Full wwPDB X-ray Structure Validation Report (i)

Mar 23, 2024 – 10:26 AM EDT

PDB ID	:	5KXI
Title	:	X-ray structure of the human Alpha4Beta2 nicotinic receptor
Authors	:	Morales-Perez, C.L.; Noviello, C.M.; Hibbs, R.E.
Deposited on	:	2016-07-20
Resolution	:	3.94 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:

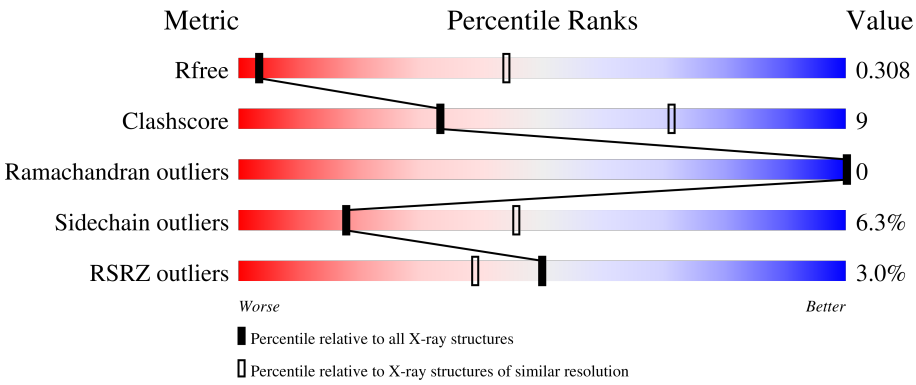
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 3.94 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	1036 (4.20-3.68)
Clashscore	141614	1009 (4.18-3.70)
Ramachandran outliers	138981	1057 (4.20-3.68)
Sidechain outliers	138945	1049 (4.20-3.68)
RSRZ outliers	127900	1007 (4.24-3.64)

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	386	3% 71% 22% • 6%
1	D	386	3% 73% 20% • 6%
2	B	403	3% 63% 24% • 11%
2	C	403	% 64% 24% • 11%
2	E	403	3% 64% 24% • 11%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14805 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 Neuronal acetylcholine receptor subunit alpha-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	363	2983	1968	482	516	17	0	0	0
1	D	363	2983	1968	482	516	17	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ASP	-	linker	UNP P43681
A	340	THR	-	linker	UNP P43681
A	341	ASP	-	linker	UNP P43681
A	342	PHE	-	linker	UNP P43681
A	343	GLU	-	linker	UNP P43681
A	344	ARG	-	linker	UNP P43681
D	339	ASP	-	linker	UNP P43681
D	340	THR	-	linker	UNP P43681
D	341	ASP	-	linker	UNP P43681
D	342	PHE	-	linker	UNP P43681
D	343	GLU	-	linker	UNP P43681
D	344	ARG	-	linker	UNP P43681

- Molecule 2 is a protein called Neuronal acetylcholine receptor subunit beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	358	2913	1915	459	521	18	0	0	0
2	C	358	2913	1915	459	521	18	0	0	0
2	E	358	2913	1915	459	521	18	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	331	ASP	-	linker	UNP P17787
B	332	ASP	-	linker	UNP P17787
B	333	ASP	-	linker	UNP P17787
B	334	GLN	-	linker	UNP P17787
B	335	GLU	-	linker	UNP P17787
B	336	ARG	-	linker	UNP P17787
B	394	SER	-	expression tag	UNP P17787
B	395	ALA	-	expression tag	UNP P17787
B	396	TRP	-	expression tag	UNP P17787
B	397	SER	-	expression tag	UNP P17787
B	398	HIS	-	expression tag	UNP P17787
B	399	PRO	-	expression tag	UNP P17787
B	400	GLN	-	expression tag	UNP P17787
B	401	PHE	-	expression tag	UNP P17787
B	402	GLU	-	expression tag	UNP P17787
B	403	LYS	-	expression tag	UNP P17787
C	331	ASP	-	linker	UNP P17787
C	332	ASP	-	linker	UNP P17787
C	333	ASP	-	linker	UNP P17787
C	334	GLN	-	linker	UNP P17787
C	335	GLU	-	linker	UNP P17787
C	336	ARG	-	linker	UNP P17787
C	394	SER	-	expression tag	UNP P17787
C	395	ALA	-	expression tag	UNP P17787
C	396	TRP	-	expression tag	UNP P17787
C	397	SER	-	expression tag	UNP P17787
C	398	HIS	-	expression tag	UNP P17787
C	399	PRO	-	expression tag	UNP P17787
C	400	GLN	-	expression tag	UNP P17787
C	401	PHE	-	expression tag	UNP P17787
C	402	GLU	-	expression tag	UNP P17787
C	403	LYS	-	expression tag	UNP P17787
E	331	ASP	-	linker	UNP P17787
E	332	ASP	-	linker	UNP P17787
E	333	ASP	-	linker	UNP P17787
E	334	GLN	-	linker	UNP P17787
E	335	GLU	-	linker	UNP P17787
E	336	ARG	-	linker	UNP P17787
E	394	SER	-	expression tag	UNP P17787
E	395	ALA	-	expression tag	UNP P17787
E	396	TRP	-	expression tag	UNP P17787
E	397	SER	-	expression tag	UNP P17787
E	398	HIS	-	expression tag	UNP P17787

