Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 05:03 PM BST

PDB ID	:	6YJP
Title	:	Crystal structure of a complex between glycosylated NKp30 and its deglycosylated tumour ligand B7-H6
Authors	:	Skalova, T.; Dohnalek, J.; Skorepa, O.; Kalouskova, B.; Pazicky, S.; Blaha, J.; Vanek, O.
Deposited on	:	2020-04-04
Resolution	:	3.10 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 ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

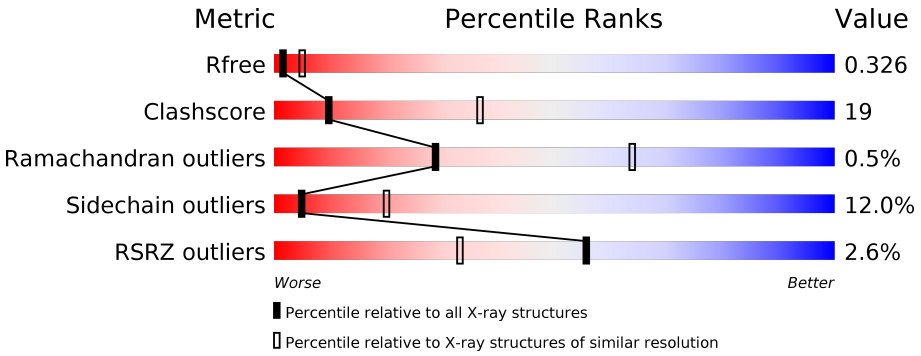
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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	C	234	59% 33%
1	D	234	2% 56% 29% 6% 9%
1	E	234	7% 61% 27% 9%
2	A	126	% 61% 23% 12%
2	B	126	58% 24% 6% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6907 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 Natural cytotoxicity triggering receptor 3 ligand 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	225	Total	C	N	O	S	0	0	0
			1766	1122	293	341	10			
1	D	214	Total	C	N	O	S	0	0	0
			1678	1071	277	321	9			
1	E	214	Total	C	N	O	S	0	0	0
			1685	1073	278	325	9			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	22	ILE	-	expression tag	UNP Q68D85
C	23	THR	-	expression tag	UNP Q68D85
C	212	SER	CYS	engineered mutation	UNP Q68D85
C	245	GLY	-	expression tag	UNP Q68D85
C	246	THR	-	expression tag	UNP Q68D85
C	247	HIS	-	expression tag	UNP Q68D85
C	248	HIS	-	expression tag	UNP Q68D85
C	249	HIS	-	expression tag	UNP Q68D85
C	250	HIS	-	expression tag	UNP Q68D85
C	251	HIS	-	expression tag	UNP Q68D85
C	252	HIS	-	expression tag	UNP Q68D85
C	253	HIS	-	expression tag	UNP Q68D85
C	254	HIS	-	expression tag	UNP Q68D85
C	255	GLY	-	expression tag	UNP Q68D85
D	22	ILE	-	expression tag	UNP Q68D85
D	23	THR	-	expression tag	UNP Q68D85
D	212	SER	CYS	engineered mutation	UNP Q68D85
D	245	GLY	-	expression tag	UNP Q68D85
D	246	THR	-	expression tag	UNP Q68D85
D	247	HIS	-	expression tag	UNP Q68D85
D	248	HIS	-	expression tag	UNP Q68D85
D	249	HIS	-	expression tag	UNP Q68D85
D	250	HIS	-	expression tag	UNP Q68D85

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Chain	Residue	Modelled	Actual	Comment	Reference
D	251	HIS	-	expression tag	UNP Q68D85
D	252	HIS	-	expression tag	UNP Q68D85
D	253	HIS	-	expression tag	UNP Q68D85
D	254	HIS	-	expression tag	UNP Q68D85
D	255	GLY	-	expression tag	UNP Q68D85
E	22	ILE	-	expression tag	UNP Q68D85
E	23	THR	-	expression tag	UNP Q68D85
E	212	SER	CYS	engineered mutation	UNP Q68D85
E	245	GLY	-	expression tag	UNP Q68D85
E	246	THR	-	expression tag	UNP Q68D85
E	247	HIS	-	expression tag	UNP Q68D85
E	248	HIS	-	expression tag	UNP Q68D85
E	249	HIS	-	expression tag	UNP Q68D85
E	250	HIS	-	expression tag	UNP Q68D85
E	251	HIS	-	expression tag	UNP Q68D85
E	252	HIS	-	expression tag	UNP Q68D85
E	253	HIS	-	expression tag	UNP Q68D85
E	254	HIS	-	expression tag	UNP Q68D85
E	255	GLY	-	expression tag	UNP Q68D85

- Molecule 2 is a protein called Natural cytotoxicity triggering receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	111	Total	C	N	O	S	0	0	0
			854	535	161	156	2			
2	B	111	Total	C	N	O	S	0	0	0
			854	535	161	156	2			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ILE	-	expression tag	UNP O14931
A	17	THR	-	expression tag	UNP O14931
A	18	GLY	-	expression tag	UNP O14931
A	131	GLY	-	expression tag	UNP O14931
A	132	THR	-	expression tag	UNP O14931
A	133	HIS	-	expression tag	UNP O14931
A	134	HIS	-	expression tag	UNP O14931
A	135	HIS	-	expression tag	UNP O14931
A	136	HIS	-	expression tag	UNP O14931
A	137	HIS	-	expression tag	UNP O14931
A	138	HIS	-	expression tag	UNP O14931

