Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 11:23 AM JST

PDB ID	:	5X2M
Title	:	Crystal structure of the medaka fish taste receptor T1r2a-T1r3 ligand binding domains in complex with L-glutamine
Authors	:	Nuemket, N.; Yasui, N.; Atsumi, N.; Yamashita, A.
Deposited on	:	2017-02-02
Resolution	:	2.21 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:

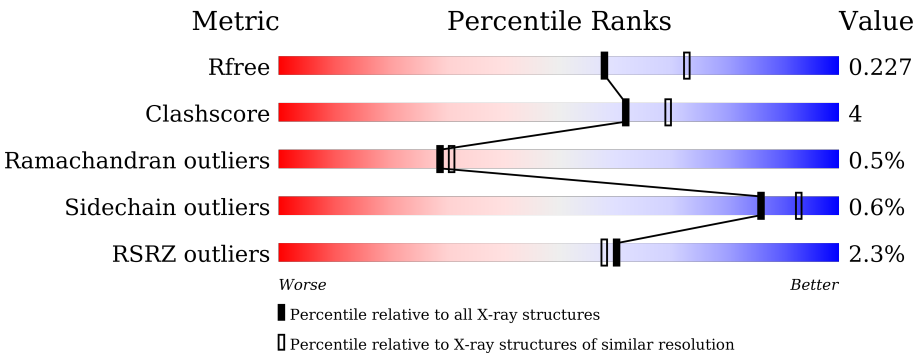
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.21 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	.% 87% 7% 7%
1	C	461	2% 84% 8% 7%
2	B	478	2% 84% 11% 5%
2	D	478	7% 71% 17% • 12%
3	H	225	.% 89% 8% •
3	J	225	.% 85% 10% • •

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Mol	Chain	Length	Quality of chain
4	K	217	94% 6%
4	L	217	93% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	D	905	-	-	-	X

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 21519 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	3413	2206	565	624	18	0	2	0
1	C	427	3388	2186	562	622	18	0	1	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	452	3557	2287	570	685	15	0	2	0
2	D	422	3304	2123	531	637	13	0	1	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

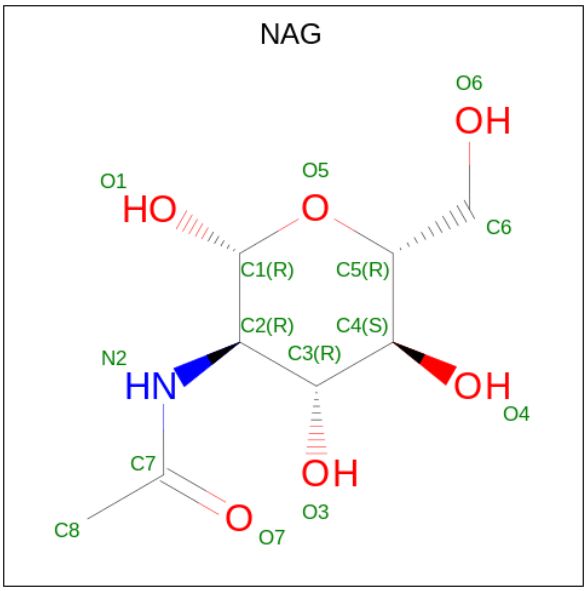
- Molecule 3 is a protein called Fab16A Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	219	1662	1056	274	324	8	0	0	0
			Total	C	N	O	S			
3	J	217	1647	1048	271	320	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	217	1679	1040	288	345	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	B	1	14	8	1	5	0	0

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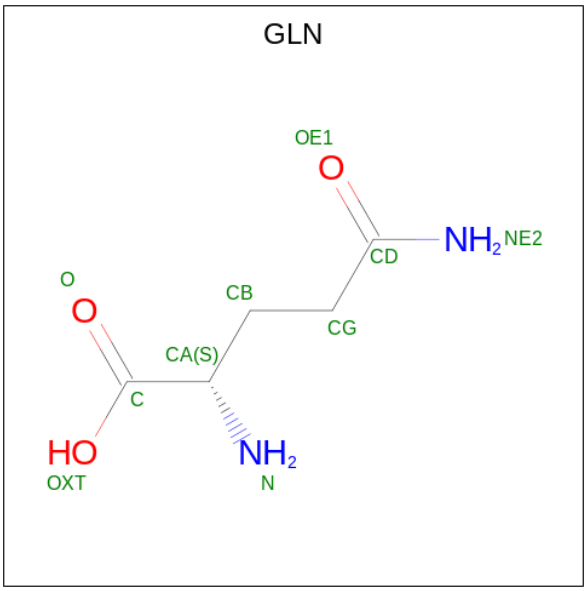
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	C	1	14	8	1	5	0	0
			Total	C	N	O		
5	C	1	14	8	1	5	0	0
			Total	C	N	O		
5	C	1	14	8	1	5	0	0
			Total	C	N	O		
5	C	1	14	8	1	5	0	0
			Total	C	N	O		
5	C	1	14	8	1	5	0	0
			Total	C	N	O		
5	C	1	14	8	1	5	0	0
			Total	C	N	O		
5	C	1	14	8	1	5	0	0
			Total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

- Molecule 6 is GLUTAMINE (three-letter code: GLN) (formula: $C_5H_{10}N_2O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 10 5 2 3	0	0
6	B	1	Total C N O 10 5 2 3	0	0
6	C	1	Total C N O 10 5 2 3	0	0
6	D	1	Total C N O 10 5 2 3	0	0

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

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

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

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

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
9	L	1	1	1	0	0

- Molecule 10 is water.

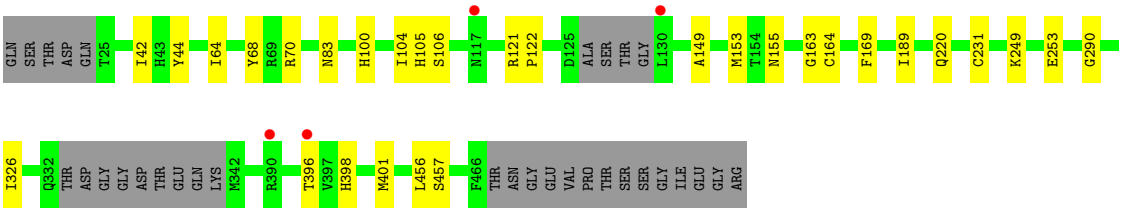
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	191	191	191	0	0
			Total	O		
10	B	100	100	100	0	0
			Total	O		
10	C	149	149	149	0	0
			Total	O		
10	D	46	46	46	0	0
			Total	O		
10	H	81	81	81	0	0
			Total	O		
10	L	73	73	73	0	0
			Total	O		
10	J	47	47	47	0	0
			Total	O		
10	K	88	88	88	0	0

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.

