



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:59 PM GMT

PDB ID : 4GRW  
Title : Structure of a complex of human IL-23 with 3 Nanobodies (Llama vHHs)  
Authors : Desmyter, A.; Spinelli, S.; Button, C.; Saunders, M.; de Haard, H.; Romme-  
laere, H.; Union, A.; Cambillau, C.  
Deposited on : 2012-08-27  
Resolution : 2.55 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

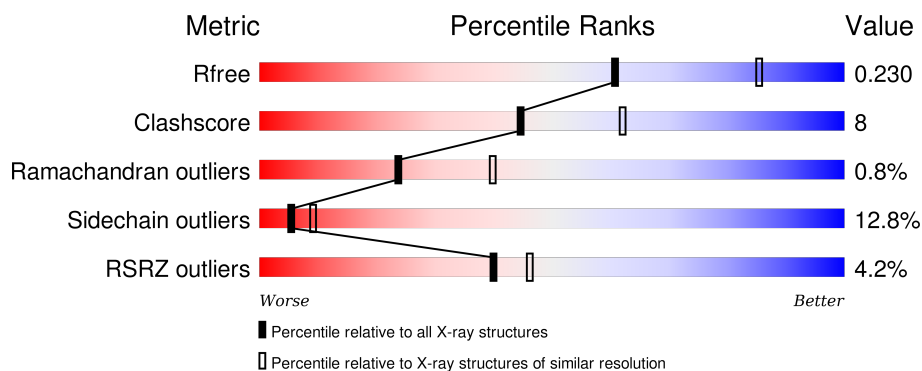
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	189	<div> <div>3%</div> <div>52% 12% 5% 31%</div> </div>
1	C	189	<div> <div>%</div> <div>63% • 32%</div> </div>
2	B	328	<div> <div>2%</div> <div>71% 15% • 11%</div> </div>
2	D	328	<div> <div>3%</div> <div>71% 14% • 11%</div> </div>
3	E	125	<div> <div>%</div> <div>81% 18% •</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	125	
4	F	126	
4	J	126	
5	H	123	
5	I	123	

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
6	NAG	B	402	X	-	-	-
6	NAG	D	402	X	-	-	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13131 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 Interleukin-23 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	130	Total	C	N	O	S	0	0	0
			1010	647	181	177	5			
1	C	129	Total	C	N	O	S	0	0	0
			1002	643	179	175	5			

- Molecule 2 is a protein called Interleukin-12 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	293	Total	C	N	O	S	0	0	0
			2331	1478	382	459	12			
2	D	292	Total	C	N	O	S	0	0	0
			2319	1467	379	461	12			

- Molecule 3 is a protein called Nanobody 124C4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	125	Total	C	N	O	S	0	0	0
			938	586	161	187	4			
3	G	125	Total	C	N	O	S	0	0	0
			937	586	161	186	4			

- Molecule 4 is a protein called Nanobody 37D5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	125	Total	C	N	O	S	0	0	0
			954	596	161	192	5			
4	J	122	Total	C	N	O	S	0	0	0
			932	583	158	186	5			

- Molecule 5 is a protein called Nanobody 22E11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	123	Total	C	N	O	S	0	0	0
			938	585	168	182	3			
5	I	123	Total	C	N	O	S	0	0	0
			938	585	168	182	3			

- Molecule 6 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	5	Total	C	N	O	0	0
			61	34	2	25		
6	D	5	Total	C	N	O	0	0
			61	34	2	25		

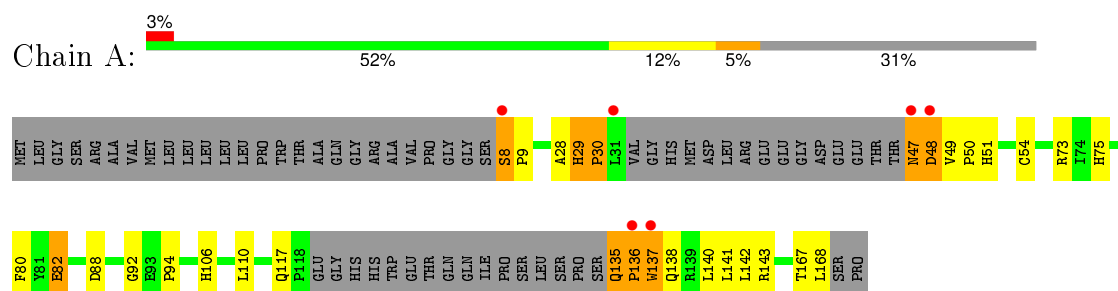
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	24	Total	O	0	0
			24	24		
7	B	143	Total	O	0	0
			143	143		
7	C	48	Total	O	0	0
			48	48		
7	D	187	Total	O	0	0
			187	187		
7	E	67	Total	O	0	0
			67	67		
7	F	38	Total	O	0	0
			38	38		
7	G	57	Total	O	0	0
			57	57		
7	H	50	Total	O	0	0
			50	50		
7	I	73	Total	O	0	0
			73	73		
7	J	23	Total	O	0	0
			23	23		

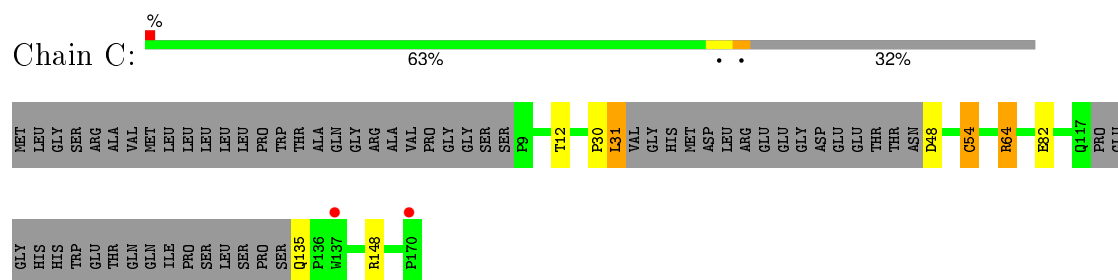
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