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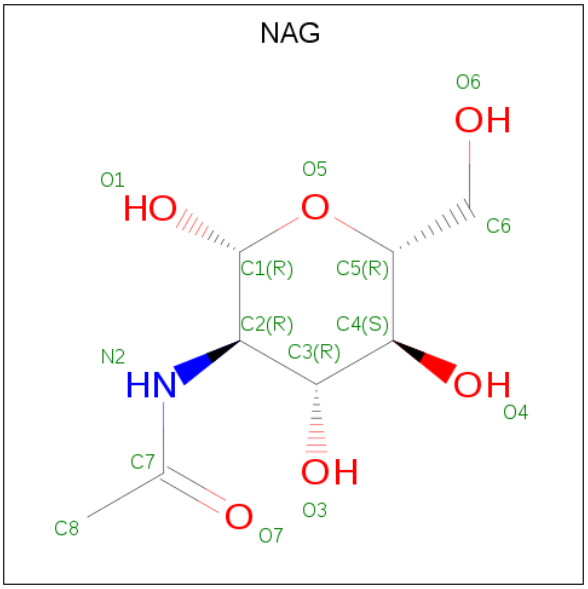
Chain	Residue	Modelled	Actual	Comment	Reference
A	139	HIS	-	expression tag	UNP O14931
A	140	HIS	-	expression tag	UNP O14931
A	141	GLY	-	expression tag	UNP O14931
B	16	ILE	-	expression tag	UNP O14931
B	17	THR	-	expression tag	UNP O14931
B	18	GLY	-	expression tag	UNP O14931
B	131	GLY	-	expression tag	UNP O14931
B	132	THR	-	expression tag	UNP O14931
B	133	HIS	-	expression tag	UNP O14931
B	134	HIS	-	expression tag	UNP O14931
B	135	HIS	-	expression tag	UNP O14931
B	136	HIS	-	expression tag	UNP O14931
B	137	HIS	-	expression tag	UNP O14931
B	138	HIS	-	expression tag	UNP O14931
B	139	HIS	-	expression tag	UNP O14931
B	140	HIS	-	expression tag	UNP O14931
B	141	GLY	-	expression tag	UNP O14931

- 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
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

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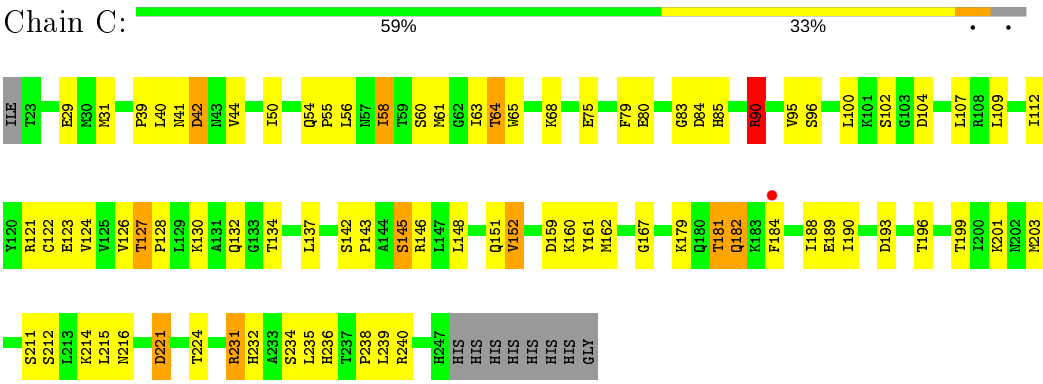
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		

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.

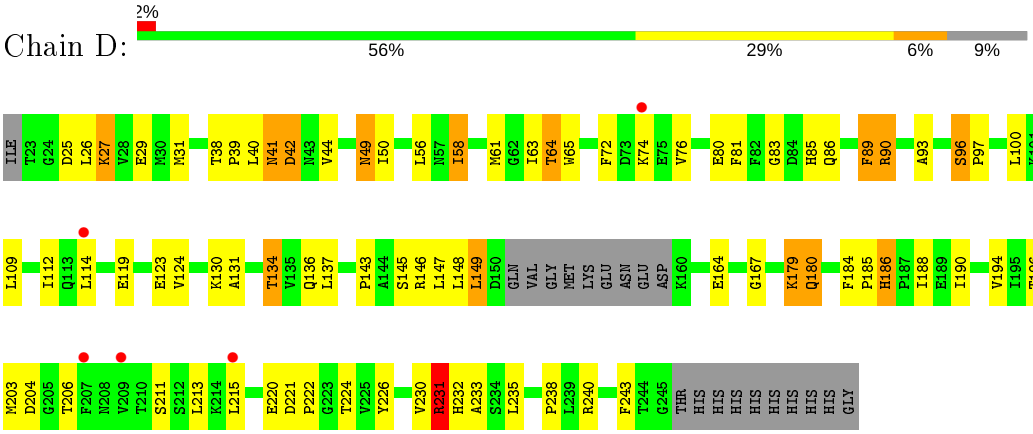
- Molecule 1: Natural cytotoxicity triggering receptor 3 ligand 1

Chain C:



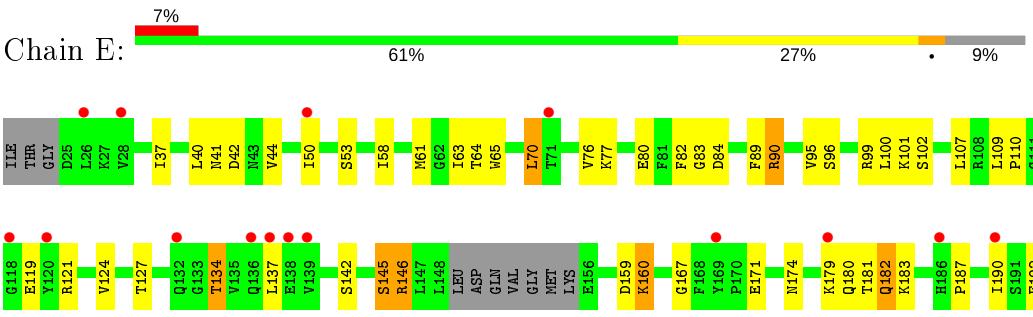
- Molecule 1: Natural cytotoxicity triggering receptor 3 ligand 1