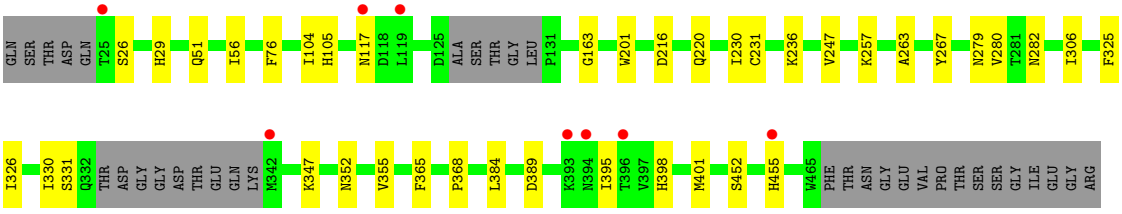
• Molecule 1: Taste receptor, type 1, member 2a

Chain A:



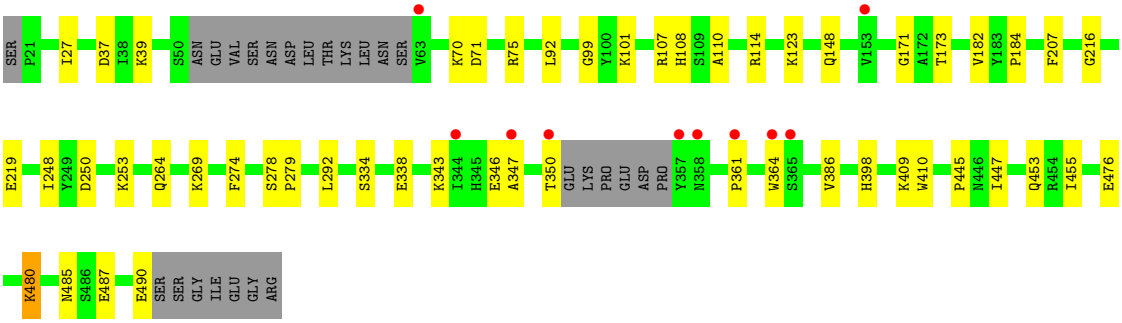
• Molecule 1: Taste receptor, type 1, member 2a

Chain C:



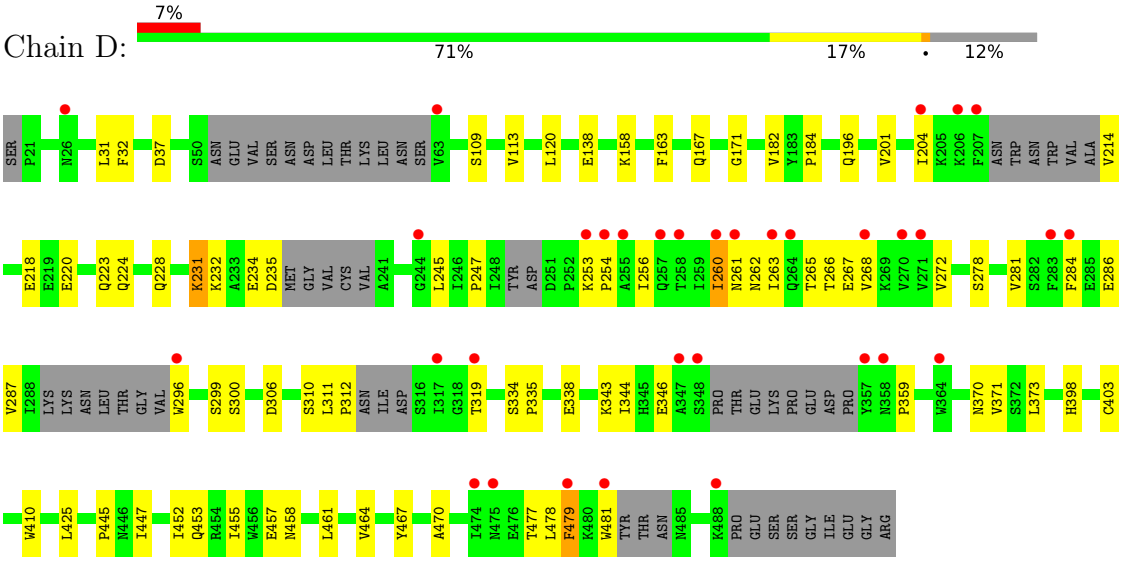
• Molecule 2: Taste receptor, type 1, member 3

Chain B:



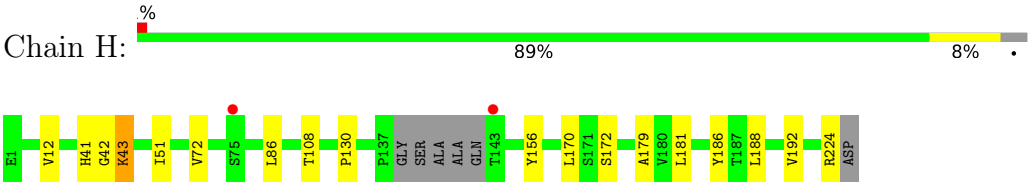
• Molecule 2: Taste receptor, type 1, member 3

Chain D:



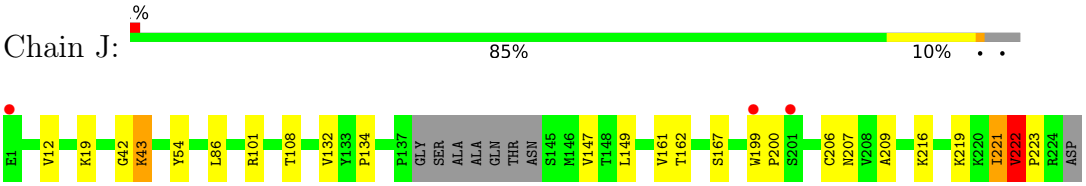
- Molecule 3: Fab16A Heavy chain

Chain H:



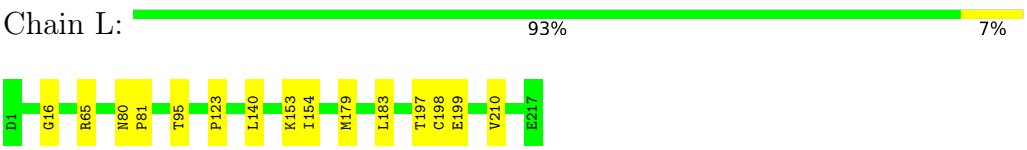
- Molecule 3: Fab16A Heavy chain

Chain J:



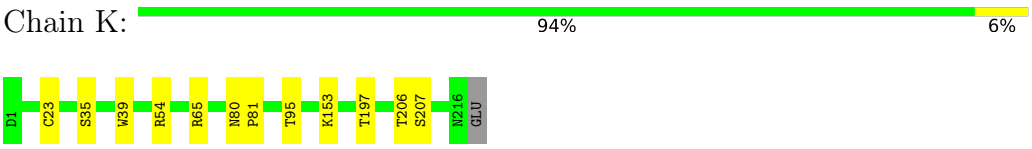
- Molecule 4: Fab16A Light chain

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	99.66Å 116.36Å 129.48Å 90.00° 92.20° 90.00°	Depositor
Resolution (Å)	49.89 – 2.21 49.89 – 2.21	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.89-2.21) 96.2 (49.89-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.173 , 0.227 0.175 , 0.227	Depositor DCC
R_{free} test set	7155 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 40.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	21519	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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, CA, 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	0.45	0/3507	0.55	0/4761
1	C	0.43	0/3478	0.53	0/4722
2	B	0.39	0/3645	0.52	0/4957
2	D	0.38	0/3375	0.53	0/4575
3	H	0.41	0/1706	0.55	0/2331
3	J	0.40	0/1691	0.60	2/2310 (0.1%)
4	K	0.41	0/1707	0.55	0/2320
4	L	0.44	0/1716	0.55	0/2332
All	All	0.42	0/20825	0.54	2/28308 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	J	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	222	VAL	C-N-CD	-6.96	105.28	120.60
3	J	222	VAL	C-N-CA	5.61	145.55	122.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	J	221	ILE	Peptide

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	3413	0	3343	20	0
1	C	3388	0	3311	25	0
2	B	3557	0	3511	37	0
2	D	3304	0	3255	58	1
3	H	1662	0	1642	11	0
3	J	1647	0	1629	20	0
4	K	1670	0	1596	6	1
4	L	1679	0	1602	9	0
5	A	98	0	91	2	0
5	B	98	0	91	2	0
5	C	98	0	91	3	0
5	D	84	0	78	3	0
6	A	10	0	7	0	0
6	B	10	0	7	4	0
6	C	10	0	7	0	0
6	D	10	0	7	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
9	L	1	0	0	0	0
10	A	191	0	0	4	0
10	B	100	0	0	7	0
10	C	149	0	0	2	0
10	D	46	0	0	6	0
10	H	81	0	0	1	0
10	J	47	0	0	3	0
10	K	88	0	0	0	0
10	L	73	0	0	0	0
All	All	21519	0	20268	181	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 4.