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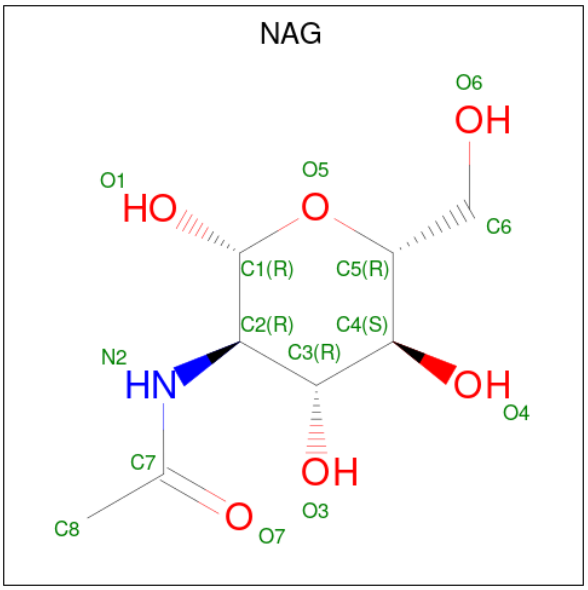
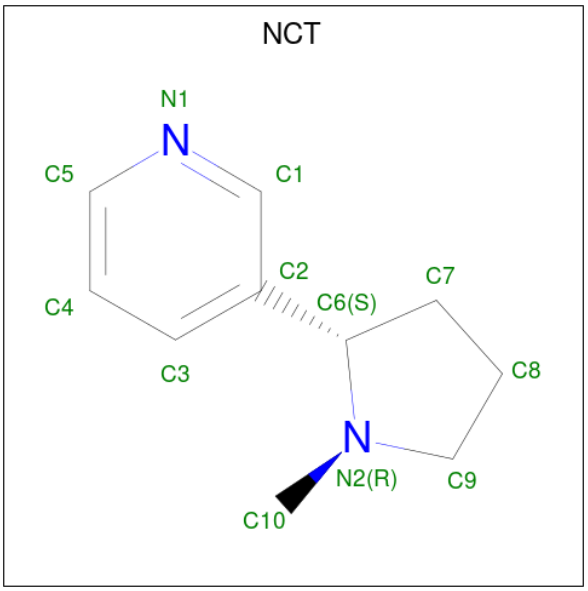
Chain	Residue	Modelled	Actual	Comment	Reference
E	399	PRO	-	expression tag	UNP P17787
E	400	GLN	-	expression tag	UNP P17787
E	401	PHE	-	expression tag	UNP P17787
E	402	GLU	-	expression tag	UNP P17787
E	403	LYS	-	expression tag	UNP P17787

- Molecule 3 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		
3	A	1	14	8	1	5	0	0
3	B	1	14	8	1	5	0	0
3	C	1	14	8	1	5	0	0
3	D	1	14	8	1	5	0	0
3	E	1	14	8	1	5	0	0

- Molecule 4 is (S)-3-(1-METHYLPYRROLIDIN-2-YL)PYRIDINE (three-letter code: NCT) (formula: $C_{10}H_{14}N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 12 10 2	0	0
4	D	1	Total C N 12 10 2	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 6 is water.

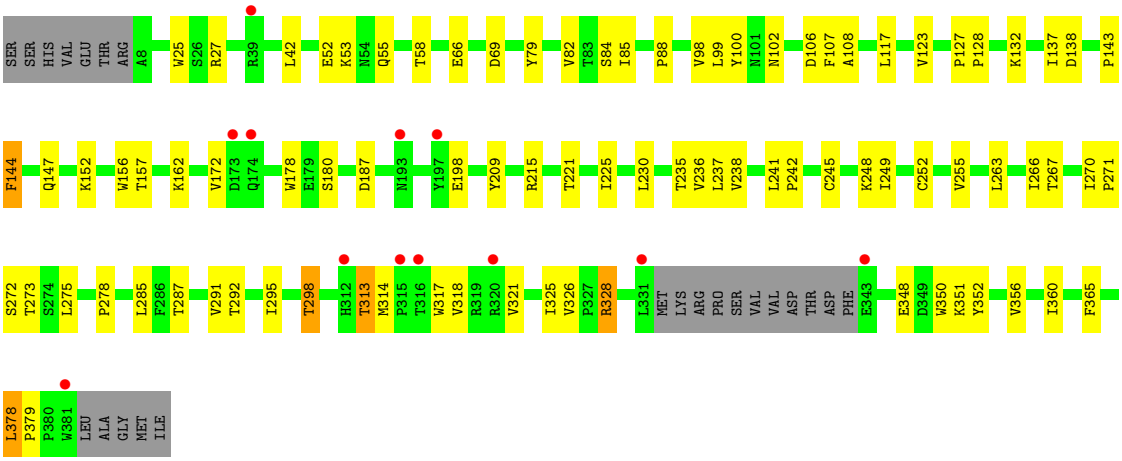
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 1 1	0	0
6	B	1	Total O 1 1	0	0
6	C	1	Total O 1 1	0	0
6	D	1	Total O 1 1	0	0
6	E	1	Total O 1 1	0	0

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.

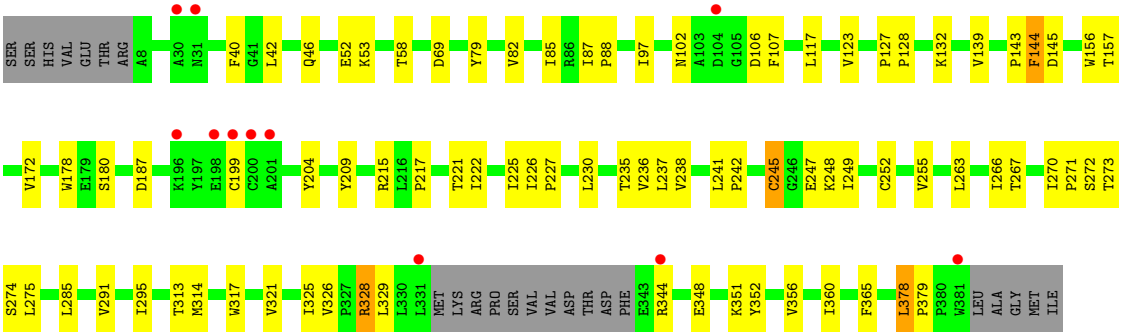
• Molecule 1: Neuronal acetylcholine receptor subunit alpha-4

Chain A:



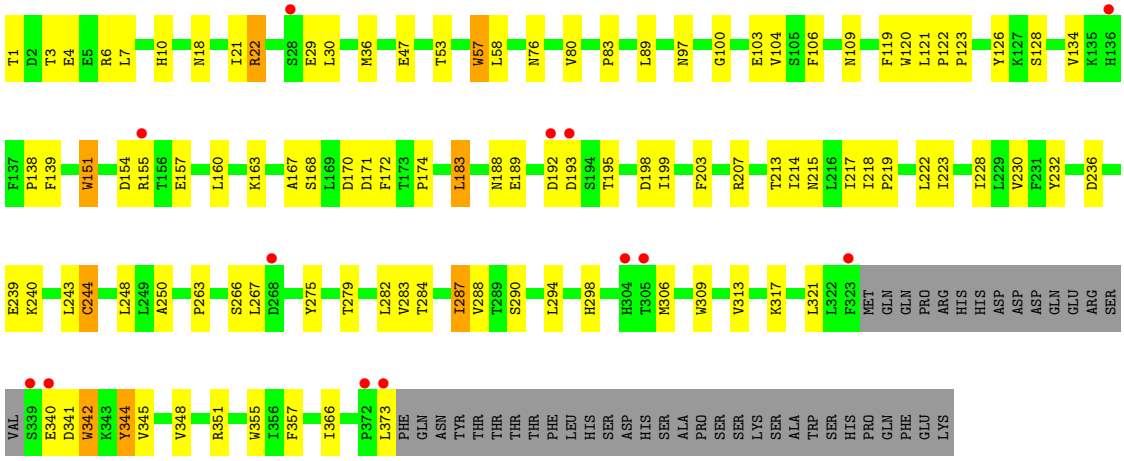
• Molecule 1: Neuronal acetylcholine receptor subunit alpha-4