Chain D:



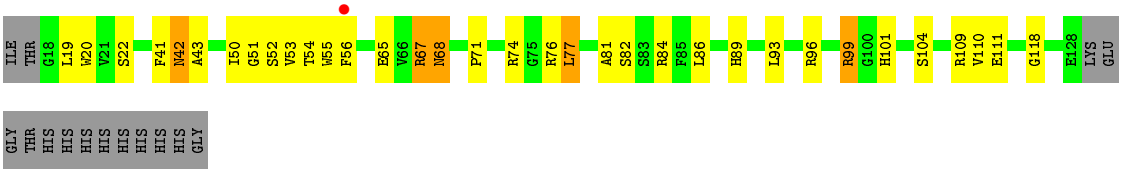
- Molecule 1: Natural cytotoxicity triggering receptor 3 ligand 1

Chain E:



- Molecule 2: Natural cytotoxicity triggering receptor 3

Chain A:



- Molecule 2: Natural cytotoxicity triggering receptor 3

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	166.04Å 86.46Å 111.30Å 90.00° 97.58° 90.00°	Depositor
Resolution (Å)	48.95 – 3.10 48.90 – 3.10	Depositor EDS
% Data completeness (in resolution range)	94.7 (48.95-3.10) 94.7 (48.90-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0258 (LORESTR pipeline))	Depositor
R, R_{free}	0.272 , 0.322 0.272 , 0.326	Depositor DCC
R_{free} test set	1348 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	91.5	Xtriage
Anisotropy	0.649	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 101.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6907	wwPDB-VP
Average B, all atoms (Å^2)	155.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	C	0.34	0/1808	0.82	1/2456 (0.0%)
1	D	0.36	0/1718	0.84	3/2334 (0.1%)
1	E	0.34	0/1725	0.81	1/2343 (0.0%)
2	A	0.35	0/873	0.86	4/1184 (0.3%)
2	B	0.37	0/873	0.76	0/1184
All	All	0.35	0/6997	0.82	9/9501 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	67	ARG	NE-CZ-NH2	-7.15	116.73	120.30
1	E	183	LYS	CB-CA-C	6.23	122.85	110.40
1	C	90	ARG	CB-CG-CD	6.01	127.24	111.60
2	A	99	ARG	CG-CD-NE	5.75	123.88	111.80
1	D	180	GLN	CB-CA-C	5.64	121.69	110.40
2	A	67	ARG	CD-NE-CZ	5.51	131.32	123.60
2	A	67	ARG	CB-CG-CD	5.50	125.91	111.60
1	D	231	ARG	CG-CD-NE	-5.33	100.62	111.80
1	D	179	LYS	CB-CA-C	-5.29	99.81	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1766	0	1723	80	0
1	D	1678	0	1644	82	0
1	E	1685	0	1641	57	0
2	A	854	0	839	32	0
2	B	854	0	839	30	0
3	A	14	0	13	1	0
3	B	14	0	13	1	0
3	C	14	0	13	0	0
3	D	14	0	13	0	0
3	E	14	0	13	2	0
All	All	6907	0	6751	263	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 19.