All (181) 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:D:479:PHE:HB3	2:D:481:TRP:HE1	1.23	1.02
3:J:167:SER:H	3:J:207:ASN:HD21	1.19	0.87
2:B:92:LEU:O	2:B:398:HIS:ND1	2.07	0.87
2:B:334:SER:O	10:B:1001:HOH:O	1.97	0.82
2:D:455:ILE:HD13	5:D:903:NAG:H83	1.63	0.81
2:B:338:GLU:N	10:B:1001:HOH:O	2.02	0.76
1:C:231:CYS:SG	10:J:346:HOH:O	2.42	0.76
3:J:222:VAL:HG23	3:J:223:PRO:HA	1.69	0.75
2:B:107:ARG:HH12	6:B:951:GLN:HE21	1.39	0.71
1:A:396:THR:O	10:A:1001:HOH:O	2.09	0.70
4:L:154:ILE:HD11	4:L:183:LEU:HD21	1.73	0.70
3:J:147:VAL:HG21	3:J:199:TRP:HD1	1.56	0.68
1:C:389:ASP:OD1	10:C:1001:HOH:O	2.11	0.68
2:B:346:GLU:OE2	10:B:1002:HOH:O	2.12	0.68
2:D:235:ASP:OD2	10:D:1001:HOH:O	2.11	0.68
2:D:138:GLU:OE2	10:D:1002:HOH:O	2.12	0.68
2:B:453:GLN:NE2	2:B:480:LYS:O	2.25	0.68
1:A:231:CYS:SG	10:H:380:HOH:O	2.52	0.68
2:B:269:LYS:NZ	2:B:490:GLU:HB2	2.09	0.67
2:D:481:TRP:O	10:D:1003:HOH:O	2.13	0.66
2:D:479:PHE:HB3	2:D:481:TRP:NE1	2.05	0.62
2:D:266:THR:HB	2:D:268:VAL:HG13	1.81	0.61
2:D:306:ASP:O	2:D:310:SER:N	2.34	0.61
3:J:42:GLY:O	3:J:43:LYS:HB2	2.01	0.60
2:B:148:GLN:HE21	6:B:951:GLN:NE2	2.00	0.59
2:D:319:THR:HG21	2:D:481:TRP:HA	1.85	0.59
4:L:199:GLU:HG3	4:L:210:VAL:HG12	1.85	0.59
1:C:230:ILE:O	3:J:101:ARG:NH1	2.35	0.59
1:C:330:ILE:HG21	1:C:355:VAL:HG22	1.85	0.58
2:D:218:GLU:HB3	2:D:247:PRO:HA	1.85	0.58
2:D:284:PHE:O	2:D:287:VAL:HG22	2.03	0.58
2:B:173:THR:HG1	6:B:951:GLN:N	2.02	0.58
2:D:338:GLU:HG2	2:D:371:VAL:HG21	1.87	0.57
1:A:44:TYR:HB2	1:A:64:ILE:HD11	1.87	0.56
2:B:485:ASN:ND2	2:B:487:GLU:OE1	2.39	0.56
2:D:455:ILE:HD12	2:D:458:ASN:HB2	1.88	0.56
2:D:37:ASP:HB3	2:D:410:TRP:CZ2	2.41	0.56
2:D:214:VAL:HG12	2:D:272:VAL:HB	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:42:GLY:O	3:H:43:LYS:HB2	2.06	0.56
3:J:149:LEU:HB3	3:J:221:ILE:HG21	1.87	0.55
5:A:901:NAG:H81	10:A:1086:HOH:O	2.05	0.55
2:B:269:LYS:HZ2	2:B:490:GLU:HB2	1.71	0.55
2:D:260:ILE:HD12	2:D:286:GLU:HB2	1.89	0.54
3:J:147:VAL:HG21	3:J:199:TRP:CD1	2.40	0.54
1:A:398:HIS:HB2	1:A:401:MET:HE2	1.88	0.54
2:B:361:PRO:O	2:B:364:TRP:HD1	1.91	0.54
3:J:200:PRO:HG3	3:J:223:PRO:HG3	1.89	0.54
2:D:311:LEU:HB3	2:D:312:PRO:CD	2.37	0.54
2:B:264:GLN:HG2	2:B:292:LEU:HD21	1.90	0.54
1:A:149:ALA:O	1:A:153:MET:HG2	2.08	0.53
2:D:478:LEU:N	10:D:1005:HOH:O	2.42	0.53
2:D:260:ILE:HA	2:D:263:ILE:CG1	2.38	0.53
2:D:218:GLU:HB2	2:D:245:LEU:HG	1.90	0.53
1:C:201:TRP:CE2	1:C:257:LYS:HD3	2.44	0.53
3:J:209:ALA:HB2	3:J:216:LYS:HE2	1.91	0.53
2:B:347:ALA:O	2:B:350:THR:OG1	2.19	0.52
2:D:452:ILE:HD12	2:D:461:LEU:HD12	1.91	0.51
1:C:398:HIS:H	1:C:401:MET:CE	2.24	0.51
2:D:262:ASN:HA	2:D:265:THR:HG22	1.93	0.51
3:H:12:VAL:HG21	3:H:86:LEU:HD13	1.93	0.51
2:B:445:PRO:HB2	2:B:447:ILE:HG12	1.92	0.51
3:J:222:VAL:HG23	3:J:223:PRO:CA	2.40	0.51
2:D:477:THR:N	10:D:1005:HOH:O	2.43	0.51
2:D:201:VAL:O	2:D:204:ILE:HG13	2.11	0.50
2:D:31:LEU:HD21	2:D:344:ILE:HD11	1.93	0.50
2:D:334:SER:HB2	2:D:335:PRO:HD3	1.93	0.50
2:D:256:ILE:O	2:D:260:ILE:HG13	2.11	0.49
3:H:181:LEU:HB2	3:H:186:TYR:CE1	2.47	0.49
3:J:12:VAL:HG11	3:J:86:LEU:HD13	1.94	0.49
3:J:149:LEU:HD21	3:J:199:TRP:NE1	2.28	0.49
2:B:269:LYS:HZ1	2:B:490:GLU:HB2	1.76	0.49
2:D:370:ASN:HD22	5:D:902:NAG:H83	1.77	0.48
5:C:901:NAG:H81	10:C:1028:HOH:O	2.12	0.48
1:C:279:ASN:HD22	5:C:903:NAG:H83	1.78	0.48
1:A:164[A]:CYS:SG	1:A:169:PHE:CE2	3.07	0.48
1:C:263:ALA:HB1	1:C:267:TYR:HB2	1.95	0.48
4:K:65:ARG:HD2	4:K:81:PRO:O	2.14	0.48
1:C:455:HIS:HB2	3:J:54:TYR:OH	2.13	0.48
2:D:278:SER:O	2:D:281:VAL:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:ILE:HG22	2:B:279:PRO:HG3	1.95	0.48
1:A:42:ILE:HD12	1:A:68:TYR:HA	1.96	0.48
1:C:452:SER:O	1:C:455:HIS:ND1	2.44	0.47
2:D:196:GLN:HE22	2:D:300:SER:H	1.62	0.47
2:B:278:SER:HB2	2:B:279:PRO:HD3	1.96	0.47
2:D:167:GLN:NE2	10:D:1009:HOH:O	2.47	0.47
1:C:347:LYS:NZ	5:C:904:NAG:H81	2.29	0.47
3:J:108:THR:HA	4:K:95:THR:O	2.14	0.47
4:K:153:LYS:HB2	4:K:197:THR:HB	1.95	0.47
2:B:455:ILE:HG13	5:B:904:NAG:H83	1.96	0.47
2:D:234:GLU:HG2	2:D:235:ASP:N	2.30	0.47
2:B:70:LYS:HE2	5:B:903:NAG:H81	1.96	0.47
2:B:343:LYS:NZ	10:B:1009:HOH:O	2.47	0.47
1:A:104:ILE:O	1:A:104:ILE:HG13	2.14	0.46
1:C:236:LYS:HD3	1:C:247:VAL:HG22	1.96	0.46
2:D:455:ILE:CD1	2:D:458:ASN:HD22	2.29	0.46
1:C:398:HIS:H	1:C:401:MET:HE3	1.80	0.46