Chain D:



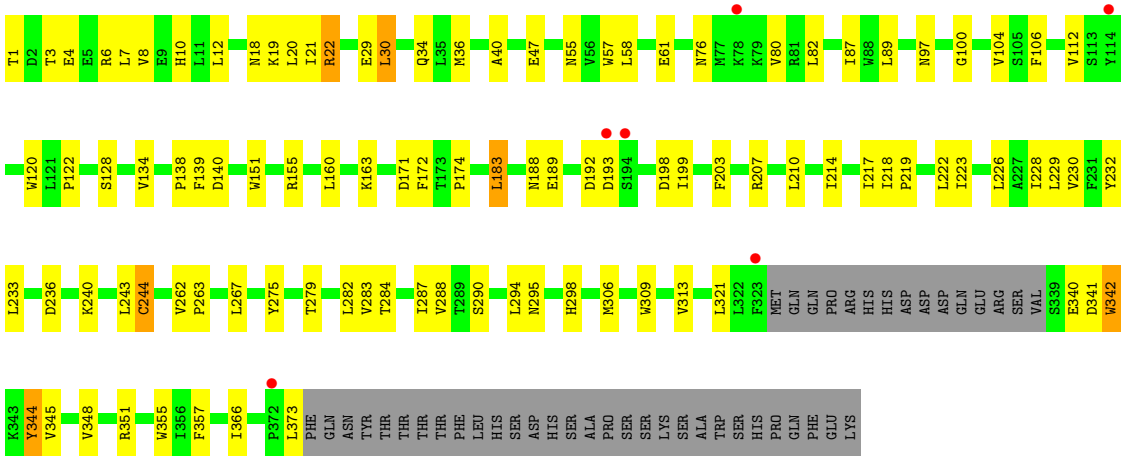
• Molecule 2: Neuronal acetylcholine receptor subunit beta-2

Chain B:



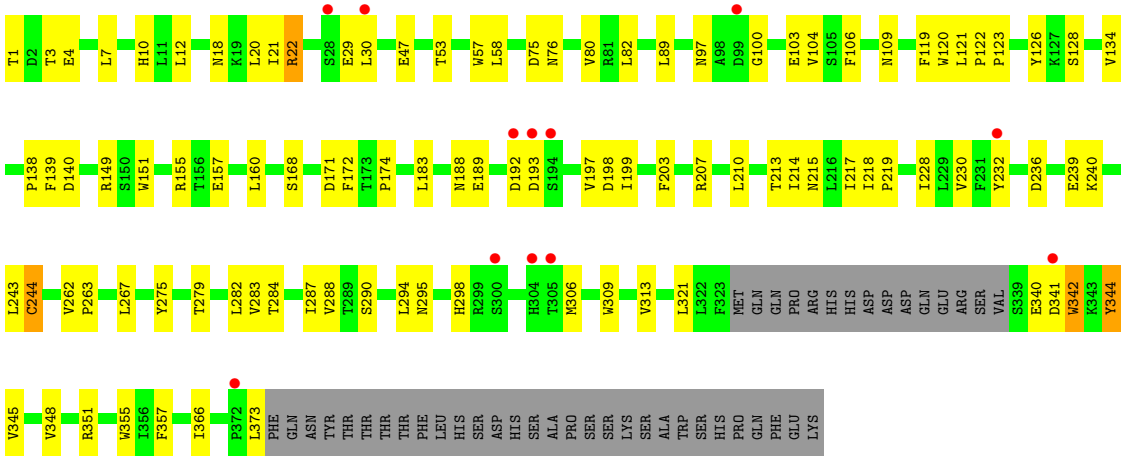
- Molecule 2: Neuronal acetylcholine receptor subunit beta-2

Chain C:



- Molecule 2: Neuronal acetylcholine receptor subunit beta-2

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	127.10Å 132.63Å 202.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.94 25.00 – 3.94	Depositor EDS
% Data completeness (in resolution range)	86.8 (25.00-3.94) 86.8 (25.00-3.94)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.10 (at 3.97Å)	Xtriage
Refinement program	PHENIX (1.10_2155)	Depositor
R, R_{free}	0.285 , 0.307 0.285 , 0.308	Depositor DCC
R_{free} test set	1331 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	159.8	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 66.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	14805	wwPDB-VP
Average B, all atoms (Å^2)	170.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: NCT, NA, 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	0.26	0/3068	0.46	1/4191 (0.0%)
1	D	0.25	0/3068	0.45	1/4191 (0.0%)
2	B	0.26	0/2993	0.47	0/4089
2	C	0.26	0/2993	0.47	0/4089
2	E	0.26	0/2993	0.47	0/4089
All	All	0.26	0/15115	0.46	2/20649 (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	D	378	LEU	CA-CB-CG	5.54	128.03	115.30
1	A	378	LEU	CA-CB-CG	5.42	127.76	115.30

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	2983	0	3015	60	0
1	D	2983	0	3015	59	0
2	B	2913	0	2936	59	0
2	C	2913	0	2936	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	2913	0	2936	53	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
3	D	14	0	13	0	0
3	E	14	0	13	0	0
4	A	12	0	14	2	0
4	D	12	0	14	4	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
All	All	14805	0	14931	255	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 9.

