102, 140	0
3	H	223/225 (99%)	-0.25	1 (0%) 92 91	28, 45, 87, 109	0
3	J	219/225 (97%)	-0.21	5 (2%) 60 58	31, 49, 84, 117	0
4	K	216/217 (99%)	-0.45	0 100 100	32, 41, 58, 105	0
4	L	216/217 (99%)	-0.42	0 100 100	29, 39, 60, 88	0
All	All	2641/2762 (95%)	-0.07	83 (3%) 49 47	27, 44, 84, 140	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	287	VAL	7.1
1	C	394	ASN	7.1
2	D	474	ILE	6.2
2	D	255	ALA	5.6
2	B	364	TRP	5.6
2	D	240	VAL	5.4
1	A	128	THR	5.3
2	D	322	GLY	4.5
2	D	292	LEU	4.3
2	B	353	PRO	4.1
2	D	271	VAL	4.1
2	D	236	MET	4.1
1	C	341	LYS	4.0
2	D	263	ILE	4.0
2	D	364	TRP	4.0
3	J	139	SER	3.9

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Mol	Chain	Res	Type	RSRZ
2	D	284	PHE	3.9
2	D	469	SER	3.8
2	D	241	ALA	3.8
2	B	352	LYS	3.8
2	D	314	ILE	3.7
2	D	355	ASP	3.7
1	C	453	SER	3.6
2	D	205	LYS	3.6
2	D	259	ILE	3.6
1	C	395	ILE	3.6
2	D	213	ALA	3.5
1	C	450	PHE	3.5
1	C	454	ILE	3.4
2	D	258	THR	3.4
2	D	211	TRP	3.4
2	D	63	VAL	3.3
3	J	138	GLY	3.2
1	A	130	LEU	3.1
2	D	270	VAL	3.1
2	D	357	TYR	3.0
1	A	390	ARG	3.0
1	A	183[A]	HIS	3.0
1	A	452	SER	3.0
3	J	1	GLU	2.9
2	D	317	ILE	2.9
2	D	235	ASP	2.9
2	D	201	VAL	2.9
3	H	138	GLY	2.8
2	D	479	PHE	2.8
2	D	272	VAL	2.8
2	D	212	VAL	2.8
2	D	475	ASN	2.8
1	C	183[A]	HIS	2.8
2	B	356	PRO	2.7
2	D	290	LYS	2.6
2	D	356	PRO	2.6
2	D	321	ILE	2.6
1	C	117	ASN	2.6
1	A	393	LYS	2.5
1	C	340	GLN	2.5
2	D	237	GLY	2.5
2	D	62	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	208	ASN	2.5
2	D	256	ILE	2.3
2	D	295	VAL	2.3
3	J	200	PRO	2.3
1	C	327	TYR	2.3
2	D	288	ILE	2.3
3	J	199	TRP	2.2
2	D	316	SER	2.2
2	B	64	SER	2.2
2	D	209	TRP	2.2
2	D	51	ASN	2.2
2	D	453	GLN	2.2
1	C	129	GLY	2.2
1	A	394	ASN	2.2
2	D	257	GLN	2.2
1	C	342	MET	2.1
2	D	296	TRP	2.1
2	D	265	THR	2.1
2	D	473	SER	2.1
2	B	491	SER	2.1
2	D	207	PHE	2.1
1	C	351	SER	2.0
2	D	206	LYS	2.0
2	D	61	ASN	2.0
1	C	128	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 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, 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	B-factors(Å^2)	Q<0.9
5	NAG	D	903	14/15	0.54	0.31	106,106,106,106	0
5	NAG	A	903	14/15	0.69	0.26	108,110,111,111	0
5	NAG	A	902	14/15	0.73	0.38	97,98,98,98	0
5	NAG	B	904	14/15	0.77	0.38	107,107,108,108	0
5	NAG	A	907	14/15	0.84	0.24	85,85,86,86	0
5	NAG	B	903	14/15	0.84	0.16	86,86,86,86	0
5	NAG	D	902	14/15	0.85	0.17	67,67,67,67	0
5	NAG	C	902	14/15	0.85	0.33	91,91,92,92	0
5	NAG	C	903	14/15	0.86	0.16	62,63,63,63	0
5	NAG	B	905	14/15	0.86	0.24	67,68,69,69	0
5	NAG	B	902	14/15	0.86	0.21	75,76,77,77	0
5	NAG	C	904	14/15	0.89	0.20	66,66,67,67	0
5	NAG	D	904	14/15	0.89	0.29	75,75,76,76	0
5	NAG	C	907	14/15	0.90	0.16	64,65,65,65	0
5	NAG	D	901	14/15	0.91	0.11	50,51,51,51	0
5	NAG	A	906	14/15	0.91	0.13	61,61,61,61	0
5	NAG	C	905	14/15	0.92	0.11	52,53,53,53	0
5	NAG	A	904	14/15	0.93	0.24	60,60,61,61	0
5	NAG	A	905	14/15	0.94	0.16	62,62,63,63	0
5	NAG	C	906	14/15	0.95	0.09	55,56,57,57	0
5	NAG	A	901	14/15	0.95	0.12	39,39,39,40	0
5	NAG	B	901	14/15	0.96	0.09	48,50,52,52	0
5	NAG	C	901	14/15	0.96	0.11	39,39,40,40	0
6	ALA	D	951	6/6	0.96	0.18	44,44,44,45	0
7	NA	C	961	1/1	0.96	0.06	39,39,39,39	0
6	ALA	A	951	6/6	0.97	0.20	31,31,32,32	0
6	ALA	C	951	6/6	0.97	0.24	36,36,37,37	0
6	ALA	B	951	6/6	0.98	0.14	31,31,31,31	0
7	NA	A	961	1/1	0.99	0.07	35,35,35,35	0
8	CL	B	971	1/1	0.99	0.13	34,34,34,34	0
8	CL	D	971	1/1	0.99	0.12	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.