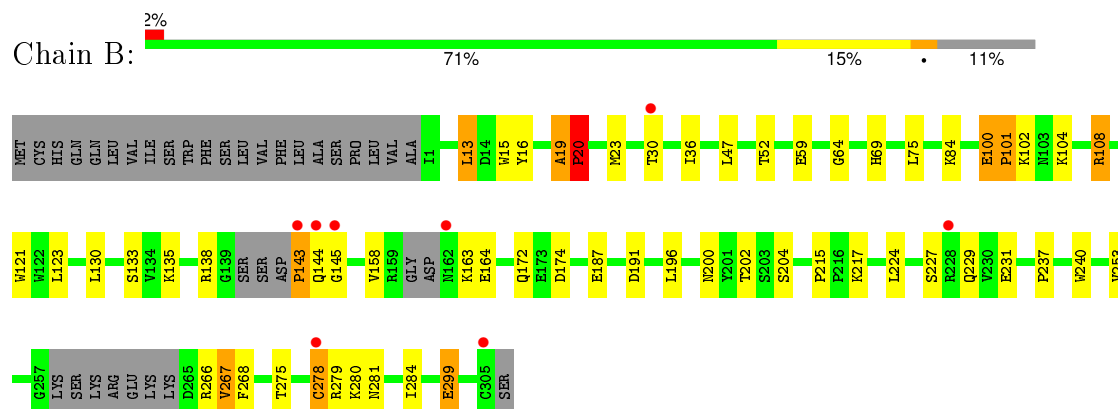
- Molecule 1: Interleukin-23 subunit alpha