All (255) 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:97:ASN:HB3	2:B:100:GLY:HA3	1.52	0.91
2:C:97:ASN:HB3	2:C:100:GLY:HA3	1.53	0.90
2:E:97:ASN:HB3	2:E:100:GLY:HA3	1.53	0.88
1:A:325:ILE:HG21	1:A:360:ILE:HD11	1.58	0.83
1:D:325:ILE:HG21	1:D:360:ILE:HD11	1.62	0.79
1:D:241:LEU:HD12	1:D:242:PRO:HD2	1.66	0.78
1:A:241:LEU:HD12	1:A:242:PRO:HD2	1.65	0.77
1:A:230:LEU:HB3	2:E:284:THR:HG21	1.69	0.75
1:D:143:PRO:HD3	1:D:225:ILE:HD11	1.72	0.71
1:D:156:TRP:CZ2	2:E:123:PRO:HG3	2.27	0.69
1:A:156:TRP:CZ2	2:B:123:PRO:HG3	2.28	0.69
2:B:138:PRO:HD3	2:B:217:ILE:HD11	1.75	0.68
2:B:21:ILE:HD11	2:C:8:VAL:HG21	1.75	0.68
1:D:157:THR:HG21	2:E:109:ASN:HB2	1.76	0.67
2:C:138:PRO:HD3	2:C:217:ILE:HD11	1.76	0.67
1:A:143:PRO:HD3	1:A:225:ILE:HD11	1.76	0.66
2:B:47:GLU:OE2	2:B:207:ARG:NH2	2.30	0.65
2:C:20:LEU:HD22	1:D:88:PRO:HG3	1.79	0.64
2:E:134:VAL:HG21	2:E:263:PRO:HD2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:214:ILE:HA	2:E:218:ILE:HD12	1.78	0.64
1:D:249:ILE:HD11	2:E:239:GLU:HB3	1.80	0.63
2:E:47:GLU:OE2	2:E:207:ARG:NH2	2.30	0.63
2:C:284:THR:HG21	1:D:230:LEU:HB3	1.80	0.62
1:A:249:ILE:HD11	2:B:239:GLU:HB3	1.81	0.62
1:D:52:GLU:OE2	1:D:215:ARG:NH2	2.32	0.62
1:A:378:LEU:HG	1:A:379:PRO:HD3	1.82	0.61
1:D:378:LEU:HG	1:D:379:PRO:HD3	1.81	0.61
2:C:192:ASP:OD1	2:C:193:ASP:N	2.34	0.60
2:B:228:ILE:HD12	2:B:357:PHE:HB3	1.84	0.60
2:E:138:PRO:HD3	2:E:217:ILE:HD11	1.84	0.60
2:E:192:ASP:OD1	2:E:193:ASP:N	2.35	0.59
2:C:155:ARG:NH1	2:C:189:GLU:OE2	2.34	0.59
2:C:21:ILE:HD11	1:D:85:ILE:HD11	1.85	0.59
2:B:192:ASP:OD1	2:B:193:ASP:N	2.36	0.59
2:B:214:ILE:HA	2:B:218:ILE:HD12	1.85	0.59
1:D:238:VAL:HG11	1:D:252:CYS:SG	2.44	0.58
2:C:342:TRP:HA	2:C:342:TRP:CE3	2.39	0.58
1:D:348:GLU:HA	1:D:351:LYS:HG2	1.86	0.58
2:E:160:LEU:HB3	2:E:199:ILE:HD11	1.84	0.58
2:B:160:LEU:HB3	2:B:199:ILE:HD11	1.86	0.58
2:B:266:SER:HB3	2:C:210:LEU:HB3	1.86	0.58
2:E:306:MET:HG3	2:E:309:TRP:HB2	1.84	0.58
1:D:58:THR:HG22	1:D:132:LYS:HG2	1.86	0.58
2:C:47:GLU:OE2	2:C:207:ARG:NH2	2.37	0.57
2:B:342:TRP:HA	2:B:342:TRP:CE3	2.40	0.57
2:C:160:LEU:HB3	2:C:199:ILE:HD11	1.85	0.57
1:D:325:ILE:HA	1:D:328:ARG:HB3	1.87	0.57
2:B:155:ARG:NH1	2:B:189:GLU:OE2	2.38	0.56
2:C:230:VAL:HG22	2:C:243:LEU:HG	1.87	0.56
1:A:248:LYS:HG3	1:A:298:THR:HG23	1.87	0.56
1:A:237:LEU:HD21	2:E:288:VAL:HA	1.88	0.56
2:C:240:LYS:HD3	2:C:294:LEU:HD21	1.88	0.56
2:E:342:TRP:HA	2:E:342:TRP:CE3	2.40	0.56
1:A:325:ILE:HA	1:A:328:ARG:HB3	1.88	0.55
2:E:140:ASP:OD1	2:E:207:ARG:NH1	2.39	0.55
2:C:306:MET:HG3	2:C:309:TRP:HB2	1.88	0.55
1:A:238:VAL:HG11	1:A:252:CYS:SG	2.47	0.55
1:D:102:ASN:HD22	1:D:107:PHE:HA	1.71	0.55
2:B:306:MET:HG3	2:B:309:TRP:HB2	1.89	0.55
2:C:120:TRP:CE2	2:C:122:PRO:HG3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:240:LYS:HD3	2:B:294:LEU:HD21	1.90	0.54
2:B:321:LEU:HD21	2:B:351:ARG:HB3	1.88	0.54
2:E:344:TYR:O	2:E:348:VAL:HG23	2.08	0.54
2:C:214:ILE:HA	2:C:218:ILE:HD12	1.89	0.54
2:B:106:PHE:HB3	2:B:123:PRO:HD2	1.89	0.54
2:B:279:THR:O	2:B:283:VAL:HG23	2.08	0.54
2:B:230:VAL:HG22	2:B:243:LEU:HG	1.90	0.54
2:C:279:THR:O	2:C:283:VAL:HG23	2.08	0.54
2:C:344:TYR:O	2:C:348:VAL:HG23	2.08	0.53
2:E:106:PHE:HB3	2:E:123:PRO:HD2	1.90	0.53
2:E:240:LYS:HD3	2:E:294:LEU:HD21	1.90	0.53
2:B:120:TRP:CE2	2:B:122:PRO:HG3	2.43	0.53
2:C:228:ILE:HD12	2:C:357:PHE:HB3	1.91	0.53
2:E:279:THR:O	2:E:283:VAL:HG23	2.08	0.53
2:C:321:LEU:HD21	2:C:351:ARG:HB3	1.91	0.53
2:E:313:VAL:HG11	2:E:345:VAL:HG13	1.91	0.53
2:B:344:TYR:O	2:B:348:VAL:HG23	2.08	0.53
2:C:1:THR:HA	2:C:4:GLU:HB2	1.89	0.53
1:A:291:VAL:O	1:A:295:ILE:HG13	2.09	0.52
2:E:321:LEU:HD21	2:E:351:ARG:HB3	1.89	0.52
1:A:102:ASN:HD22	1:A:107:PHE:HA	1.75	0.52
1:A:348:GLU:HA	1:A:351:LYS:HG2	1.92	0.52
2:E:120:TRP:CE2	2:E:122:PRO:HG3	2.44	0.52
1:A:42:LEU:HB3	1:A:172:VAL:HG13	1.92	0.52
2:B:22:ARG:NH2	2:B:29:GLU:O	2.40	0.52
2:E:155:ARG:NH1	2:E:189:GLU:OE2	2.43	0.52
1:A:252:CYS:HB3	1:A:295:ILE:HG12	1.91	0.51
2:E:228:ILE:HD12	2:E:357:PHE:HB3	1.92	0.51