1:C:365:PHE:C	1:C:368:PRO:HD2	2.36	0.46
1:A:155:ASN:ND2	2:B:114:ARG:HH22	2.14	0.46
2:D:464:VAL:HG12	2:D:478:LEU:HB2	1.98	0.45
2:D:373:LEU:HD21	5:D:902:NAG:H81	1.99	0.45
1:A:189:ILE:HG13	1:A:220:GLN:HB2	1.97	0.45
2:D:196:GLN:NE2	2:D:299:SER:HA	2.31	0.45
2:B:108:HIS:CE1	2:B:110:ALA:HB3	2.51	0.45
3:J:199:TRP:HH2	3:J:221:ILE:O	1.99	0.45
1:C:56:ILE:HG12	1:C:105:HIS:CG	2.51	0.45
3:J:19:LYS:NZ	10:J:302:HOH:O	2.50	0.45
2:B:101:LYS:HD2	10:B:1083:HOH:O	2.17	0.45
2:B:39:LYS:HA	2:B:99:GLY:O	2.17	0.45
2:D:182:VAL:O	2:D:184:PRO:HD3	2.17	0.44
2:D:425:LEU:HD23	2:D:425:LEU:HA	1.84	0.44
2:D:445:PRO:HB2	2:D:447:ILE:HG12	1.98	0.44
1:A:326:ILE:HD13	1:A:326:ILE:HA	1.78	0.44
2:B:409:LYS:NZ	10:B:1013:HOH:O	2.50	0.44
2:D:109:SER:O	2:D:113:VAL:HG23	2.17	0.44
3:H:130:PRO:HB3	3:H:156:TYR:HB3	1.98	0.44
2:B:148:GLN:HE21	6:B:951:GLN:HE22	1.66	0.44
2:D:455:ILE:HD11	2:D:458:ASN:HD22	1.82	0.44
3:H:43:LYS:HA	3:H:43:LYS:HD2	1.65	0.44
3:H:224:ARG:CZ	4:L:123:PRO:HG2	2.47	0.44
1:C:257:LYS:NZ	1:C:282:ASN:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:ASP:O	2:B:75:ARG:HG3	2.18	0.44
1:C:26:SER:HB3	1:C:29:HIS:CE1	2.53	0.44
2:D:284:PHE:HE1	2:D:296:TRP:CE3	2.34	0.43
1:A:456:LEU:HD12	1:A:457:SER:N	2.34	0.43
2:D:296:TRP:CD1	2:D:296:TRP:N	2.86	0.43
3:H:51:ILE:HD13	3:H:72:VAL:HG13	1.99	0.43
1:C:326:ILE:O	1:C:330:ILE:HG12	2.18	0.43
2:D:120:LEU:HD13	2:D:163:PHE:CE1	2.53	0.43
3:H:179:ALA:HA	3:H:188:LEU:HB3	2.00	0.43
2:D:260:ILE:HA	2:D:263:ILE:HG12	1.99	0.43
1:C:76:PHE:HB2	1:C:325:PHE:CD2	2.54	0.43
3:J:134:PRO:HD3	3:J:219:LYS:HZ2	1.84	0.43
2:D:453:GLN:OE1	2:D:455:ILE:HG23	2.18	0.43
2:B:37:ASP:HB3	2:B:410:TRP:CZ2	2.54	0.43
4:L:65:ARG:HD2	4:L:81:PRO:O	2.18	0.43
2:B:207:PHE:HE1	2:B:476:GLU:HG3	1.83	0.42
3:J:101:ARG:NH2	10:J:303:HOH:O	2.52	0.42
2:B:108:HIS:HE1	2:B:110:ALA:HB3	1.84	0.42
1:C:365:PHE:HA	1:C:368:PRO:HG2	2.01	0.42
3:H:108:THR:HA	4:L:95:THR:O	2.19	0.42
3:H:170:LEU:HD13	3:H:192:VAL:HG21	2.01	0.42
1:A:290:GLY:HA3	10:A:1023:HOH:O	2.18	0.42
4:L:80:ASN:HA	4:L:81:PRO:HA	1.94	0.42
2:B:253:LYS:HE2	10:B:1018:HOH:O	2.19	0.42
1:C:201:TRP:NE1	1:C:257:LYS:HD3	2.35	0.42
1:C:280:VAL:O	1:C:306:ILE:HA	2.20	0.42
2:D:284:PHE:HA	2:D:287:VAL:HG13	2.01	0.42
2:D:343:LYS:O	2:D:346:GLU:HG2	2.19	0.42
2:D:398:HIS:CE1	2:D:403:CYS:HB2	2.55	0.42
2:D:220:GLU:OE2	2:D:224:GLN:HG3	2.19	0.42
2:D:455:ILE:CD1	2:D:458:ASN:HB2	2.48	0.42
4:L:16:GLY:HA2	4:L:81:PRO:HB2	2.02	0.42
3:J:132:VAL:O	3:J:219:LYS:NZ	2.40	0.42
1:A:249:LYS:HE2	1:A:253:GLU:OE2	2.20	0.42
2:B:485:ASN:OD1	2:B:485:ASN:N	2.53	0.42
4:L:153:LYS:HB2	4:L:197:THR:HB	2.02	0.42
2:B:75:ARG:HB3	2:B:386:VAL:HG21	2.02	0.41
3:H:41:HIS:O	3:H:43:LYS:HD3	2.21	0.41
2:D:260:ILE:HG22	2:D:260:ILE:O	2.21	0.41
2:D:253:LYS:HB2	2:D:254:PRO:HD3	2.02	0.41
2:D:467:TYR:OH	2:D:470:ALA:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ASN:HD22	5:A:901:NAG:H83	1.85	0.41
1:A:70:ARG:NH2	10:A:1017:HOH:O	2.52	0.41
1:A:104:ILE:HG23	1:A:105:HIS:ND1	2.36	0.41
1:A:398:HIS:H	1:A:401:MET:CE	2.34	0.41
2:B:37:ASP:O	2:B:123:LYS:NZ	2.54	0.41
1:C:104:ILE:HG12	2:D:158:LYS:HD3	2.02	0.41
2:D:228:GLN:O	2:D:231:LYS:HB3	2.21	0.41
4:L:140:LEU:HD22	4:L:179:MET:HE1	2.02	0.41
3:J:162:THR:OG1	3:J:209:ALA:HB3	2.21	0.41
1:A:100:HIS:ND1	1:A:106:SER:HB2	2.36	0.41
1:A:121:ARG:HA	1:A:122:PRO:HD3	1.78	0.41
2:B:182:VAL:O	2:B:184:PRO:HD3	2.21	0.41
1:C:216:ASP:O	1:C:220:GLN:HG2	2.21	0.41
2:D:32:PHE:CG	2:D:359:PRO:HG2	2.55	0.41
4:K:35:SER:O	4:K:54:ARG:HA	2.20	0.41
2:B:216:GLY:HA2	2:B:274:PHE:O	2.21	0.40
4:K:23:CYS:HB2	4:K:39:TRP:CH2	2.56	0.40
1:C:384:LEU:HD22	1:C:395:ILE:CG2	2.51	0.40
4:K:80:ASN:HA	4:K:81:PRO:HA	1.99	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:310:SER:OG	4:K:206:THR:O[2_846]	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	425/461 (92%)	409 (96%)	15 (4%)	1 (0%)	47 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	422/461 (92%)	403 (96%)	17 (4%)	2 (0%)	29	31
2	B	448/478 (94%)	437 (98%)	9 (2%)	2 (0%)	34	37
2	D	405/478 (85%)	382 (94%)	17 (4%)	6 (2%)	10	8
3	H	215/225 (96%)	209 (97%)	5 (2%)	1 (0%)	29	31
3	J	213/225 (95%)	205 (96%)	6 (3%)	2 (1%)	17	16
4	K	214/217 (99%)	207 (97%)	7 (3%)	0	100	100
4	L	215/217 (99%)	207 (96%)	8 (4%)	0	100	100
All	All	2557/2762 (93%)	2459 (96%)	84 (3%)	14 (0%)	29	31