- Molecule 1: Interleukin-23 subunit alpha

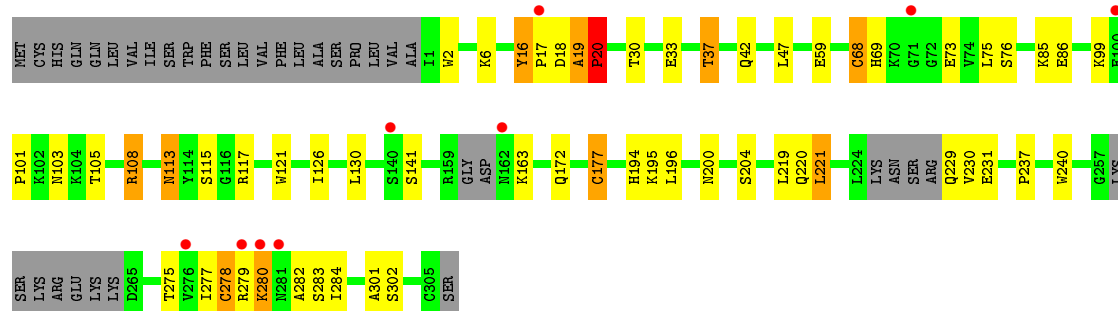


- Molecule 2: Interleukin-12 subunit beta

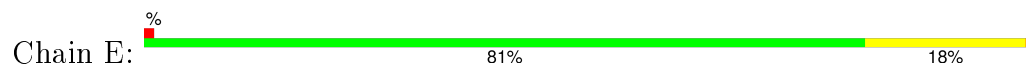


- Molecule 2: Interleukin-12 subunit beta

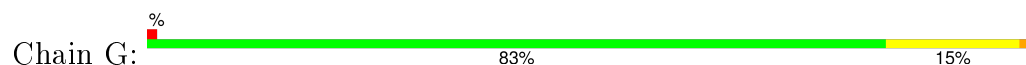




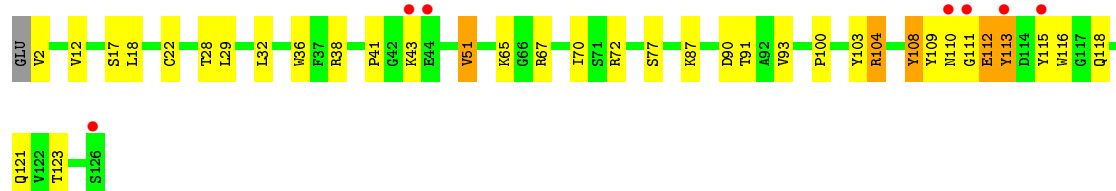
• Molecule 3: Nanobody 124C4



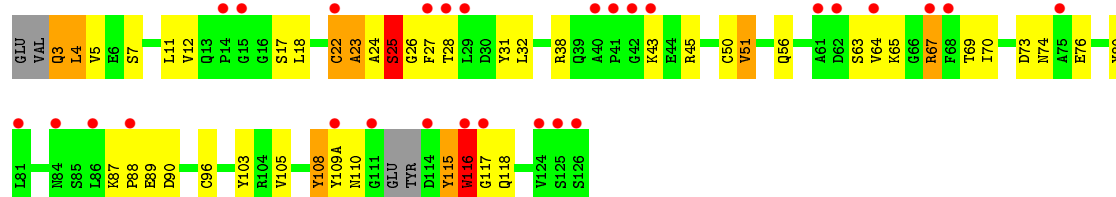
• Molecule 3: Nanobody 124C4



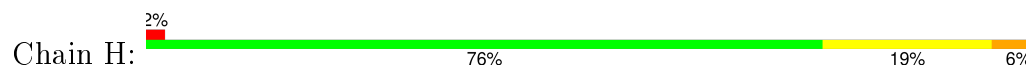
• Molecule 4: Nanobody 37D5

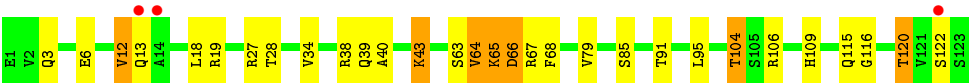


• Molecule 4: Nanobody 37D5

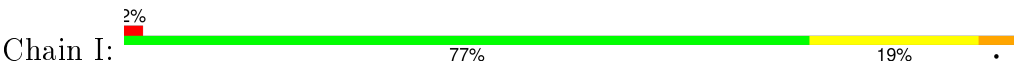


• Molecule 5: Nanobody 22E11





● Molecule 5: Nanobody 22E11





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.27Å 135.14Å 139.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.83 – 2.55 43.83 – 2.55	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.83-2.55) 99.8 (43.83-2.55)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.01 (at 2.54Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, $R_{free}$	0.183 , 0.218 0.192 , 0.230	Depositor DCC
$R_{free}$ test set	1940 reflections (3.16%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.5	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 66.5	EDS
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 63329 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13131	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.55	0/1034	0.73	1/1405 (0.1%)
1	C	0.50	0/1026	0.65	0/1393
2	B	0.50	0/2387	0.75	1/3241 (0.0%)
2	D	0.52	2/2375 (0.1%)	0.72	0/3228
3	E	0.54	0/958	0.73	0/1300
3	G	0.51	0/957	0.77	0/1299
4	F	0.54	0/975	0.69	0/1323
4	J	0.55	0/952	0.77	1/1290 (0.1%)
5	H	0.56	0/960	0.71	0/1302
5	I	0.49	0/960	0.68	0/1302
All	All	0.53	2/12584 (0.0%)	0.72	3/17083 (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
1	A	0	3
2	B	0	1
4	F	0	2
4	J	0	7
5	H	0	2
5	I	0	1
6	B	1	0
6	D	1	0
All	All	2	16

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	20	PRO	N-CD	5.53	1.55	1.47
2	D	16	TYR	CE1-CZ	-5.03	1.32	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	110	ASN	C-N-CA	6.78	136.53	122.30
1	A	29	HIS	C-N-CD	5.85	140.69	128.40
2	B	20	PRO	CA-N-CD	-5.54	103.75	111.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	402	NAG	C1
6	D	402	NAG	C1

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	28	ALA	Peptide
1	A	30	PRO	Peptide
1	A	47	ASN	Peptide
2	B	143	PRO	Peptide
4	F	112	GLU	Peptide
4	F	113	TYR	Peptide
5	H	65	LYS	Peptide
5	H	66	ASP	Peptide
5	I	17	SER	Peptide
4	J	108	TYR	Mainchain
4	J	115	TYR	Peptide
4	J	116	TRP	Peptide
4	J	117	GLY	Peptide
4	J	23	ALA	Peptide
4	J	24	ALA	Peptide
4	J	25	SER	Peptide

## 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	A	1010	0	1006	31	0
1	C	1002	0	1001	6	0
2	B	2331	0	2244	31	0
2	D	2319	0	2215	38	0
3	E	938	0	890	8	0
3	G	937	0	887	9	0
4	F	954	0	888	30	0
4	J	932	0	869	24	0
5	H	938	0	893	11	0
5	I	938	0	893	16	0
6	B	61	0	52	3	0
6	D	61	0	52	7	0
7	A	24	0	0	0	0
7	B	143	0	0	1	0
7	C	48	0	0	1	0
7	D	187	0	0	2	0
7	E	67	0	0	0	0
7	F	38	0	0	0	0
7	G	57	0	0	0	0
7	H	50	0	0	0	0
7	I	73	0	0	1	0
7	J	23	0	0	0	0
All	All	13131	0	11890	189	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 8.