All (263) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:THR:HG23	1:E:80:GLU:HG2	1.25	1.15
1:C:90:ARG:HD3	1:C:109:LEU:HD22	1.22	1.07
2:A:43:ALA:HA	2:A:89:HIS:CD2	1.89	1.07
1:D:90:ARG:HD3	1:D:109:LEU:HD23	1.37	1.02
2:A:56:PHE:CE1	2:A:65:GLU:HG2	1.94	1.02
2:A:43:ALA:CA	2:A:89:HIS:CD2	2.42	1.02
1:D:179:LYS:HG3	1:D:190:ILE:HD11	1.40	1.02
1:C:63:ILE:HD11	1:C:100:LEU:HD13	1.42	0.99
1:C:143:PRO:HD2	1:C:235:LEU:HD21	1.50	0.94
1:C:143:PRO:CD	1:C:235:LEU:HD21	1.98	0.93
2:A:43:ALA:HB1	2:A:89:HIS:HD2	1.34	0.91
1:E:145:SER:HB2	1:E:239:LEU:HD21	1.51	0.90
1:E:63:ILE:HD11	1:E:100:LEU:HD13	1.52	0.89
2:B:29:THR:HG21	2:B:35:ALA:HB2	1.55	0.88
1:C:148:LEU:HD12	1:C:162:MET:SD	2.13	0.87
1:C:58:ILE:HA	1:C:61:MET:HE3	1.57	0.87
1:E:64:THR:HG23	1:E:80:GLU:CG	2.05	0.87
2:A:43:ALA:HA	2:A:89:HIS:CG	2.09	0.86
2:B:76:ARG:HH12	2:B:99:ARG:HB2	1.39	0.85
1:D:196:THR:HG22	1:D:211:SER:OG	1.76	0.84
1:D:119:GLU:HB2	1:D:136:GLN:HE22	1.43	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:HIS:O	1:D:235:LEU:HB2	1.79	0.83
1:D:63:ILE:HD12	1:D:124:VAL:HG22	1.61	0.82
1:E:179:LYS:HG3	1:E:190:ILE:HD11	1.62	0.82
1:D:202:ASN:HD22	1:D:206:THR:HG23	1.45	0.80
2:A:56:PHE:HE1	2:A:65:GLU:HG2	1.44	0.80
1:C:196:THR:HG22	1:C:211:SER:OG	1.82	0.80
1:D:220:GLU:OE2	1:D:226:TYR:CE1	2.35	0.80
2:A:43:ALA:CB	2:A:89:HIS:HD2	1.95	0.79
1:C:148:LEU:HB2	1:C:162:MET:HB2	1.63	0.79
1:D:220:GLU:OE2	1:D:226:TYR:HE1	1.67	0.78
1:C:127:THR:HG23	2:A:51:GLY:O	1.84	0.77
1:E:40:LEU:HD13	1:E:114:LEU:HG	1.67	0.77
2:A:43:ALA:CB	2:A:89:HIS:CD2	2.68	0.76
1:C:143:PRO:CG	1:C:235:LEU:HD21	2.14	0.76
1:C:64:THR:HG23	1:C:80:GLU:HG3	1.67	0.76
2:A:43:ALA:HB1	2:A:89:HIS:CD2	2.19	0.76
1:C:201:LYS:HG3	1:C:207:PHE:CE1	2.21	0.75
1:E:235:LEU:HD13	1:E:237:THR:O	1.87	0.74
2:B:48:LEU:CD1	2:B:86:LEU:HB3	2.19	0.73
2:B:68:ASN:HB3	2:B:75:GLY:HA2	1.71	0.72
1:D:179:LYS:HG2	1:D:226:TYR:CD1	2.25	0.72
1:D:64:THR:HG23	1:D:80:GLU:HG3	1.71	0.71
1:C:148:LEU:HB3	1:C:151:GLN:HB3	1.71	0.71
2:B:43:ALA:HA	2:B:89:HIS:CG	2.26	0.71
1:D:213:LEU:HD21	1:D:215:LEU:CD1	2.20	0.71
1:D:112:ILE:CD1	1:D:137:LEU:HD21	2.21	0.71
1:C:112:ILE:CD1	1:C:137:LEU:HD21	2.20	0.70
1:C:232:HIS:HB3	1:C:235:LEU:HD23	1.73	0.70
1:D:123:GLU:HG2	1:D:130:LYS:HE2	1.73	0.70
1:D:119:GLU:HB2	1:D:136:GLN:NE2	2.06	0.69
1:E:112:ILE:HD11	1:E:137:LEU:HD21	1.74	0.69
1:E:112:ILE:CD1	1:E:137:LEU:HD21	2.23	0.68
1:E:179:LYS:HE2	1:E:226:TYR:HE2	1.57	0.68
1:C:112:ILE:HD11	1:C:137:LEU:HD21	1.75	0.67
1:D:112:ILE:HD11	1:D:137:LEU:HD21	1.74	0.67
1:E:90:ARG:HD3	1:E:109:LEU:HD22	1.77	0.67
2:B:102:ASP:OD1	2:B:102:ASP:N	2.28	0.66
1:C:145:SER:HB2	1:C:239:LEU:HD21	1.76	0.66
1:C:143:PRO:HD2	1:C:235:LEU:CD2	2.25	0.66
1:C:63:ILE:CD1	1:C:95:VAL:HG11	2.25	0.66
1:C:63:ILE:HD11	1:C:100:LEU:CD1	2.22	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:LEU:HD12	1:D:114:LEU:HD21	1.77	0.65
1:D:146:ARG:HG3	1:E:102:SER:HB3	1.79	0.65
1:D:213:LEU:HD21	1:D:215:LEU:HD11	1.78	0.65
2:B:37:LEU:HD21	2:B:125:LEU:HD13	1.79	0.65
2:A:43:ALA:C	2:A:89:HIS:CD2	2.69	0.65
1:E:77:LYS:HD3	1:E:80:GLU:OE2	1.96	0.65
1:C:68:LYS:HG3	1:C:75:GLU:OE2	1.97	0.64
2:A:77:LEU:HD21	2:A:93:LEU:HD11	1.79	0.64
2:B:77:LEU:O	2:B:77:LEU:HD12	1.97	0.64
2:B:30:LEU:H	2:B:30:LEU:HD12	1.63	0.64
1:C:40:LEU:HD13	1:C:114:LEU:HG	1.79	0.64
1:E:50:ILE:HD13	1:E:124:VAL:HG11	1.80	0.64
1:C:90:ARG:HD3	1:C:109:LEU:CD2	2.14	0.63
1:D:196:THR:HG22	1:D:211:SER:HG	1.63	0.63
1:C:128:PRO:O	2:A:52:SER:HA	1.99	0.62
2:B:48:LEU:HD11	2:B:86:LEU:HB3	1.80	0.62
1:C:90:ARG:CD	1:C:109:LEU:HD22	2.14	0.62
1:D:146:ARG:HG2	1:D:148:LEU:CD2	2.30	0.62
1:C:201:LYS:HG3	1:C:207:PHE:HE1	1.62	0.62
1:E:182:GLN:NE2	1:E:222:PRO:O	2.33	0.61
1:C:160:LYS:HG3	1:C:214:LYS:HG3	1.83	0.61
1:E:145:SER:HB2	1:E:239:LEU:CD2	2.28	0.61
1:E:64:THR:CG2	1:E:80:GLU:HG2	2.16	0.61
1:D:194:VAL:CG2	1:D:213:LEU:HD13	2.30	0.61
2:A:56:PHE:HE1	2:A:65:GLU:CG	2.13	0.60
1:E:110:PRO:HB3	3:E:301:NAG:H82	1.82	0.60
2:A:99:ARG:NH1	2:A:101:HIS:NE2	2.49	0.60