1:D:266:ILE:HG22	1:D:270:ILE:HD11	1.93	0.51
1:A:100:TYR:HB2	1:A:152:LYS:HB3	1.92	0.51
2:E:230:VAL:HG22	2:E:243:LEU:HG	1.92	0.51
2:C:22:ARG:NH2	2:C:29:GLU:O	2.41	0.51
2:C:288:VAL:HA	1:D:237:LEU:HD21	1.92	0.51
2:C:313:VAL:HG11	2:C:345:VAL:HG13	1.92	0.51
1:D:291:VAL:O	1:D:295:ILE:HG13	2.10	0.51
1:A:52:GLU:OE2	1:A:215:ARG:NH2	2.44	0.50
1:D:204:TYR:CZ	4:D:402:NCT:HC3	2.46	0.50
2:B:342:TRP:HA	2:B:342:TRP:HE3	1.76	0.50
1:D:314:MET:HB2	1:D:317:TRP:CD1	2.47	0.50
4:A:402:NCT:HC82	2:B:57:TRP:CZ3	2.47	0.50
2:C:342:TRP:HA	2:C:342:TRP:HE3	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:LEU:HD23	2:B:80:VAL:HG21	1.94	0.49
1:A:138:ASP:O	1:A:147:GLN:NE2	2.40	0.49
1:A:102:ASN:ND2	1:A:106:ASP:O	2.44	0.49
1:A:263:LEU:O	1:A:267:THR:HG23	2.12	0.49
1:A:266:ILE:HG22	1:A:270:ILE:HD11	1.93	0.49
2:E:213:THR:HA	2:E:217:ILE:HD12	1.94	0.49
1:D:145:ASP:OD1	1:D:215:ARG:NH1	2.45	0.49
2:B:134:VAL:HG21	2:B:263:PRO:HD2	1.93	0.49
1:D:172:VAL:HG22	1:D:209:TYR:CD1	2.47	0.49
2:E:214:ILE:O	2:E:219:PRO:HD3	2.13	0.49
2:C:188:ASN:HB2	2:C:198:ASP:HB2	1.95	0.49
1:D:267:THR:HG21	2:E:215:ASN:HB3	1.94	0.49
1:A:58:THR:HG22	1:A:132:LYS:HG2	1.94	0.49
1:A:352:TYR:O	1:A:356:VAL:HG23	2.13	0.49
2:E:188:ASN:HB2	2:E:198:ASP:HB2	1.93	0.49
1:A:178:TRP:NE1	1:A:180:SER:HB2	2.28	0.48
2:B:36:MET:HB2	2:B:163:LYS:HB2	1.95	0.48
2:B:313:VAL:HG11	2:B:345:VAL:HG13	1.94	0.48
2:C:134:VAL:HG21	2:C:263:PRO:HD2	1.95	0.48
2:E:172:PHE:CE2	2:E:174:PRO:HA	2.48	0.48
2:C:214:ILE:O	2:C:219:PRO:HD3	2.14	0.48
1:D:178:TRP:NE1	1:D:180:SER:HB2	2.29	0.48
1:A:313:THR:HG1	1:A:350:TRP:HZ2	1.59	0.48
1:A:117:LEU:HD23	1:A:123:VAL:HB	1.96	0.48
1:D:263:LEU:O	1:D:267:THR:HG23	2.13	0.48
1:D:314:MET:HB2	1:D:317:TRP:HD1	1.78	0.48
2:B:287:ILE:HG21	2:C:226:LEU:HD11	1.94	0.48
1:D:241:LEU:HD23	1:D:248:LYS:HA	1.96	0.48
2:B:214:ILE:O	2:B:219:PRO:HD3	2.12	0.48
1:D:252:CYS:HB3	1:D:295:ILE:HG12	1.95	0.48
2:E:1:THR:HA	2:E:4:GLU:HB2	1.96	0.48
2:E:7:LEU:HD23	2:E:80:VAL:HG21	1.96	0.48
1:D:352:TYR:O	1:D:356:VAL:HG23	2.14	0.47
1:A:156:TRP:CD1	4:A:402:NCT:HC1	2.49	0.47
2:C:97:ASN:O	1:D:46:GLN:NE2	2.47	0.47
2:C:7:LEU:HD23	2:C:80:VAL:HG21	1.96	0.47
1:D:221:THR:HA	1:D:225:ILE:HD12	1.96	0.47
1:D:117:LEU:HD23	1:D:123:VAL:HB	1.96	0.47
1:A:221:THR:HA	1:A:225:ILE:HD12	1.97	0.47
2:C:223:ILE:O	2:C:226:LEU:HB2	2.15	0.47
1:A:321:VAL:O	1:A:326:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:THR:HA	2:B:4:GLU:HB2	1.97	0.46
1:A:285:LEU:HD22	2:B:214:ILE:HG23	1.96	0.46
2:B:188:ASN:HB2	2:B:198:ASP:HB2	1.96	0.46
2:C:58:LEU:HD21	2:C:104:VAL:HG11	1.97	0.46
2:E:342:TRP:HA	2:E:342:TRP:HE3	1.78	0.46
1:A:79:TYR:O	1:A:82:VAL:HG22	2.16	0.46
1:D:139:VAL:HG21	1:D:271:PRO:HD2	1.98	0.46
2:B:294:LEU:HD12	2:C:233:LEU:HD11	1.98	0.46
1:D:40:PHE:HZ	1:D:97:ILE:HG21	1.81	0.45
1:A:172:VAL:HG22	1:A:209:TYR:CD1	2.50	0.45
2:C:290:SER:O	2:C:294:LEU:HG	2.16	0.45
1:D:321:VAL:O	1:D:326:VAL:HG23	2.16	0.45
1:A:98:VAL:HA	1:A:108:ALA:HB2	1.97	0.45
2:C:172:PHE:CE2	2:C:174:PRO:HA	2.52	0.45
1:A:267:THR:HG21	2:B:215:ASN:HB3	1.99	0.45
1:D:79:TYR:O	1:D:82:VAL:HG22	2.16	0.45
1:D:266:ILE:O	1:D:270:ILE:HG13	2.17	0.45
2:C:36:MET:HB2	2:C:163:LYS:HB2	1.99	0.45
1:D:42:LEU:HB3	1:D:172:VAL:HG13	1.99	0.45
1:A:55:GLN:HE21	1:A:271:PRO:HB2	1.82	0.45
2:E:183:LEU:HD21	2:E:203:PHE:CE2	2.52	0.45
1:D:267:THR:HA	1:D:270:ILE:HD12	1.99	0.45
2:E:58:LEU:HD23	2:E:122:PRO:HD2	1.99	0.45
2:E:230:VAL:HG11	2:E:244:CYS:SG	2.57	0.45
2:B:213:THR:HA	2:B:217:ILE:HD12	1.99	0.44
2:B:58:LEU:HD23	2:B:122:PRO:HD2	1.99	0.44
1:D:52:GLU:O	1:D:271:PRO:HB3	2.16	0.44
2:C:183:LEU:HD21	2:C:203:PHE:CE2	2.53	0.44
4:D:402:NCT:HC72	2:E:121:LEU:HD11	1.99	0.44
2:E:134:VAL:HG11	2:E:262:VAL:HG22	2.00	0.44
1:A:314:MET:HB2	1:A:317:TRP:CD1	2.53	0.44
2:B:230:VAL:HG11	2:B:244:CYS:SG	2.58	0.44
1:D:348:GLU:HA	1:D:351:LYS:CG	2.47	0.44
2:B:172:PHE:CE2	2:B:174:PRO:HA	2.53	0.44
2:B:290:SER:O	2:B:294:LEU:HG	2.17	0.44
1:A:292:THR:HG21	2:B:222:LEU:HB3	1.99	0.44
2:C:294:LEU:HD13	1:D:245:CYS:SG	2.57	0.44