All (189) 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:200:ASN:HD21	6:D:402:NAG:C1	1.31	1.44
2:B:200:ASN:HD21	6:B:402:NAG:C1	1.36	1.30
1:A:137:TRP:HB3	1:A:138:GLN:HB3	1.18	1.18
1:A:137:TRP:HB3	1:A:138:GLN:CB	1.79	1.11
2:D:19:ALA:HB1	2:D:20:PRO:CA	1.82	1.10
2:B:19:ALA:HB1	2:B:20:PRO:HA	1.30	1.05
1:A:135:GLN:HE21	1:A:135:GLN:HA	1.14	1.05
2:D:19:ALA:CB	2:D:20:PRO:HA	1.78	1.04
5:H:104:THR:HG21	5:H:109:HIS:HD2	1.23	1.00
5:H:104:THR:HG21	5:H:109:HIS:CD2	1.98	0.99
5:I:104:THR:HG21	5:I:109:HIS:HD2	1.28	0.98
5:I:104:THR:HG21	5:I:109:HIS:CD2	2.01	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:104:ARG:NH1	4:F:113:TYR:CB	2.31	0.93
4:J:73:ASP:HB2	4:J:80:TYR:HE2	1.34	0.93
1:A:137:TRP:CB	1:A:138:GLN:HB3	1.99	0.92
2:D:19:ALA:HB1	2:D:20:PRO:HA	0.93	0.92
1:A:137:TRP:HB3	1:A:138:GLN:CA	2.01	0.90
1:A:135:GLN:NE2	1:A:135:GLN:HA	1.87	0.88
1:A:136:PRO:O	1:A:137:TRP:HB2	1.75	0.87
2:B:19:ALA:CB	2:B:20:PRO:HA	2.07	0.83
5:H:104:THR:CG2	5:H:109:HIS:HD2	1.91	0.83
4:F:67:ARG:NH2	4:F:90:ASP:OD2	2.14	0.81
5:I:104:THR:CG2	5:I:109:HIS:HD2	1.92	0.81
4:F:109:TYR:CZ	4:F:111:GLY:HA2	2.16	0.80
2:B:200:ASN:HD22	6:B:402:NAG:C1	1.93	0.79
4:J:115:TYR:HB3	4:J:116:TRP:O	1.82	0.78
4:F:104:ARG:HH12	4:F:113:TYR:CB	1.96	0.77
4:J:63:SER:O	4:J:67:ARG:NH1	2.18	0.77
4:F:103:TYR:O	4:F:108:TYR:O	2.04	0.75
2:B:253:VAL:HB	2:B:267:VAL:HG13	1.68	0.74
2:D:16:TYR:HB2	2:D:17:PRO:CD	2.18	0.73
1:A:47:ASN:OD1	2:D:277:ILE:HD11	1.89	0.73
4:J:73:ASP:HB2	4:J:80:TYR:CE2	2.22	0.72
1:C:54:CYS:HG	2:D:177:CYS:HG	1.37	0.71
4:F:109:TYR:CE1	4:F:111:GLY:HA2	2.26	0.70
4:F:112:GLU:HA	4:F:112:GLU:OE2	1.91	0.69
4:J:22:CYS:CB	4:J:96:CYS:SG	2.78	0.69
2:D:219:LEU:HD11	2:D:301:ALA:HB1	1.74	0.69
4:J:4:LEU:HA	4:J:23:ALA:O	1.93	0.69
4:F:104:ARG:HD3	4:F:110:ASN:HB2	1.73	0.69
5:H:40:ALA:HB3	5:H:43:LYS:HG3	1.76	0.68
4:F:109:TYR:CZ	4:F:111:GLY:CA	2.77	0.68
2:B:280:LYS:O	2:B:281:ASN:HB2	1.95	0.67
2:B:144:GLN:HA	2:B:144:GLN:NE2	2.11	0.65
2:B:145:GLY:O	2:B:174:ASP:N	2.27	0.65
5:I:27:ARG:NH1	5:I:77:ASN:OD1	2.31	0.64
2:D:16:TYR:HB2	2:D:17:PRO:HD2	1.78	0.64
2:D:221:LEU:HB2	2:D:230:VAL:HG11	1.79	0.63
4:F:29:LEU:HD23	4:F:32:LEU:HD12	1.81	0.63
2:B:13:LEU:CD1	2:B:15:TRP:HB2	2.30	0.62
1:A:50:PRO:HD3	1:A:80:PHE:CD2	2.34	0.62
1:A:137:TRP:CB	1:A:138:GLN:CB	2.66	0.62
2:B:215:PRO:HG3	2:B:299:GLU:HG2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:PRO:HG2	1:A:137:TRP:CD1	2.34	0.62
1:A:135:GLN:CA	1:A:135:GLN:HE21	2.03	0.61
4:J:67:ARG:NH2	4:J:90:ASP:OD2	2.34	0.61
3:G:8:GLY:O	3:G:18:LEU:HD21	2.00	0.60
2:B:138:ARG:O	2:B:143:PRO:HB2	2.02	0.59
4:J:5:VAL:N	4:J:23:ALA:O	2.32	0.59
2:B:19:ALA:HB1	2:B:20:PRO:CA	2.19	0.58
2:D:19:ALA:CB	2:D:20:PRO:CA	2.57	0.58
4:F:109:TYR:CE1	4:F:111:GLY:CA	2.86	0.58
2:B:278:CYS:SG	2:B:284:ILE:HD11	2.44	0.58
2:D:172:GLN:HE22	3:E:103:TRP:HH2	1.52	0.58
5:H:64:VAL:HG11	5:H:68:PHE:CD2	2.39	0.57
1:A:47:ASN:N	1:A:48:ASP:HB2	2.19	0.57
2:B:13:LEU:HD13	2:B:15:TRP:HB2	1.85	0.57
1:A:48:ASP:HB2	2:D:277:ILE:HD13	1.85	0.56
2:D:37:THR:HG22	2:D:69:HIS:HB2	1.87	0.56
4:F:104:ARG:CD	4:F:110:ASN:HB2	2.34	0.56
4:F:115:TYR:CD1	4:F:116:TRP:N	2.73	0.56
2:D:278:CYS:SG	2:D:284:ILE:HD11	2.46	0.56
4:J:50:CYS:HB2	4:J:105:VAL:HG21	1.88	0.55
5:I:43:LYS:HD3	5:I:44:GLU:H	1.71	0.55
4:J:3:GLN:HB3	4:J:25:SER:O	2.06	0.55
1:A:137:TRP:HB3	1:A:138:GLN:C	2.27	0.55
1:A:94:PRO:CG	1:A:140:LEU:HD21	2.37	0.55
1:A:136:PRO:O	1:A:137:TRP:CB	2.50	0.54
1:A:94:PRO:HG2	1:A:140:LEU:HD21	1.89	0.54
4:J:51:VAL:HG13	4:J:70:ILE:HG23	1.87	0.54
1:A:8:SER:N	1:A:9:PRO:HD3	2.22	0.54
2:B:19:ALA:CB	2:B:20:PRO:CA	2.83	0.54
5:I:1:GLU:HA	7:I:247:HOH:O	2.07	0.54
2:B:108:ARG:HD2	2:B:121:TRP:CZ2	2.41	0.54
1:C:64:ARG:HG3	3:E:31:ASP:OD2	2.08	0.54
1:A:137:TRP:CG	1:A:138:GLN:HB3	2.42	0.54
2:B:224:LEU:HD12	2:B:229:GLN:HG2	1.90	0.54
3:G:13:GLN:NE2	3:G:13:GLN:H	2.07	0.52
2:B:143:PRO:O	2:B:145:GLY:N	2.42	0.52
4:J:26:GLY:N	4:J:27:PHE:CD1	2.78	0.52
1:C:12:THR:HG22	7:C:225:HOH:O	2.10	0.52
7:D:572:HOH:O	5:I:109:HIS:HE1	1.92	0.52
4:J:3:GLN:HA	4:J:3:GLN:OE1	2.10	0.52
4:F:51:VAL:HG13	4:F:70:ILE:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:PRO:O	1:C:31:LEU:HB2	2.10	0.52
4:J:25:SER:OG	4:J:26:GLY:HA2	2.09	0.51
2:D:115:SER:HB2	3:E:103:TRP:CE2	2.45	0.51
1:A:47:ASN:N	1:A:48:ASP:CB	2.74	0.51
4:J:26:GLY:N	4:J:27:PHE:HD1	2.08	0.51
4:F:103:TYR:C	4:F:108:TYR:O	2.48	0.51
5:H:12:VAL:HG11	5:H:18:LEU:HD23	1.93	0.50