1:C:56:LEU:HB3	1:C:61:MET:CE	2.31	0.60
1:D:231:ARG:HG2	1:D:235:LEU:HD21	1.82	0.60
1:C:161:TYR:CE1	1:C:215:LEU:HD12	2.37	0.59
2:B:59:GLU:HB3	2:B:61:VAL:HG13	1.83	0.59
1:D:63:ILE:CD1	1:D:124:VAL:HG22	2.31	0.59
2:B:81:ALA:HB3	2:B:84:ARG:HG3	1.85	0.58
1:D:202:ASN:HD22	1:D:206:THR:CG2	2.16	0.58
1:C:50:ILE:HD13	1:C:124:VAL:HG11	1.86	0.58
1:D:231:ARG:HG3	1:D:238:PRO:HG3	1.86	0.57
2:A:68:ASN:N	2:A:68:ASN:OD1	2.37	0.57
1:E:63:ILE:HD11	1:E:100:LEU:CD1	2.31	0.57
2:B:77:LEU:C	2:B:77:LEU:HD12	2.24	0.57
1:D:179:LYS:HG2	1:D:226:TYR:HD1	1.65	0.56
1:E:119:GLU:HG3	1:E:134:THR:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:LYS:HE3	1:C:207:PHE:HE1	1.70	0.56
1:D:185:PRO:HG2	1:D:186:HIS:CE1	2.41	0.56
2:A:56:PHE:CE1	2:A:65:GLU:CG	2.81	0.55
1:E:90:ARG:HH11	1:E:109:LEU:HD22	1.71	0.55
1:D:179:LYS:HG2	1:D:226:TYR:CE1	2.42	0.55
2:B:76:ARG:NH1	2:B:99:ARG:HB2	2.15	0.55
1:E:61:MET:HE1	1:E:100:LEU:HG	1.87	0.55
2:B:48:LEU:HD12	2:B:86:LEU:HB3	1.86	0.55
1:C:75:GLU:O	1:C:75:GLU:HG3	2.05	0.55
1:C:121:ARG:NH2	1:C:132:GLN:OE1	2.40	0.55
2:A:19:LEU:HB3	2:A:118:GLY:HA3	1.88	0.55
2:B:29:THR:HG21	2:B:35:ALA:CB	2.33	0.54
1:E:112:ILE:HD11	1:E:137:LEU:CD2	2.38	0.54
1:C:184:PHE:CG	1:D:49:ASN:OD1	2.61	0.54
1:C:79:PHE:HE2	1:C:95:VAL:HB	1.72	0.53
1:C:232:HIS:HB3	1:C:235:LEU:CD2	2.37	0.53
1:E:145:SER:CB	1:E:239:LEU:HD21	2.32	0.53
1:C:143:PRO:CD	1:C:235:LEU:CD2	2.79	0.53
1:C:63:ILE:HD13	1:C:95:VAL:HG11	1.91	0.52
1:D:146:ARG:HG2	1:D:148:LEU:HD22	1.91	0.52
2:A:81:ALA:HB3	2:A:84:ARG:HG3	1.92	0.52
1:C:123:GLU:HG2	1:C:130:LYS:HE2	1.91	0.52
1:C:39:PRO:O	1:C:42:ASP:HB2	2.09	0.52
1:E:242:ASN:OD1	1:E:242:ASN:N	2.42	0.52
1:D:231:ARG:HG2	1:D:235:LEU:HD11	1.91	0.52
1:D:146:ARG:NH1	1:E:101:LYS:HD2	2.25	0.52
1:D:58:ILE:HA	1:D:61:MET:HE1	1.90	0.52
1:C:160:LYS:HG3	1:C:214:LYS:CG	2.39	0.51
1:C:201:LYS:HE3	1:C:207:PHE:CE1	2.46	0.51
1:D:232:HIS:H	1:D:235:LEU:HG	1.76	0.51
1:D:232:HIS:CG	1:D:233:ALA:H	2.28	0.51
1:D:232:HIS:CG	1:D:233:ALA:N	2.78	0.51
2:A:42:ASN:HB2	3:A:201:NAG:O5	2.10	0.51
1:D:226:TYR:HB2	1:D:243:PHE:CZ	2.45	0.50
1:C:184:PHE:CD1	1:D:49:ASN:OD1	2.64	0.50
1:E:61:MET:CE	1:E:100:LEU:HG	2.40	0.50
1:E:182:GLN:HE21	1:E:223:GLY:HA3	1.77	0.50
2:B:50:ILE:HD12	2:B:50:ILE:H	1.75	0.50
2:A:20:TRP:CD2	2:B:30:LEU:HD21	2.46	0.50
1:D:119:GLU:HG3	1:D:134:THR:HG22	1.92	0.50
1:D:232:HIS:O	1:D:235:LEU:CB	2.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:LEU:HB3	1:C:61:MET:HE1	1.94	0.49
1:C:56:LEU:HB3	1:C:61:MET:HE2	1.94	0.49
1:E:83:GLY:O	1:E:84:ASP:HB3	2.11	0.49
1:C:182:GLN:NE2	1:C:182:GLN:O	2.45	0.49
1:D:81:PHE:HD1	1:D:86:GLN:HB3	1.77	0.49
2:B:19:LEU:HD11	2:B:42:ASN:HB3	1.94	0.49
1:D:72:PHE:HB3	1:D:74:LYS:HE2	1.94	0.49
1:D:56:LEU:HD13	1:D:61:MET:SD	2.52	0.49
1:C:119:GLU:HG3	1:C:134:THR:HG22	1.93	0.49
1:C:167:GLY:HA2	1:C:206:THR:CG2	2.43	0.48
1:C:63:ILE:CD1	1:C:100:LEU:HD13	2.30	0.48
1:D:123:GLU:CG	1:D:130:LYS:HE2	2.41	0.48
1:D:44:VAL:HG11	1:D:112:ILE:CD1	2.44	0.48
1:E:182:GLN:NE2	1:E:223:GLY:HA3	2.29	0.48
1:C:130:LYS:HE3	2:A:111:GLU:OE1	2.14	0.48
2:B:68:ASN:O	2:B:75:GLY:N	2.47	0.48
1:C:146:ARG:HH11	1:E:225:VAL:HG22	1.78	0.48
1:D:146:ARG:HH12	1:E:101:LYS:HD2	1.79	0.47
2:B:20:TRP:HB2	3:B:201:NAG:O6	2.14	0.47
1:E:179:LYS:HE2	1:E:226:TYR:CE2	2.44	0.47
1:D:26:LEU:HD12	1:D:27:LYS:N	2.29	0.47
2:A:55:TRP:CG	2:A:93:LEU:HD13	2.49	0.47
2:B:78:ALA:HB1	2:B:79:PRO:HD2	1.96	0.47
1:C:54:GLN:HB3	1:C:55:PRO:HD2	1.97	0.47
1:D:167:GLY:HA2	1:D:206:THR:CG2	2.44	0.47
1:D:147:LEU:O	1:E:102:SER:HB2	2.14	0.47
1:D:40:LEU:HD12	1:D:114:LEU:CD2	2.44	0.47
1:D:149:LEU:HG	1:D:149:LEU:H	1.35	0.47
1:E:40:LEU:O	1:E:41:ASN:HB2	2.14	0.47
1:E:63:ILE:CD1	1:E:95:VAL:HG11	2.44	0.47
1:C:151:GLN:HG3	1:C:152:VAL:N	2.30	0.47
1:E:160:LYS:HB2	1:E:160:LYS:HE3	1.65	0.46
1:E:167:GLY:HA2	1:E:206:THR:CG2	2.45	0.46
1:D:222:PRO:C	1:D:224:THR:H	2.18	0.46
1:E:171:GLU:OE2	1:E:199:THR:HG23	2.16	0.46
2:A:53:VAL:HG23	2:A:110:VAL:HG22	1.96	0.46
1:C:204:ASP:OD1	1:C:206:THR:HG22	2.14	0.46