1:D:144:PHE:CD2	1:D:217:PRO:HG3	2.53	0.44
2:E:22:ARG:NH2	2:E:29:GLU:O	2.47	0.44
1:A:314:MET:HB2	1:A:317:TRP:HD1	1.82	0.43
2:C:275:TYR:O	2:C:279:THR:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:149:ARG:HD3	2:E:197:VAL:O	2.18	0.43
2:B:275:TYR:O	2:B:279:THR:HG22	2.17	0.43
2:E:275:TYR:O	2:E:279:THR:HG22	2.18	0.43
1:A:235:THR:HG22	1:A:255:VAL:HG11	2.01	0.43
1:A:266:ILE:O	1:A:270:ILE:HG13	2.18	0.43
2:B:22:ARG:CZ	2:B:157:GLU:HG3	2.49	0.43
2:C:230:VAL:HG11	2:C:244:CYS:SG	2.58	0.43
2:E:12:LEU:HD11	2:E:82:LEU:HD22	2.01	0.43
1:A:137:ILE:HB	1:A:271:PRO:HG3	2.01	0.43
2:B:284:THR:HG21	2:C:222:LEU:HB3	2.00	0.43
2:E:119:PHE:CE2	2:E:121:LEU:HD22	2.54	0.43
2:B:119:PHE:CE2	2:B:121:LEU:HD22	2.55	0.42
1:D:222:ILE:O	1:D:227:PRO:HD3	2.19	0.42
1:A:27:ARG:HD2	1:A:162:LYS:HB3	2.01	0.42
2:B:248:LEU:HD13	2:B:284:THR:HG23	2.02	0.42
1:D:241:LEU:HD21	1:D:247:GLU:HB2	2.01	0.42
1:D:274:SER:HB3	2:E:210:LEU:HB3	2.02	0.42
1:A:52:GLU:O	1:A:271:PRO:HB3	2.20	0.42
2:E:22:ARG:CZ	2:E:157:GLU:HG3	2.50	0.42
2:E:53:THR:HA	2:E:126:TYR:O	2.20	0.42
1:A:88:PRO:HG3	2:E:20:LEU:HD22	2.02	0.42
1:A:157:THR:HG21	2:B:109:ASN:HB2	2.00	0.42
1:A:287:THR:O	1:A:291:VAL:HG23	2.20	0.42
1:D:143:PRO:CD	1:D:225:ILE:HD11	2.46	0.42
2:C:22:ARG:NH2	2:C:30:LEU:HA	2.35	0.42
2:C:140:ASP:OD1	2:C:207:ARG:NH1	2.52	0.42
1:D:222:ILE:HA	1:D:226:ILE:HD12	2.01	0.42
1:D:285:LEU:HD22	2:E:214:ILE:HG23	2.02	0.42
1:A:84:SER:HA	1:A:117:LEU:O	2.19	0.42
2:C:12:LEU:HD11	2:C:82:LEU:HD22	2.02	0.42
2:B:3:THR:HG22	2:B:6:ARG:HH21	1.85	0.41
2:B:167:ALA:HB3	2:B:183:LEU:HD13	2.00	0.41
2:C:3:THR:HG22	2:C:6:ARG:HH21	1.84	0.41
2:C:40:ALA:HB3	2:C:55:ASN:ND2	2.35	0.41
2:E:290:SER:O	2:E:294:LEU:HG	2.20	0.41
1:A:85:ILE:HD11	2:E:21:ILE:HD11	2.03	0.41
1:A:99:LEU:HA	1:A:152:LYS:O	2.19	0.41
2:B:58:LEU:HD21	2:B:104:VAL:HG11	2.01	0.41
2:B:183:LEU:HD21	2:B:203:PHE:CE2	2.55	0.41
2:C:40:ALA:HB3	2:C:55:ASN:HD21	1.86	0.41
1:A:25:TRP:CD2	2:B:83:PRO:HG3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ILE:CG2	1:A:270:ILE:HD11	2.51	0.41
1:D:236:VAL:HG22	1:D:365:PHE:HB3	2.02	0.41
1:A:313:THR:HG22	1:A:318:VAL:HG21	2.02	0.41
1:A:348:GLU:HA	1:A:351:LYS:CG	2.50	0.41
1:D:356:VAL:O	1:D:360:ILE:HG13	2.21	0.41
2:B:223:ILE:HD13	2:B:250:ALA:HB1	2.02	0.41
2:B:288:VAL:HG23	2:C:229:LEU:HD13	2.03	0.41
2:C:19:LYS:HG3	2:C:87:ILE:C	2.41	0.41
2:C:82:LEU:HD12	2:C:112:VAL:HG21	2.01	0.41
1:D:235:THR:HG22	1:D:255:VAL:HG11	2.03	0.41
1:A:356:VAL:O	1:A:360:ILE:HG13	2.20	0.41
2:B:154:ASP:HB3	2:B:195:THR:O	2.21	0.41
1:D:87:ILE:HD12	1:D:117:LEU:HD12	2.03	0.41
1:D:127:PRO:HA	1:D:128:PRO:HD3	1.90	0.41
1:D:199:CYS:SG	4:D:402:NCT:HC71	2.61	0.41
2:B:317:LYS:HD3	2:B:317:LYS:HA	1.75	0.41
2:E:183:LEU:HD21	2:E:203:PHE:CD2	2.56	0.41
1:A:143:PRO:HD2	1:A:144:PHE:CE1	2.57	0.40
1:A:198:GLU:HB3	2:B:170:ASP:CG	2.42	0.40
2:B:53:THR:HA	2:B:126:TYR:O	2.21	0.40
2:C:134:VAL:HG11	2:C:262:VAL:HG22	2.03	0.40
2:B:151:TRP:HH2	2:C:106:PHE:HB3	1.86	0.40
1:D:325:ILE:HG22	1:D:329:LEU:HD23	2.02	0.40
2:E:3:THR:HG21	2:E:75:ASP:CG	2.41	0.40
1:A:127:PRO:HA	1:A:128:PRO:HD3	1.89	0.40
1:A:270:ILE:HD13	1:A:278:PRO:CG	2.51	0.40
2:C:34:GLN:HB2	2:C:61:GLU:HB2	2.03	0.40
1:A:236:VAL:HG22	1:A:365:PHE:HB3	2.03	0.40
1:D:102:ASN:ND2	1:D:106:ASP:O	2.54	0.40
1:D:157:THR:HA	4:D:402:NCT:C5	2.50	0.40
2:E:58:LEU:HD21	2:E:104:VAL:HG11	2.02	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	359/386 (93%)	338 (94%)	21 (6%)	0	100	100
1	D	359/386 (93%)	338 (94%)	21 (6%)	0	100	100
2	B	354/403 (88%)	332 (94%)	22 (6%)	0	100	100
2	C	354/403 (88%)	330 (93%)	24 (7%)	0	100	100
2	E	354/403 (88%)	332 (94%)	22 (6%)	0	100	100
All	All	1780/1981 (90%)	1670 (94%)	110 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	338/359 (94%)	326 (96%)	12 (4%)	35	60
1	D	338/359 (94%)	327 (97%)	11 (3%)	38	62
2	B	335/379 (88%)	307 (92%)	28 (8%)	11	38
2	C	335/379 (88%)	308 (92%)	27 (8%)	11	39
2	E	335/379 (88%)	307 (92%)	28 (8%)	11	38
All	All	1681/1855 (91%)	1575 (94%)	106 (6%)	18	46