2:D:19:ALA:HB3	7:D:521:HOH:O	2.11	0.50
1:A:75:HIS:CE1	1:A:117:GLN:HB2	2.47	0.50
1:A:47:ASN:HB2	2:D:277:ILE:CD1	2.42	0.50
2:D:86:GLU:OE1	5:I:52:ARG:NH2	2.46	0.49
2:D:117:ARG:HB2	2:D:172:GLN:NE2	2.28	0.49
3:G:87:THR:HG23	3:G:118:THR:HA	1.93	0.49
3:E:12:VAL:HG11	3:E:86:LEU:HD23	1.96	0.48
2:D:200:ASN:HD22	6:D:402:NAG:C1	2.09	0.48
2:B:217:LYS:NZ	3:G:54:ALA:O	2.46	0.48
2:D:101:PRO:HG2	2:D:105:THR:HG21	1.95	0.48
2:D:113:ASN:HD22	2:D:115:SER:H	1.61	0.47
5:H:64:VAL:HG11	5:H:68:PHE:CE2	2.49	0.47
5:H:64:VAL:CG1	5:H:68:PHE:CD2	2.98	0.47
1:A:94:PRO:HB3	4:J:108:TYR:CZ	2.49	0.47
5:H:95:LEU:HD12	5:H:116:GLY:CA	2.45	0.47
2:D:200:ASN:ND2	6:D:402:NAG:H82	2.30	0.47
5:I:104:THR:CG2	5:I:109:HIS:CD2	2.78	0.47
2:D:68:CYS:HB2	2:D:76:SER:O	2.15	0.46
2:B:16:TYR:CD1	4:F:41:PRO:HB2	2.51	0.46
1:C:30:PRO:HD2	4:F:100:PRO:HG3	1.96	0.46
2:B:266:ARG:NH2	4:J:25:SER:OG	2.48	0.46
4:J:27:PHE:CD1	4:J:27:PHE:N	2.84	0.46
3:G:93:ALA:HB3	3:G:108:MET:HE2	1.98	0.46
2:B:237:PRO:HG2	2:B:240:TRP:HB2	1.96	0.46
2:D:117:ARG:HB2	2:D:172:GLN:HE21	1.81	0.46
2:D:68:CYS:HB3	2:D:75:LEU:HB2	1.97	0.46
1:A:137:TRP:CB	1:A:138:GLN:CA	2.84	0.45
4:F:22:CYS:HB2	4:F:36:TRP:CZ2	2.52	0.45
5:I:28:THR:HG22	5:I:98:GLU:OE1	2.16	0.45
3:G:14:PRO:HG2	3:G:121:SER:HA	1.99	0.45
2:D:18:ASP:O	2:D:19:ALA:HB3	2.17	0.45
4:F:67:ARG:HH22	4:F:90:ASP:CG	2.20	0.45
4:F:32:LEU:O	4:F:72:ARG:NH1	2.46	0.45
5:H:34:VAL:HB	5:H:79:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:95:LEU:HD12	5:I:116:GLY:CA	2.47	0.45
5:I:88:PRO:HA	5:I:121:VAL:HB	1.99	0.45
6:D:403:BMA:H61	6:D:405:MAN:H2	1.60	0.45
5:I:27:ARG:HD2	5:I:53:TRP:CD1	2.52	0.44
2:D:279:ARG:HB2	2:D:282:ALA:HB2	1.99	0.44
1:A:49:VAL:HG23	1:A:51:HIS:CE1	2.52	0.44
4:J:25:SER:CB	4:J:26:GLY:HA2	2.47	0.44
4:F:91:THR:HG23	4:F:123:THR:HA	1.99	0.44
2:D:237:PRO:HG2	2:D:240:TRP:HB2	2.00	0.44
4:F:110:ASN:C	4:F:112:GLU:H	2.20	0.43
2:D:200:ASN:HD21	6:D:402:NAG:H82	1.84	0.43
2:D:2:TRP:CH2	6:D:402:NAG:H2	2.52	0.43
2:D:30:THR:HG21	2:D:75:LEU:HD13	2.01	0.43
2:B:30:THR:HG21	2:B:75:LEU:HD13	1.99	0.43
2:D:126:ILE:HG21	2:D:194:HIS:CD2	2.54	0.43
2:D:108:ARG:HD3	2:D:121:TRP:CZ2	2.53	0.43
3:G:79:MET:HE1	3:G:117:VAL:HG21	2.01	0.43
3:G:95:VAL:HG22	3:G:108:MET:HE1	2.01	0.42
4:F:111:GLY:C	4:F:113:TYR:H	2.22	0.42
4:F:110:ASN:C	4:F:112:GLU:N	2.69	0.42
3:E:19:ARG:HG3	3:E:82:GLN:NE2	2.34	0.42
5:I:68:PHE:N	5:I:68:PHE:CD1	2.86	0.42
3:E:97:ALA:HB3	3:E:112:MET:HE2	2.01	0.42
4:J:64:VAL:HA	4:J:67:ARG:NH1	2.34	0.42
1:A:47:ASN:HB2	2:D:277:ILE:HD12	2.00	0.42
2:B:64:GLY:HA2	2:B:196:LEU:HD21	2.01	0.42
4:J:4:LEU:CA	4:J:23:ALA:O	2.66	0.42
2:B:100:GLU:HA	2:B:101:PRO:C	2.40	0.42
4:F:116:TRP:CE3	4:F:116:TRP:HA	2.55	0.42
4:F:111:GLY:C	4:F:113:TYR:N	2.73	0.42
1:A:82:GLU:OE2	1:A:106:HIS:HE1	2.03	0.41
6:D:402:NAG:H83	6:D:402:NAG:H3	2.02	0.41
5:I:34:VAL:HB	5:I:79:VAL:HG21	2.01	0.41
2:D:221:LEU:H	2:D:221:LEU:HD23	1.84	0.41
4:F:115:TYR:HD1	4:F:116:TRP:H	1.67	0.41
1:A:30:PRO:HG3	4:J:32:LEU:HD21	2.03	0.41
4:F:110:ASN:ND2	4:F:112:GLU:HB2	2.36	0.41
4:F:93:VAL:HG22	4:F:121:GLN:HG2	2.03	0.41
2:B:36:ILE:HA	2:B:69:HIS:O	2.20	0.41
1:A:143:ARG:NH1	4:J:103:TYR:OH	2.51	0.40
6:B:402:NAG:H82	7:B:627:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:13:GLN:H	3:G:13:GLN:HE21	1.69	0.40
5:H:91:THR:HG23	5:H:120:THR:HA	2.03	0.40
2:B:215:PRO:CG	2:B:299:GLU:HG2	2.51	0.40
2:B:266:ARG:HD3	2:B:268:PHE:CE2	2.56	0.40
2:B:16:TYR:CE1	4:F:41:PRO:HB2	2.56	0.40
3:E:108:PRO:HG2	3:E:110:TYR:CZ	2.56	0.40
2:B:133:SER:HB3	2:B:191:ASP:HB2	2.03	0.40
1:C:54:CYS:CB	2:D:177:CYS:HG	2.32	0.40
2:B:13:LEU:HD11	2:B:15:TRP:HB2	2.04	0.40
4:J:26:GLY:H	4:J:27:PHE:HD1	1.69	0.40
3:E:68:PHE:HA	3:E:82:GLN:O	2.21	0.40
5:I:67:ARG:C	5:I:68:PHE:HD1	2.25	0.40
1:A:167:THR:OG1	1:A:168:LEU:HD12	2.22	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	124/189 (66%)	118 (95%)	2 (2%)	4 (3%)	5	6
1	C	123/189 (65%)	120 (98%)	3 (2%)	0	100	100
2	B	285/328 (87%)	269 (94%)	14 (5%)	2 (1%)	26	44
2	D	284/328 (87%)	268 (94%)	13 (5%)	3 (1%)	17	30
3	E	123/125 (98%)	123 (100%)	0	0	100	100
3	G	123/125 (98%)	122 (99%)	1 (1%)	0	100	100
4	F	123/126 (98%)	118 (96%)	5 (4%)	0	100	100
4	J	118/126 (94%)	109 (92%)	7 (6%)	2 (2%)	11	18
5	H	121/123 (98%)	118 (98%)	2 (2%)	1 (1%)	24	40
5	I	121/123 (98%)	120 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1545/1782 (87%)	1485 (96%)	48 (3%)	12 (1%)	24	40