1:E:44:VAL:HG11	1:E:112:ILE:CD1	2.46	0.46
1:E:44:VAL:HG11	1:E:112:ILE:HD13	1.96	0.46
1:D:112:ILE:HD11	1:D:137:LEU:CD2	2.42	0.46
1:C:112:ILE:HD11	1:C:137:LEU:CD2	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:CYS:HB3	2:B:91:ALA:O	2.16	0.46
1:D:40:LEU:C	1:D:40:LEU:HD23	2.37	0.46
1:D:26:LEU:HG	1:D:131:ALA:HB2	1.97	0.45
1:E:110:PRO:HB3	3:E:301:NAG:C8	2.44	0.45
1:D:145:SER:OG	1:D:230:VAL:HG21	2.17	0.45
1:E:146:ARG:NH1	1:E:146:ARG:HG3	2.31	0.45
1:E:146:ARG:HG3	1:E:146:ARG:HH11	1.82	0.45
1:D:167:GLY:HA2	1:D:206:THR:HG21	1.97	0.45
1:D:143:PRO:HD3	1:D:232:HIS:CD2	2.52	0.45
2:A:71:PRO:O	2:A:74:ARG:HG3	2.16	0.45
2:B:73:PHE:N	2:B:73:PHE:CD1	2.84	0.45
2:B:41:PHE:CZ	2:B:89:HIS:HA	2.51	0.45
1:C:44:VAL:HG11	1:C:112:ILE:CD1	2.46	0.45
1:C:104:ASP:HA	1:D:184:PHE:HZ	1.82	0.45
1:C:193:ASP:OD2	1:C:216:ASN:ND2	2.44	0.45
1:D:231:ARG:CG	1:D:238:PRO:HG3	2.46	0.45
1:C:63:ILE:HD11	1:C:100:LEU:HD22	1.98	0.45
2:A:41:PHE:CZ	2:A:89:HIS:HA	2.52	0.44
1:C:148:LEU:CB	1:C:162:MET:HB2	2.40	0.44
1:D:213:LEU:HD21	1:D:215:LEU:HD12	1.95	0.44
1:D:204:ASP:OD1	1:D:206:THR:HG22	2.18	0.44
1:C:181:THR:HG22	1:C:224:THR:HG23	1.99	0.44
1:E:204:ASP:OD1	1:E:206:THR:HG22	2.18	0.44
1:C:188:ILE:HG21	1:D:29:GLU:OE1	2.18	0.44
2:B:100:GLY:N	2:B:102:ASP:OD1	2.51	0.44
1:E:50:ILE:HD13	1:E:124:VAL:CG1	2.48	0.44
1:E:96:SER:HB3	1:E:99:ARG:HB2	2.00	0.44
2:A:20:TRP:CH2	2:A:22:SER:HB3	2.52	0.43
1:E:112:ILE:HD13	1:E:137:LEU:HD21	2.00	0.43
1:E:146:ARG:CG	1:E:146:ARG:HH11	2.31	0.43
2:B:82:SER:O	2:B:86:LEU:HG	2.18	0.43
1:E:63:ILE:HD13	1:E:95:VAL:HG11	2.00	0.43
1:C:142:SER:HA	1:C:234:SER:OG	2.18	0.43
2:B:100:GLY:HA2	2:B:127:VAL:HG11	2.01	0.43
1:C:79:PHE:CE2	1:C:95:VAL:HB	2.53	0.43
1:D:44:VAL:HG11	1:D:112:ILE:HD12	2.01	0.43
1:C:196:THR:HG22	1:C:211:SER:HG	1.81	0.43
2:A:20:TRP:HE3	2:A:20:TRP:O	2.01	0.43
1:C:146:ARG:HH11	1:E:225:VAL:CG2	2.32	0.43
1:E:196:THR:HG22	1:E:211:SER:OG	2.19	0.43
1:D:147:LEU:HD23	1:D:147:LEU:HA	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:GLU:CD	1:D:226:TYR:OH	2.57	0.43
1:C:112:ILE:HD13	1:C:137:LEU:HD21	2.01	0.42
2:B:65:GLU:OE1	2:B:65:GLU:N	2.39	0.42
1:D:50:ILE:HD13	1:D:124:VAL:HG11	2.02	0.42
1:E:142:SER:HA	1:E:234:SER:OG	2.19	0.42
1:D:179:LYS:CG	1:D:226:TYR:HD1	2.30	0.42
1:E:65:TRP:CE2	1:E:107:LEU:HB2	2.54	0.42
2:A:76:ARG:HD2	2:A:96:ARG:O	2.20	0.42
2:A:76:ARG:HH12	2:A:99:ARG:HB2	1.84	0.42
2:A:82:SER:O	2:A:86:LEU:HG	2.20	0.42
1:C:65:TRP:CE2	1:C:107:LEU:HB2	2.54	0.42
1:D:25:ASP:O	1:D:27:LYS:HG3	2.18	0.42
1:D:65:TRP:CE2	1:D:107:LEU:HB2	2.54	0.42
1:D:90:ARG:HG2	1:D:93:ALA:HB2	2.01	0.42
1:C:221:ASP:N	1:C:221:ASP:OD1	2.53	0.42
1:C:90:ARG:HG2	1:C:90:ARG:O	2.20	0.42
1:C:104:ASP:OD1	1:D:184:PHE:CZ	2.73	0.41
1:D:63:ILE:HD11	1:D:100:LEU:HD11	2.01	0.41
1:D:202:ASN:ND2	1:D:206:THR:HG23	2.25	0.41
1:D:40:LEU:O	1:D:41:ASN:HB2	2.20	0.41
1:C:130:LYS:HB2	2:A:52:SER:CB	2.50	0.41
1:C:29:GLU:HB3	1:D:188:ILE:HD13	2.02	0.41
1:D:194:VAL:HG22	1:D:213:LEU:HD13	2.01	0.41
1:D:39:PRO:O	1:D:42:ASP:HB2	2.20	0.41
1:D:96:SER:HA	1:D:97:PRO:HD3	1.92	0.41
1:D:38:THR:HA	1:D:39:PRO:HD3	1.88	0.41
1:C:146:ARG:NH1	1:E:225:VAL:HG22	2.35	0.41
1:D:89:PHE:CD1	1:D:89:PHE:N	2.88	0.41
1:C:40:LEU:O	1:C:41:ASN:HB2	2.21	0.41
2:B:61:VAL:HG23	2:B:63:GLY:N	2.35	0.41
1:E:70:LEU:HA	1:E:70:LEU:HD22	1.76	0.41
1:E:89:PHE:N	1:E:89:PHE:CD1	2.89	0.41
1:C:231:ARG:HG3	1:C:238:PRO:HG3	2.03	0.41
1:C:61:MET:HG3	1:C:126:VAL:HG22	2.02	0.40
1:C:63:ILE:CD1	1:C:100:LEU:HD22	2.51	0.40
1:C:122:CYS:O	1:C:132:GLN:HA	2.22	0.40
1:C:179:LYS:HB3	1:C:190:ILE:HD11	2.03	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	C	223/234 (95%)	204 (92%)	17 (8%)	2 (1%)	17 52
1	D	210/234 (90%)	196 (93%)	13 (6%)	1 (0%)	29 64
1	E	210/234 (90%)	197 (94%)	12 (6%)	1 (0%)	29 64
2	A	109/126 (86%)	102 (94%)	7 (6%)	0	100 100
2	B	109/126 (86%)	101 (93%)	8 (7%)	0	100 100
All	All	861/954 (90%)	800 (93%)	57 (7%)	4 (0%)	29 64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	83	GLY
1	D	83	GLY
1	E	182	GLN
1	C	152	VAL