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	231	LYS
3	J	43	LYS
2	B	250	ASP
1	C	117	ASN
2	D	267	GLU
2	D	232	LYS
2	D	260	ILE
3	H	43	LYS
2	D	479	PHE
2	D	171	GLY
3	J	222	VAL
1	A	163	GLY
2	B	171	GLY
1	C	163	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	384/407 (94%)	384 (100%)	0	100	100
1	C	381/407 (94%)	378 (99%)	3 (1%)	81	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	406/428 (95%)	402 (99%)	4 (1%)	76	86
2	D	376/428 (88%)	374 (100%)	2 (0%)	88	94
3	H	189/192 (98%)	188 (100%)	1 (0%)	88	94
3	J	187/192 (97%)	185 (99%)	2 (1%)	73	85
4	K	190/191 (100%)	189 (100%)	1 (0%)	88	94
4	L	191/191 (100%)	190 (100%)	1 (0%)	88	94
All	All	2304/2436 (95%)	2290 (99%)	14 (1%)	86	93

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	27	ILE
2	B	219[A]	GLU
2	B	219[B]	GLU
2	B	480	LYS
1	C	51	GLN
1	C	331	SER
1	C	352	ASN
2	D	261	ASN
2	D	457	GLU
3	H	172	SER
4	L	198	CYS
3	J	161	VAL
3	J	206	CYS
4	K	207	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	ASN
1	A	441	ASN
2	B	167	GLN
2	B	243	GLN
1	C	441	ASN
2	D	26	ASN
2	D	148	GLN
2	D	167	GLN
2	D	196	GLN
2	D	261	ASN

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Mol	Chain	Res	Type
2	D	441	GLN
4	L	214	ASN
3	J	41	HIS
3	J	207	ASN
4	K	216	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 37 ligands modelled in this entry, 6 are monoatomic - leaving 31 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	A	902	1	14,14,15	0.55	0	17,19,21	1.07	1 (5%)
5	NAG	A	904	1	14,14,15	0.47	0	17,19,21	1.53	1 (5%)
5	NAG	D	904	2	14,14,15	0.50	0	17,19,21	0.66	0
5	NAG	C	907	1	14,14,15	0.54	0	17,19,21	1.10	2 (11%)
5	NAG	B	902	2	14,14,15	0.50	0	17,19,21	1.37	3 (17%)
5	NAG	A	906	1	14,14,15	0.51	0	17,19,21	1.05	1 (5%)
5	NAG	A	905	1	14,14,15	0.50	0	17,19,21	1.28	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	D	906	2	14,14,15	0.46	0	17,19,21	1.17	2 (11%)
6	GLN	D	951	-	8,9,9	0.83	1 (12%)	10,11,11	1.12	2 (20%)
5	NAG	B	907	2	14,14,15	0.79	1 (7%)	17,19,21	1.63	3 (17%)
5	NAG	C	902	1	14,14,15	0.56	0	17,19,21	0.79	0
5	NAG	D	902	2	14,14,15	0.53	0	17,19,21	1.83	3 (17%)
5	NAG	B	906	2	14,14,15	0.49	0	17,19,21	0.74	1 (5%)
5	NAG	B	905	2	14,14,15	0.47	0	17,19,21	1.51	2 (11%)
5	NAG	C	906	1	14,14,15	0.53	0	17,19,21	1.11	3 (17%)
5	NAG	D	903	2	14,14,15	0.39	0	17,19,21	1.73	3 (17%)
5	NAG	B	901	2	14,14,15	0.63	0	17,19,21	0.92	1 (5%)
6	GLN	C	951	-	8,9,9	0.75	0	10,11,11	0.76	0
5	NAG	C	905	1	14,14,15	0.57	0	17,19,21	1.56	2 (11%)
5	NAG	D	905	2	14,14,15	0.73	0	17,19,21	1.61	3 (17%)
5	NAG	B	903	2	14,14,15	0.48	0	17,19,21	1.31	1 (5%)
5	NAG	A	907	1	14,14,15	0.54	0	17,19,21	0.98	2 (11%)
5	NAG	C	901	1	14,14,15	0.54	0	17,19,21	1.26	2 (11%)
5	NAG	D	901	2	14,14,15	0.47	0	17,19,21	1.14	1 (5%)
5	NAG	C	903	1	14,14,15	0.48	0	17,19,21	1.14	1 (5%)
6	GLN	A	951	-	8,9,9	0.80	0	10,11,11	0.94	1 (10%)
5	NAG	A	903	1	14,14,15	0.56	0	17,19,21	0.70	0
5	NAG	A	901	1	14,14,15	0.57	0	17,19,21	1.47	2 (11%)
5	NAG	B	904	2	14,14,15	0.43	0	17,19,21	2.34	2 (11%)
5	NAG	C	904	1	14,14,15	0.52	0	17,19,21	1.27	2 (11%)
6	GLN	B	951	-	8,9,9	0.78	0	10,11,11	1.43	2 (20%)

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	A	902	1	-	2/6/23/26	0/1/1/1
5	NAG	A	904	1	-	2/6/23/26	0/1/1/1
5	NAG	D	904	2	-	2/6/23/26	0/1/1/1
5	NAG	C	907	1	-	2/6/23/26	0/1/1/1
5	NAG	B	902	2	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	906	1	-	4/6/23/26	0/1/1/1
5	NAG	A	905	1	-	4/6/23/26	0/1/1/1
5	NAG	D	906	2	-	2/6/23/26	0/1/1/1
6	GLN	D	951	-	-	1/9/9/9	-
5	NAG	B	907	2	-	3/6/23/26	0/1/1/1
5	NAG	C	902	1	-	2/6/23/26	0/1/1/1
5	NAG	D	902	2	-	4/6/23/26	0/1/1/1
5	NAG	B	906	2	-	2/6/23/26	0/1/1/1
5	NAG	B	905	2	-	2/6/23/26	0/1/1/1
5	NAG	C	906	1	-	3/6/23/26	0/1/1/1
5	NAG	D	903	2	-	2/6/23/26	0/1/1/1
5	NAG	B	901	2	-	4/6/23/26	0/1/1/1
6	GLN	C	951	-	-	0/9/9/9	-
5	NAG	C	905	1	-	3/6/23/26	0/1/1/1
5	NAG	D	905	2	-	3/6/23/26	0/1/1/1
5	NAG	B	903	2	-	4/6/23/26	0/1/1/1
5	NAG	A	907	1	-	2/6/23/26	0/1/1/1
5	NAG	C	901	1	-	2/6/23/26	0/1/1/1
5	NAG	D	901	2	-	4/6/23/26	0/1/1/1
5	NAG	C	903	1	-	4/6/23/26	0/1/1/1
6	GLN	A	951	-	-	0/9/9/9	-
5	NAG	A	903	1	-	4/6/23/26	0/1/1/1
5	NAG	A	901	1	-	2/6/23/26	0/1/1/1
5	NAG	B	904	2	-	4/6/23/26	0/1/1/1
5	NAG	C	904	1	-	2/6/23/26	0/1/1/1
6	GLN	B	951	-	-	0/9/9/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	951	GLN	OXT-C	-2.09	1.23	1.30
5	B	907	NAG	O5-C1	-2.06	1.40	1.43