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	A	136	PRO
2	B	19	ALA
2	D	19	ALA
4	J	116	TRP
1	A	137	TRP
2	D	280	LYS
5	H	66	ASP
2	B	101	PRO
2	D	195	LYS
1	A	92	GLY
4	J	88	PRO

### 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	109/159 (69%)	99 (91%)	10 (9%)	11	20
1	C	108/159 (68%)	101 (94%)	7 (6%)	21	37
2	B	263/297 (89%)	235 (89%)	28 (11%)	8	15
2	D	262/297 (88%)	233 (89%)	29 (11%)	8	13
3	E	96/97 (99%)	82 (85%)	14 (15%)	4	6
3	G	95/97 (98%)	85 (90%)	10 (10%)	8	15
4	F	100/103 (97%)	86 (86%)	14 (14%)	4	7
4	J	97/103 (94%)	72 (74%)	25 (26%)	0	1
5	H	98/99 (99%)	78 (80%)	20 (20%)	1	2
5	I	98/99 (99%)	85 (87%)	13 (13%)	5	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1326/1510 (88%)	1156 (87%)	170 (13%)	<b>5</b> <b>9</b>

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	29	HIS
1	A	54	CYS
1	A	73	ARG
1	A	82	GLU
1	A	88	ASP
1	A	110	LEU
1	A	135	GLN
1	A	141	LEU
1	A	142	LEU
2	B	13	LEU
2	B	20	PRO
2	B	23	MET
2	B	47	LEU
2	B	52	THR
2	B	59	GLU
2	B	84	LYS
2	B	100	GLU
2	B	102	LYS
2	B	104	LYS
2	B	108	ARG
2	B	123	LEU
2	B	130	LEU
2	B	135	LYS
2	B	158	VAL
2	B	163	LYS
2	B	164	GLU
2	B	172	GLN
2	B	187	GLU
2	B	202	THR
2	B	204	SER
2	B	227	SER
2	B	231	GLU
2	B	267	VAL
2	B	275	THR
2	B	278	CYS
2	B	279	ARG