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	C	199/207 (96%)	176 (88%)	23 (12%)	5 22
1	D	189/207 (91%)	166 (88%)	23 (12%)	5 19
1	E	190/207 (92%)	165 (87%)	25 (13%)	4 17
2	A	91/104 (88%)	83 (91%)	8 (9%)	10 36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	91/104 (88%)	79 (87%)	12 (13%)	4 17
All	All	760/829 (92%)	669 (88%)	91 (12%)	5 20

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	31	MET
1	C	42	ASP
1	C	58	ILE
1	C	60	SER
1	C	64	THR
1	C	84	ASP
1	C	85	HIS
1	C	90	ARG
1	C	96	SER
1	C	102	SER
1	C	127	THR
1	C	145	SER
1	C	159	ASP
1	C	181	THR
1	C	182	GLN
1	C	189	GLU
1	C	199	THR
1	C	203	MET
1	C	212	SER
1	C	221	ASP
1	C	231	ARG
1	C	236	HIS
1	C	240	ARG
1	D	27	LYS
1	D	31	MET
1	D	41	ASN
1	D	42	ASP
1	D	49	ASN
1	D	58	ILE
1	D	64	THR
1	D	76	VAL
1	D	85	HIS
1	D	89	PHE
1	D	90	ARG
1	D	96	SER
1	D	102	SER