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	904	NAG	C1-O5-C5	8.08	123.14	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	903	NAG	C1-O5-C5	5.40	119.50	112.19
5	D	902	NAG	C1-O5-C5	5.37	119.47	112.19
5	A	904	NAG	C1-O5-C5	5.22	119.26	112.19
5	C	905	NAG	C1-O5-C5	5.13	119.14	112.19
5	B	905	NAG	C1-O5-C5	4.99	118.95	112.19
5	A	901	NAG	C1-O5-C5	4.64	118.47	112.19
5	B	903	NAG	C1-O5-C5	4.30	118.01	112.19
5	A	905	NAG	C1-O5-C5	4.21	117.90	112.19
5	B	907	NAG	C4-C3-C2	3.76	116.53	111.02
5	B	907	NAG	C3-C4-C5	3.76	116.94	110.24
5	D	902	NAG	C4-C3-C2	-3.75	105.52	111.02
5	B	904	NAG	O5-C1-C2	3.72	117.16	111.29
5	C	903	NAG	C1-O5-C5	3.44	116.85	112.19
5	D	905	NAG	C6-C5-C4	3.39	120.95	113.00
5	D	905	NAG	O5-C1-C2	-3.24	106.17	111.29
6	B	951	GLN	OXT-C-CA	3.23	124.40	113.38
5	C	904	NAG	C1-O5-C5	3.15	116.45	112.19
5	C	901	NAG	O5-C5-C6	3.10	112.06	107.20
5	B	907	NAG	O5-C1-C2	-2.91	106.69	111.29
6	B	951	GLN	OXT-C-O	-2.89	117.52	124.09
5	C	901	NAG	C1-O5-C5	2.70	115.85	112.19
5	C	907	NAG	C1-O5-C5	2.68	115.82	112.19
5	D	901	NAG	C1-O5-C5	2.64	115.77	112.19
6	D	951	GLN	OXT-C-O	-2.57	118.25	124.09
5	D	906	NAG	O5-C1-C2	-2.56	107.25	111.29
5	B	902	NAG	C1-O5-C5	2.50	115.58	112.19
5	B	902	NAG	C2-N2-C7	-2.49	119.36	122.90
5	C	904	NAG	C2-N2-C7	-2.46	119.39	122.90
5	C	907	NAG	C2-N2-C7	2.39	126.31	122.90
5	A	906	NAG	O5-C5-C6	2.38	110.94	107.20
5	C	906	NAG	O5-C5-C6	2.37	110.92	107.20
5	B	902	NAG	O5-C1-C2	-2.29	107.67	111.29
5	C	906	NAG	C1-O5-C5	2.28	115.28	112.19
5	D	903	NAG	O5-C5-C6	2.27	110.76	107.20
6	D	951	GLN	OXT-C-CA	2.27	121.12	113.38
5	D	906	NAG	C3-C4-C5	2.19	114.15	110.24
5	D	903	NAG	C4-C3-C2	-2.18	107.82	111.02
5	B	901	NAG	C4-C3-C2	2.15	114.17	111.02
5	C	906	NAG	C6-C5-C4	-2.14	107.98	113.00
5	A	901	NAG	O5-C1-C2	2.14	114.67	111.29
5	A	902	NAG	O5-C5-C6	2.13	110.55	107.20
6	A	951	GLN	OXT-C-CA	2.11	120.58	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	907	NAG	O5-C5-C6	2.10	110.49	107.20
5	B	906	NAG	O5-C5-C6	2.10	110.49	107.20
5	C	905	NAG	O5-C1-C2	2.09	114.60	111.29
5	A	907	NAG	C1-O5-C5	2.09	115.02	112.19
5	D	905	NAG	C4-C3-C2	2.07	114.06	111.02
5	D	902	NAG	O5-C5-C4	2.05	115.81	110.83
5	B	905	NAG	O5-C5-C6	2.02	110.37	107.20

There are no chirality outliers.