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Mol	Chain	Res	Type
2	B	299	GLU
1	C	31	LEU
1	C	48	ASP
1	C	54	CYS
1	C	64	ARG
1	C	82	GLU
1	C	135	GLN
1	C	148	ARG
2	D	6	LYS
2	D	20	PRO
2	D	33	GLU
2	D	37	THR
2	D	42	GLN
2	D	47	LEU
2	D	59	GLU
2	D	68	CYS
2	D	73	GLU
2	D	85	LYS
2	D	99	LYS
2	D	103	ASN
2	D	108	ARG
2	D	113	ASN
2	D	130	LEU
2	D	141	SER
2	D	163	LYS
2	D	177	CYS
2	D	196	LEU
2	D	204	SER
2	D	220	GLN
2	D	221	LEU
2	D	229	GLN
2	D	231	GLU
2	D	275	THR
2	D	278	CYS
2	D	280	LYS
2	D	283	SER
2	D	302	SER
3	E	3	GLN
3	E	18	LEU
3	E	28	THR
3	E	38	ARG
3	E	45	ARG

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Mol	Chain	Res	Type
3	E	59	TYR
3	E	62	ASP
3	E	78	THR
3	E	86	LEU
3	E	87	ARG
3	E	98	ARG
3	E	101	THR
3	E	105	LEU
3	E	125	SER
4	F	2	VAL
4	F	12	VAL
4	F	17	SER
4	F	18	LEU
4	F	28	THR
4	F	38	ARG
4	F	43	LYS
4	F	51	VAL
4	F	65	LYS
4	F	77	SER
4	F	87	LYS
4	F	104	ARG
4	F	108	TYR
4	F	118	GLN
3	G	12	VAL
3	G	13	GLN
3	G	28(B)	ASP
3	G	34	ARG
3	G	41	ARG
3	G	49	SER
3	G	74	THR
3	G	77	LEU
3	G	101	LEU
3	G	118	THR
5	H	3	GLN
5	H	6	GLU
5	H	12	VAL
5	H	13	GLN
5	H	19	ARG
5	H	27	ARG
5	H	28	THR
5	H	38	ARG
5	H	39	GLN

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Mol	Chain	Res	Type
5	H	43	LYS
5	H	63	SER
5	H	64	VAL
5	H	65	LYS
5	H	67	ARG
5	H	85	SER
5	H	104	THR
5	H	106	ARG
5	H	115	GLN
5	H	120	THR
5	H	122	SER
5	I	3	GLN
5	I	4	LEU
5	I	6	GLU
5	I	17	SER
5	I	18	LEU
5	I	19	ARG
5	I	27	ARG
5	I	28	THR
5	I	45	ARG
5	I	52	ARG
5	I	69	THR
5	I	104	THR
5	I	123	SER
4	J	3	GLN
4	J	4	LEU
4	J	7	SER
4	J	11	LEU
4	J	12	VAL
4	J	17	SER
4	J	18	LEU
4	J	22	CYS
4	J	25	SER
4	J	28	THR
4	J	31	TYR
4	J	38	ARG
4	J	43	LYS
4	J	45	ARG
4	J	51	VAL
4	J	56	GLN
4	J	65	LYS
4	J	67	ARG

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Mol	Chain	Res	Type
4	J	69	THR
4	J	74	ASN
4	J	76	GLU
4	J	87	LYS
4	J	89	GLU
4	J	109(A)	TYR
4	J	118	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	75	HIS
1	A	106	HIS
1	A	117	GLN
1	A	135	GLN
2	B	77	HIS
2	B	103	ASN
2	B	144	GLN
2	B	200	ASN
1	C	19	GLN
1	C	61	GLN
2	D	103	ASN
2	D	113	ASN
2	D	172	GLN
2	D	200	ASN
2	D	256	GLN
3	E	77	ASN
3	E	82	GLN
4	F	82	GLN
4	F	118	GLN
3	G	13	GLN
3	G	73	ASN
5	H	77	ASN
5	H	109	HIS
5	I	39	GLN
5	I	109	HIS
4	J	82	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 ⓘ

10 carbohydrates 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	$\# Z  > 2$
6	NAG	B	401	6	14,14,15	0.43	0	15,19,21	0.82	0
6	NAG	B	402	2,6	14,14,15	0.35	0	15,19,21	1.75	3 (20%)
6	BMA	B	403	6	11,11,12	0.45	0	14,15,17	1.30	1 (7%)
6	MAN	B	404	6	11,11,12	0.50	0	14,15,17	1.29	1 (7%)
6	MAN	B	405	6	11,11,12	0.48	0	14,15,17	1.36	2 (14%)
6	NAG	D	401	6	14,14,15	0.44	0	15,19,21	0.99	1 (6%)
6	NAG	D	402	2,6	14,14,15	0.37	0	15,19,21	2.58	3 (20%)
6	BMA	D	403	6	11,11,12	0.40	0	14,15,17	1.29	2 (14%)
6	MAN	D	404	6	11,11,12	0.46	0	14,15,17	1.21	2 (14%)
6	MAN	D	405	6	11,11,12	0.41	0	14,15,17	1.53	1 (7%)