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LYS
1	A	66	GLU
1	A	69	ASP
1	A	144	PHE
1	A	187	ASP
1	A	245	CYS
1	A	272	SER

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Mol	Chain	Res	Type
1	A	273	THR
1	A	275	LEU
1	A	298	THR
1	A	313	THR
1	A	328	ARG
2	B	10	HIS
2	B	18	ASN
2	B	22	ARG
2	B	30	LEU
2	B	57	TRP
2	B	76	ASN
2	B	89	LEU
2	B	103	GLU
2	B	128	SER
2	B	139	PHE
2	B	151	TRP
2	B	168	SER
2	B	171	ASP
2	B	183	LEU
2	B	232	TYR
2	B	236	ASP
2	B	244	CYS
2	B	267	LEU
2	B	282	LEU
2	B	287	ILE
2	B	298	HIS
2	B	340	GLU
2	B	341	ASP
2	B	342	TRP
2	B	344	TYR
2	B	355	TRP
2	B	366	ILE
2	B	373	LEU
2	C	10	HIS
2	C	18	ASN
2	C	22	ARG
2	C	30	LEU
2	C	57	TRP
2	C	76	ASN
2	C	89	LEU
2	C	128	SER
2	C	139	PHE

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Mol	Chain	Res	Type
2	C	151	TRP
2	C	171	ASP
2	C	183	LEU
2	C	232	TYR
2	C	236	ASP
2	C	244	CYS
2	C	267	LEU
2	C	282	LEU
2	C	287	ILE
2	C	295	ASN
2	C	298	HIS
2	C	340	GLU
2	C	341	ASP
2	C	342	TRP
2	C	344	TYR
2	C	355	TRP
2	C	366	ILE
2	C	373	LEU
1	D	53	LYS
1	D	69	ASP
1	D	144	PHE
1	D	187	ASP
1	D	245	CYS
1	D	272	SER
1	D	273	THR
1	D	275	LEU
1	D	313	THR
1	D	328	ARG
1	D	344	ARG
2	E	10	HIS
2	E	18	ASN
2	E	22	ARG
2	E	30	LEU
2	E	57	TRP
2	E	76	ASN
2	E	89	LEU
2	E	103	GLU
2	E	128	SER
2	E	139	PHE
2	E	151	TRP
2	E	168	SER
2	E	171	ASP

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Mol	Chain	Res	Type
2	E	232	TYR
2	E	236	ASP
2	E	244	CYS
2	E	267	LEU
2	E	282	LEU
2	E	287	ILE
2	E	295	ASN
2	E	298	HIS
2	E	340	GLU
2	E	341	ASP
2	E	342	TRP
2	E	344	TYR
2	E	355	TRP
2	E	366	ILE
2	E	373	LEU

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 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	$\#\|Z\| > 2$
3	NAG	E	500	2	14,14,15	1.81	5 (35%)	17,19,21	2.44	3 (17%)
4	NCT	A	402	-	13,13,13	1.01	0	17,17,17	1.39	2 (11%)
3	NAG	A	401	1	14,14,15	1.89	6 (42%)	17,19,21	1.37	4 (23%)
4	NCT	D	402	-	13,13,13	0.93	0	17,17,17	1.40	2 (11%)
3	NAG	B	500	2	14,14,15	1.84	5 (35%)	17,19,21	2.49	3 (17%)
3	NAG	D	401	1	14,14,15	1.88	6 (42%)	17,19,21	1.56	3 (17%)
3	NAG	C	500	2	14,14,15	1.76	5 (35%)	17,19,21	2.33	2 (11%)