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	904	NAG	O5-C5-C6-O6
5	B	903	NAG	O5-C5-C6-O6
5	A	905	NAG	O5-C5-C6-O6
5	B	901	NAG	O5-C5-C6-O6
5	D	902	NAG	C4-C5-C6-O6
5	A	903	NAG	O5-C5-C6-O6
5	B	904	NAG	C4-C5-C6-O6
5	A	901	NAG	C8-C7-N2-C2
5	A	901	NAG	O7-C7-N2-C2
5	A	902	NAG	C8-C7-N2-C2
5	A	902	NAG	O7-C7-N2-C2
5	A	903	NAG	C8-C7-N2-C2
5	A	903	NAG	O7-C7-N2-C2
5	A	904	NAG	C8-C7-N2-C2
5	A	904	NAG	O7-C7-N2-C2
5	A	905	NAG	C8-C7-N2-C2
5	A	905	NAG	O7-C7-N2-C2
5	A	906	NAG	C8-C7-N2-C2
5	A	906	NAG	O7-C7-N2-C2
5	A	907	NAG	C8-C7-N2-C2
5	A	907	NAG	O7-C7-N2-C2
5	B	901	NAG	C8-C7-N2-C2
5	B	901	NAG	O7-C7-N2-C2
5	B	902	NAG	C8-C7-N2-C2
5	B	902	NAG	O7-C7-N2-C2
5	B	903	NAG	C8-C7-N2-C2
5	B	903	NAG	O7-C7-N2-C2
5	B	904	NAG	C8-C7-N2-C2
5	B	904	NAG	O7-C7-N2-C2
5	B	905	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	B	905	NAG	O7-C7-N2-C2
5	B	906	NAG	C8-C7-N2-C2
5	B	906	NAG	O7-C7-N2-C2
5	B	907	NAG	C8-C7-N2-C2
5	B	907	NAG	O7-C7-N2-C2
5	C	901	NAG	C8-C7-N2-C2
5	C	901	NAG	O7-C7-N2-C2
5	C	902	NAG	C8-C7-N2-C2
5	C	902	NAG	O7-C7-N2-C2
5	C	903	NAG	C8-C7-N2-C2
5	C	903	NAG	O7-C7-N2-C2
5	C	904	NAG	C8-C7-N2-C2
5	C	904	NAG	O7-C7-N2-C2
5	C	905	NAG	C8-C7-N2-C2
5	C	905	NAG	O7-C7-N2-C2
5	C	906	NAG	C8-C7-N2-C2
5	C	906	NAG	O7-C7-N2-C2
5	C	907	NAG	C8-C7-N2-C2
5	C	907	NAG	O7-C7-N2-C2
5	D	901	NAG	C8-C7-N2-C2
5	D	901	NAG	O7-C7-N2-C2
5	D	902	NAG	C8-C7-N2-C2
5	D	902	NAG	O7-C7-N2-C2
5	D	903	NAG	C8-C7-N2-C2
5	D	903	NAG	O7-C7-N2-C2
5	D	904	NAG	C8-C7-N2-C2
5	D	904	NAG	O7-C7-N2-C2
5	D	905	NAG	C8-C7-N2-C2
5	D	905	NAG	O7-C7-N2-C2
5	D	906	NAG	C8-C7-N2-C2
5	D	906	NAG	O7-C7-N2-C2
5	B	901	NAG	C4-C5-C6-O6
5	A	903	NAG	C4-C5-C6-O6
5	A	906	NAG	O5-C5-C6-O6
5	A	905	NAG	C4-C5-C6-O6
5	B	903	NAG	C4-C5-C6-O6
5	C	903	NAG	C4-C5-C6-O6
5	C	903	NAG	O5-C5-C6-O6
5	A	906	NAG	C4-C5-C6-O6
5	B	902	NAG	O5-C5-C6-O6
5	B	902	NAG	C4-C5-C6-O6
5	D	902	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	D	905	NAG	O5-C5-C6-O6
5	D	901	NAG	C4-C5-C6-O6
5	D	901	NAG	O5-C5-C6-O6
5	B	907	NAG	O5-C5-C6-O6
6	D	951	GLN	CA-CB-CG-CD
5	C	906	NAG	O5-C5-C6-O6
5	C	905	NAG	O5-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	902	NAG	2	0
5	D	903	NAG	1	0
5	B	903	NAG	1	0
5	C	901	NAG	1	0
5	C	903	NAG	1	0
5	A	901	NAG	2	0
5	B	904	NAG	1	0
5	C	904	NAG	1	0
6	B	951	GLN	4	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%)	-0.35	4 (0%)	84	83	26, 39, 74, 126	0
1	C	427/461 (92%)	-0.32	8 (1%)	66	65	29, 42, 77, 130	0
2	B	452/478 (94%)	-0.25	10 (2%)	62	59	28, 50, 83, 123	0
2	D	422/478 (88%)	0.21	33 (7%)	13	11	33, 61, 116, 149	0
3	H	219/225 (97%)	-0.56	2 (0%)	84	83	28, 47, 74, 112	0
3	J	217/225 (96%)	-0.46	3 (1%)	75	73	31, 51, 84, 121	0
4	K	216/217 (99%)	-0.71	0	100	100	31, 41, 64, 92	0
4	L	217/217 (100%)	-0.62	0	100	100	27, 45, 69, 92	0
All	All	2599/2762 (94%)	-0.32	60 (2%)	60	58	26, 47, 93, 149	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	260	ILE	7.8
2	D	263	ILE	5.3
2	B	364	TRP	4.7
2	B	357	TYR	4.2
2	D	296	TRP	4.0
3	J	199	TRP	4.0
2	D	204	ILE	3.8
2	D	475	ASN	3.8
2	D	479	PHE	3.5
2	D	261	ASN	3.4
1	A	396	THR	3.3
1	C	394	ASN	3.2
2	D	271	VAL	3.2
1	C	455	HIS	3.2
2	D	357	TYR	3.2
2	D	268	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	364	TRP	3.1
2	D	254	PRO	3.1
3	H	143	THR	3.1
2	B	344	ILE	3.0
2	D	488	LYS	3.0
2	D	257	GLN	2.9
2	D	358	ASN	2.9
1	C	396	THR	2.9
1	A	130	LEU	2.9
2	D	264	GLN	2.8
2	D	270	VAL	2.8
1	C	119	LEU	2.8
2	B	358	ASN	2.8
1	C	393	LYS	2.8
2	D	347	ALA	2.7
1	C	342	MET	2.7
2	D	63	VAL	2.7
1	C	117	ASN	2.7
1	A	117	ASN	2.6
2	D	244	GLY	2.5
1	C	25	THR	2.5
2	D	255	ALA	2.5
2	D	348	SER	2.5
2	B	63	VAL	2.5
2	D	474	ILE	2.5
2	D	258	THR	2.4
3	J	1	GLU	2.4
2	B	361	PRO	2.4
2	D	206	LYS	2.4
2	D	253	LYS	2.4
2	D	284	PHE	2.2
2	B	350	THR	2.2
2	D	207	PHE	2.2
2	D	319	THR	2.2
2	B	365	SER	2.2
2	D	317	ILE	2.2
3	H	75	SER	2.2
2	D	481	TRP	2.1
2	B	347	ALA	2.1
1	A	390	ARG	2.0
3	J	201	SER	2.0
2	B	153	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	283	PHE	2.0
2	D	26	ASN	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	905	14/15	0.49	0.53	124,144,156,156	0
5	NAG	D	906	14/15	0.68	0.38	112,120,126,129	0
5	NAG	B	901	14/15	0.71	0.32	94,110,121,123	0
5	NAG	B	906	14/15	0.73	0.35	94,106,113,116	0
5	NAG	B	905	14/15	0.74	0.35	96,115,123,127	0
5	NAG	C	902	14/15	0.75	0.29	94,108,123,128	0
5	NAG	B	904	14/15	0.77	0.21	101,111,121,124	0
5	NAG	D	904	14/15	0.77	0.28	98,111,118,118	0
5	NAG	C	903	14/15	0.79	0.19	70,79,93,94	0
5	NAG	B	907	14/15	0.82	0.29	89,99,105,107	0
5	NAG	A	905	14/15	0.82	0.21	77,89,91,96	0
9	CA	L	971	1/1	0.83	0.24	97,97,97,97	0
5	NAG	D	903	14/15	0.85	0.25	81,107,114,116	0
5	NAG	A	902	14/15	0.87	0.39	88,101,105,107	0
5	NAG	C	905	14/15	0.88	0.15	72,86,93,96	0
7	NA	D	961	1/1	0.90	0.06	60,60,60,60	0
5	NAG	A	907	14/15	0.91	0.23	88,111,114,118	0
5	NAG	D	902	14/15	0.91	0.16	45,63,75,82	0
5	NAG	A	903	14/15	0.91	0.15	75,89,103,104	0
5	NAG	B	903	14/15	0.91	0.22	77,94,105,106	0
5	NAG	C	907	14/15	0.92	0.17	46,64,79,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	B	902	14/15	0.93	0.11	39,56,70,75	0
5	NAG	A	904	14/15	0.93	0.13	55,66,72,80	0
5	NAG	A	906	14/15	0.93	0.12	49,57,66,67	0
5	NAG	C	906	14/15	0.93	0.08	47,58,67,68	0
5	NAG	C	904	14/15	0.94	0.18	53,68,80,81	0
7	NA	A	961	1/1	0.94	0.06	41,41,41,41	0
6	GLN	D	951	10/10	0.95	0.18	43,49,78,84	0
5	NAG	D	901	14/15	0.96	0.14	49,62,79,83	0
6	GLN	B	951	10/10	0.96	0.17	29,38,68,78	0
8	CL	B	971	1/1	0.97	0.41	79,79,79,79	0
5	NAG	C	901	14/15	0.97	0.09	28,41,47,59	0
7	NA	C	961	1/1	0.98	0.10	39,39,39,39	0
6	GLN	C	951	10/10	0.98	0.16	24,33,39,43	0
6	GLN	A	951	10/10	0.98	0.17	26,29,39,39	0
5	NAG	A	901	14/15	0.98	0.09	28,37,44,50	0
8	CL	D	971	1/1	0.99	0.12	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.