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Mol	Chain	Res	Type
1	D	134	THR
1	D	149	LEU
1	D	164	GLU
1	D	180	GLN
1	D	186	HIS
1	D	200	ILE
1	D	203	MET
1	D	221	ASP
1	D	231	ARG
1	D	240	ARG
2	A	42	ASN
2	A	50	ILE
2	A	54	THR
2	A	67	ARG
2	A	68	ASN
2	A	77	LEU
2	A	104	SER
2	A	109	ARG
2	B	30	LEU
2	B	42	ASN
2	B	48	LEU
2	B	50	ILE
2	B	54	THR
2	B	59	GLU
2	B	68	ASN
2	B	74	ARG
2	B	99	ARG
2	B	102	ASP
2	B	104	SER
2	B	115	LEU
1	E	37	ILE
1	E	42	ASP
1	E	53	SER
1	E	58	ILE
1	E	70	LEU
1	E	76	VAL
1	E	82	PHE
1	E	90	ARG
1	E	121	ARG
1	E	127	THR
1	E	134	THR
1	E	145	SER

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Mol	Chain	Res	Type
1	E	146	ARG
1	E	159	ASP
1	E	160	LYS
1	E	174	ASN
1	E	180	GLN
1	E	181	THR
1	E	187	PRO
1	E	192	GLU
1	E	195	ILE
1	E	203	MET
1	E	220	GLU
1	E	231	ARG
1	E	242	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	151	GLN
1	C	182	GLN
1	C	202	ASN
1	D	136	GLN
1	D	180	GLN
2	A	89	HIS
2	A	90	GLN
2	A	94	HIS
2	B	68	ASN
2	B	89	HIS
2	B	94	HIS
1	E	182	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	E	301	1	14,14,15	0.52	0	17,19,21	1.10	1 (5%)
3	NAG	A	201	2	14,14,15	0.48	0	17,19,21	1.37	2 (11%)
3	NAG	B	201	2	14,14,15	0.54	0	17,19,21	1.57	4 (23%)
3	NAG	D	301	1	14,14,15	0.46	0	17,19,21	1.27	3 (17%)
3	NAG	C	301	1	14,14,15	0.39	0	17,19,21	1.64	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	301	1	-	3/6/23/26	0/1/1/1
3	NAG	A	201	2	-	3/6/23/26	0/1/1/1
3	NAG	B	201	2	-	6/6/23/26	0/1/1/1
3	NAG	D	301	1	-	2/6/23/26	0/1/1/1
3	NAG	C	301	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	301	NAG	C1-O5-C5	4.36	118.10	112.19
3	C	301	NAG	C4-C3-C2	-3.66	105.66	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	201	NAG	C2-N2-C7	3.60	128.04	122.90
3	A	201	NAG	C2-N2-C7	3.35	127.68	122.90
3	A	201	NAG	C1-O5-C5	-3.18	107.88	112.19
3	B	201	NAG	C1-C2-N2	2.84	115.34	110.49
3	E	301	NAG	C2-N2-C7	2.78	126.86	122.90
3	B	201	NAG	C4-C3-C2	-2.65	107.13	111.02
3	B	201	NAG	O5-C5-C6	2.50	111.12	107.20
3	D	301	NAG	O5-C1-C2	-2.40	107.50	111.29
3	D	301	NAG	C1-O5-C5	2.40	115.45	112.19
3	D	301	NAG	C1-C2-N2	2.33	114.46	110.49

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	301	NAG	O7-C7-N2-C2
3	D	301	NAG	C8-C7-N2-C2
3	D	301	NAG	O7-C7-N2-C2
3	C	301	NAG	O7-C7-N2-C2
3	E	301	NAG	C8-C7-N2-C2
3	C	301	NAG	C8-C7-N2-C2
3	A	201	NAG	O5-C5-C6-O6
3	B	201	NAG	C4-C5-C6-O6
3	B	201	NAG	O5-C5-C6-O6
3	A	201	NAG	C4-C5-C6-O6
3	B	201	NAG	C8-C7-N2-C2
3	B	201	NAG	O7-C7-N2-C2
3	E	301	NAG	C4-C5-C6-O6
3	A	201	NAG	C3-C2-N2-C7
3	C	301	NAG	C4-C5-C6-O6
3	B	201	NAG	C3-C2-N2-C7
3	B	201	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	301	NAG	2	0
3	A	201	NAG	1	0
3	B	201	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	C	225/234 (96%)	-0.05	1 (0%) 92 84	103, 136, 210, 250	0
1	D	214/234 (91%)	0.07	5 (2%) 60 39	107, 151, 199, 238	0
1	E	214/234 (91%)	0.26	16 (7%) 14 5	116, 168, 229, 278	0
2	A	111/126 (88%)	0.02	1 (0%) 84 69	106, 146, 218, 240	0
2	B	111/126 (88%)	-0.14	0 100 100	98, 135, 177, 194	0
All	All	875/954 (91%)	0.05	23 (2%) 56 33	98, 149, 213, 278	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	28	VAL	5.4
1	D	215	LEU	5.2
1	E	50	ILE	3.4
1	E	138	GLU	3.2
1	E	71	THR	3.2
1	E	190	ILE	3.1
1	E	136	GLN	2.8
1	E	186	HIS	2.8
1	E	26	LEU	2.8
1	E	169	TYR	2.6
1	E	114	LEU	2.6
1	E	132	GLN	2.5
1	E	179	LYS	2.5
1	C	184	PHE	2.4
1	E	118	GLY	2.3
1	D	207	PHE	2.3
1	D	209	VAL	2.2
2	A	56	PHE	2.2
1	E	120	TYR	2.1
1	E	137	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	139	VAL	2.1
1	D	74	LYS	2.1
1	D	114	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	B	201	14/15	0.86	0.17	144,168,187,193	0
3	NAG	D	301	14/15	0.88	0.19	139,161,192,194	0
3	NAG	E	301	14/15	0.90	0.27	139,174,180,186	0
3	NAG	A	201	14/15	0.90	0.17	171,182,204,212	0
3	NAG	C	301	14/15	0.97	0.24	134,147,176,204	0

6.5 Other polymers (i)

There are no such residues in this entry.