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
6	NAG	B	401	6	-	0/6/23/26	0/1/1/1
6	NAG	B	402	2,6	1/1/5/7	0/6/23/26	0/1/1/1
6	BMA	B	403	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	B	404	6	-	0/2/19/22	0/1/1/1
6	MAN	B	405	6	-	0/2/19/22	0/1/1/1
6	NAG	D	401	6	-	0/6/23/26	0/1/1/1
6	NAG	D	402	2,6	1/1/5/7	0/6/23/26	0/1/1/1
6	BMA	D	403	6	-	0/2/19/22	0/1/1/1
6	MAN	D	404	6	-	0/2/19/22	0/1/1/1
6	MAN	D	405	6	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	402	NAG	C4-C3-C2	-5.69	102.38	111.23
6	B	402	NAG	C4-C3-C2	-2.54	107.28	111.23
6	D	401	NAG	O7-C7-C8	-2.39	117.68	122.06
6	D	404	MAN	C1-O5-C5	2.26	115.11	112.25
6	B	405	MAN	C1-C2-C3	2.27	112.23	109.54
6	D	403	BMA	C3-C4-C5	2.31	114.23	110.20
6	B	402	NAG	C2-N2-C7	2.31	126.01	123.04
6	D	404	MAN	C3-C4-C5	2.50	114.56	110.20
6	B	404	MAN	C3-C4-C5	2.51	114.58	110.20
6	D	403	BMA	O5-C5-C6	2.82	113.45	107.35
6	D	402	NAG	C1-O5-C5	2.99	116.04	112.25
6	B	405	MAN	C1-O5-C5	3.83	117.11	112.25
6	B	403	BMA	C1-O5-C5	4.00	117.33	112.25
6	B	402	NAG	C1-O5-C5	4.42	117.86	112.25
6	D	405	MAN	C1-O5-C5	4.83	118.38	112.25
6	D	402	NAG	C2-N2-C7	7.13	132.19	123.04

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	D	402	NAG	C1
6	B	402	NAG	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	402	NAG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	402	NAG	6	0
6	D	403	BMA	1	0
6	D	405	MAN	1	0

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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 ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	130/189 (68%)	0.32	6 (4%) 36 42	33, 54, 87, 109	0
1	C	129/189 (68%)	0.11	2 (1%) 74 79	29, 42, 68, 102	0
2	B	293/328 (89%)	0.13	8 (2%) 58 63	28, 45, 83, 126	0
2	D	292/328 (89%)	0.06	9 (3%) 52 58	24, 40, 84, 130	0
3	E	125/125 (100%)	-0.25	1 (0%) 87 89	26, 37, 55, 94	0
3	G	125/125 (100%)	-0.18	1 (0%) 87 89	33, 44, 63, 109	0
4	F	125/126 (99%)	0.22	7 (5%) 28 33	29, 51, 85, 113	0
4	J	122/126 (96%)	1.22	28 (22%) 1 1	40, 73, 102, 118	0
5	H	123/123 (100%)	0.14	3 (2%) 62 67	28, 48, 78, 100	0
5	I	123/123 (100%)	0.09	2 (1%) 74 79	25, 41, 68, 104	0
All	All	1587/1782 (89%)	0.17	67 (4%) 40 46	24, 45, 86, 130	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	J	41	PRO	5.8
4	J	126	SER	5.6
2	D	280	LYS	5.1
2	D	100	GLU	5.0
2	B	144	GLN	4.8
1	A	47	ASN	4.2
2	B	228	ARG	4.1
1	A	136	PRO	3.7
2	D	279	ARG	3.7
2	D	281	ASN	3.6
5	H	13	GLN	3.4
4	F	115	TYR	3.4
2	B	162	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
4	F	113	TYR	3.4
4	F	43	LYS	3.3
4	J	68	PHE	3.3
4	J	117	GLY	3.3
1	A	137	TRP	3.2
4	J	114	ASP	3.2
4	J	15	GLY	3.2
4	J	40	ALA	3.2
4	J	43	LYS	3.1
1	A	31	LEU	3.1
1	A	48	ASP	3.1
4	J	86	LEU	3.1
4	F	110	ASN	3.1
4	J	125	SER	3.1
2	D	140	SER	3.0
4	J	111	GLY	2.9
3	G	121	SER	2.9
4	J	116	TRP	2.8
4	J	27	PHE	2.8
2	B	305	CYS	2.8
1	A	8	SER	2.8
4	J	61	ALA	2.8
4	J	64	VAL	2.8
4	J	109(A)	TYR	2.8
4	J	62	ASP	2.8
4	J	81	LEU	2.7
4	J	67	ARG	2.7
4	J	84	ASN	2.7
2	D	162	ASN	2.7
4	J	14	PRO	2.6
1	C	170	PRO	2.6
4	J	88	PRO	2.5
2	B	143	PRO	2.5
4	J	29	LEU	2.4
5	H	122	SER	2.4
4	F	126	SER	2.4
2	B	145	GLY	2.4
2	D	276	VAL	2.3
2	B	30	THR	2.3
4	F	44	GLU	2.3
5	I	12	VAL	2.3
4	F	111	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	278	CYS	2.3
4	J	75	ALA	2.3
4	J	124	VAL	2.3
3	E	125	SER	2.1
4	J	42	GLY	2.1
4	J	28	THR	2.1
5	H	14	ALA	2.1
5	I	13	GLN	2.1
1	C	137	TRP	2.1
2	D	17	PRO	2.1
2	D	71	GLY	2.0
4	J	22	CYS	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	D	402	14/15	0.93	0.15	0.80	16,40,89,96	0
6	NAG	B	402	14/15	0.96	0.12	-1.18	20,44,57,82	0
6	MAN	B	404	11/12	0.56	0.26	-	62,92,147,148	0
6	BMA	D	403	11/12	0.92	0.18	-	54,95,123,128	0
6	NAG	B	401	14/15	0.97	0.14	-	24,39,72,93	0
6	NAG	D	401	14/15	0.97	0.14	-	25,41,58,76	0
6	BMA	B	403	11/12	0.84	0.18	-	51,106,130,136	0
6	MAN	D	405	11/12	0.79	0.34	-	81,105,128,138	0
6	MAN	B	405	11/12	0.50	0.33	-	84,130,146,150	0
6	MAN	D	404	11/12	0.88	0.16	-	43,98,120,127	0

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.