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
3	NAG	E	500	2	-	2/6/23/26	0/1/1/1
4	NCT	A	402	-	-	0/4/14/14	0/2/2/2
3	NAG	A	401	1	-	2/6/23/26	0/1/1/1
4	NCT	D	402	-	-	0/4/14/14	0/2/2/2
3	NAG	B	500	2	-	2/6/23/26	0/1/1/1
3	NAG	D	401	1	-	2/6/23/26	0/1/1/1
3	NAG	C	500	2	-	2/6/23/26	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	NAG	O5-C1	-3.31	1.38	1.43
3	A	401	NAG	O5-C1	-3.28	1.38	1.43
3	B	500	NAG	O5-C1	-3.04	1.38	1.43
3	E	500	NAG	O5-C1	-2.89	1.39	1.43
3	D	401	NAG	O5-C5	-2.87	1.37	1.43
3	C	500	NAG	O5-C1	-2.80	1.39	1.43
3	A	401	NAG	O5-C5	-2.79	1.37	1.43
3	D	401	NAG	C7-N2	2.71	1.43	1.34
3	B	500	NAG	C7-N2	2.71	1.43	1.34
3	E	500	NAG	C7-N2	2.67	1.43	1.34
3	C	500	NAG	C7-N2	2.65	1.43	1.34
3	A	401	NAG	C7-N2	2.62	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	NAG	O5-C5	-2.59	1.38	1.43
3	E	500	NAG	O5-C5	-2.40	1.38	1.43
3	C	500	NAG	O5-C5	-2.21	1.39	1.43
3	A	401	NAG	O4-C4	-2.20	1.37	1.43
3	B	500	NAG	O4-C4	-2.16	1.37	1.43
3	C	500	NAG	O3-C3	-2.16	1.37	1.43
3	D	401	NAG	O4-C4	-2.16	1.37	1.43
3	A	401	NAG	O3-C3	-2.13	1.38	1.43
3	E	500	NAG	O4-C4	-2.12	1.38	1.43
3	C	500	NAG	O4-C4	-2.10	1.38	1.43
3	E	500	NAG	O3-C3	-2.05	1.38	1.43
3	D	401	NAG	C4-C5	-2.05	1.48	1.53
3	A	401	NAG	C4-C5	-2.05	1.48	1.53
3	B	500	NAG	O3-C3	-2.04	1.38	1.43
3	D	401	NAG	O3-C3	-2.03	1.38	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	500	NAG	C1-O5-C5	8.98	124.36	112.19
3	E	500	NAG	C1-O5-C5	8.80	124.12	112.19
3	C	500	NAG	C1-O5-C5	8.25	123.37	112.19
3	D	401	NAG	C1-O5-C5	4.39	118.14	112.19
4	D	402	NCT	C10-N2-C6	-4.07	100.46	112.83
4	A	402	NCT	C10-N2-C6	-3.98	100.74	112.83
3	B	500	NAG	O5-C1-C2	2.96	115.96	111.29
3	C	500	NAG	O5-C1-C2	2.83	115.75	111.29
3	E	500	NAG	O5-C1-C2	2.81	115.73	111.29
3	D	401	NAG	C8-C7-N2	2.81	120.86	116.10
3	A	401	NAG	C1-O5-C5	2.76	115.93	112.19
3	A	401	NAG	O5-C5-C6	2.69	111.42	107.20
3	B	500	NAG	C8-C7-N2	2.29	119.97	116.10
3	D	401	NAG	C3-C4-C5	-2.09	106.50	110.24
3	A	401	NAG	C3-C4-C5	-2.08	106.52	110.24
4	A	402	NCT	C7-C6-C2	2.06	117.60	113.61
3	E	500	NAG	C6-C5-C4	-2.05	108.21	113.00
4	D	402	NCT	C10-N2-C9	-2.04	106.31	112.70
3	A	401	NAG	C8-C7-N2	2.01	119.51	116.10

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	401	NAG	O5-C5-C6-O6
3	A	401	NAG	O5-C5-C6-O6
3	B	500	NAG	O5-C5-C6-O6
3	D	401	NAG	C4-C5-C6-O6
3	B	500	NAG	C4-C5-C6-O6
3	C	500	NAG	C4-C5-C6-O6
3	A	401	NAG	C4-C5-C6-O6
3	C	500	NAG	O5-C5-C6-O6
3	E	500	NAG	C4-C5-C6-O6
3	E	500	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	402	NCT	2	0
4	D	402	NCT	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	363/386 (94%)	-0.08	12 (3%)	46	37	123, 157, 261, 293	0
1	D	363/386 (94%)	-0.15	11 (3%)	50	39	138, 168, 234, 263	0
2	B	358/403 (88%)	-0.19	13 (3%)	42	34	122, 150, 231, 260	0
2	C	358/403 (88%)	-0.16	6 (1%)	70	60	124, 152, 251, 274	0
2	E	358/403 (88%)	-0.06	12 (3%)	45	36	130, 165, 251, 285	0
All	All	1800/1981 (90%)	-0.13	54 (3%)	50	39	122, 160, 245, 293	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	381	TRP	8.7
1	A	381	TRP	6.2
2	E	192	ASP	5.5
1	D	200	CYS	5.2
2	E	193	ASP	4.9
1	D	201	ALA	4.1
1	D	104	ASP	4.1
1	D	198	GLU	4.1
2	E	194	SER	3.8
1	D	331	LEU	3.7
1	D	199	CYS	3.7
1	A	320	ARG	3.6
2	B	304	HIS	3.5
2	E	341	ASP	3.4
1	A	174	GLN	3.4
2	B	372	PRO	3.3
1	A	331	LEU	3.2
2	E	305	THR	3.2
2	E	372	PRO	3.1
1	A	197	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	193	ASN	3.0
2	E	232	TYR	3.0
2	C	323	PHE	3.0
1	A	315	PRO	3.0
2	C	372	PRO	3.0
2	E	28	SER	2.9
2	E	99	ASP	2.9
1	A	173	ASP	2.7
2	B	339	SER	2.7
2	C	193	ASP	2.7
1	D	31	ASN	2.7
2	E	304	HIS	2.7
2	E	300	SER	2.6
1	D	344	ARG	2.6
1	A	316	THR	2.5
1	A	343	GLU	2.5
2	B	192	ASP	2.5
2	B	305	THR	2.4
1	A	312	HIS	2.4
2	C	78	LYS	2.4
2	B	28	SER	2.3
2	B	373	LEU	2.2
2	B	136	HIS	2.2
1	D	196	LYS	2.2
2	B	323	PHE	2.2
2	B	193	ASP	2.1
2	B	155	ARG	2.1
2	B	268	ASP	2.1
1	A	39	ARG	2.1
2	C	194	SER	2.1
1	D	30	ALA	2.1
2	C	114	TYR	2.1
2	B	340	GLU	2.1
2	E	30	LEU	2.0

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

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

6.3 Carbohydrates (i)

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
4	NCT	D	402	12/12	0.71	0.39	158,158,158,158	0
3	NAG	E	500	14/15	0.83	0.19	159,159,159,159	0
4	NCT	A	402	12/12	0.83	0.72	144,144,144,144	0
3	NAG	C	500	14/15	0.83	0.47	136,136,136,136	0
3	NAG	A	401	14/15	0.87	0.18	137,137,137,137	0
3	NAG	D	401	14/15	0.88	0.32	153,153,153,153	0
3	NAG	B	500	14/15	0.92	0.13	137,137,137,137	0
5	NA	A	403	1/1	0.92	0.39	84,84,84,84	0

6.5 Other polymers (i)

There are no such residues in this entry.