



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 01:08 AM BST

PDB ID : 3SE4  
Title : human IFNw-IFNAR ternary complex  
Authors : Thomas, C.; Garcia, K.C.  
Deposited on : 2011-06-10  
Resolution : 3.50 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (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

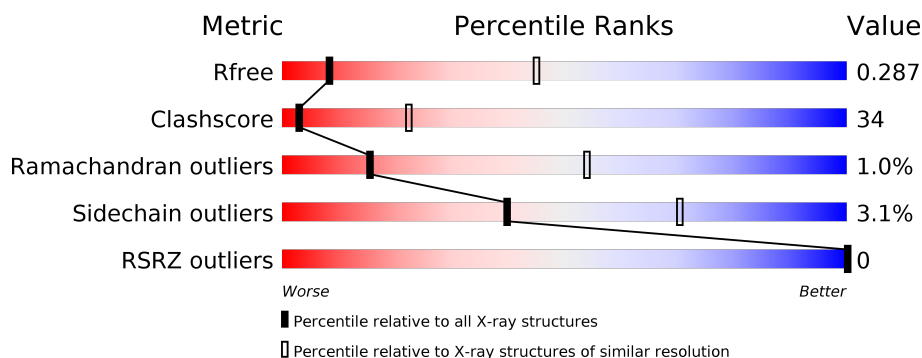
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 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  $\leq 5\%$ . 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	414	
2	B	177	
3	C	199	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4784 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 Interferon alpha/beta receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2168	1401	351	407	9			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	ALA	-	cloning artifact	UNP P17181
A	-3	ASP	-	cloning artifact	UNP P17181
A	-2	LEU	-	cloning artifact	UNP P17181
A	-1	GLY	-	cloning artifact	UNP P17181
A	0	SER	-	cloning artifact	UNP P17181

- Molecule 2 is a protein called Interferon omega-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	143	Total	C	N	O	S	0	0	0
			1133	722	206	194	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	ALA	-	cloning artifact	UNP P05000
B	-1	ASP	-	cloning artifact	UNP P05000
B	0	PRO	-	cloning artifact	UNP P05000
B	80	GLN	ASN	engineered mutation	UNP P05000

- Molecule 3 is a protein called Interferon alpha/beta receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	190	Total	C	N	O	S	0	0	0
			1469	948	237	275	9			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

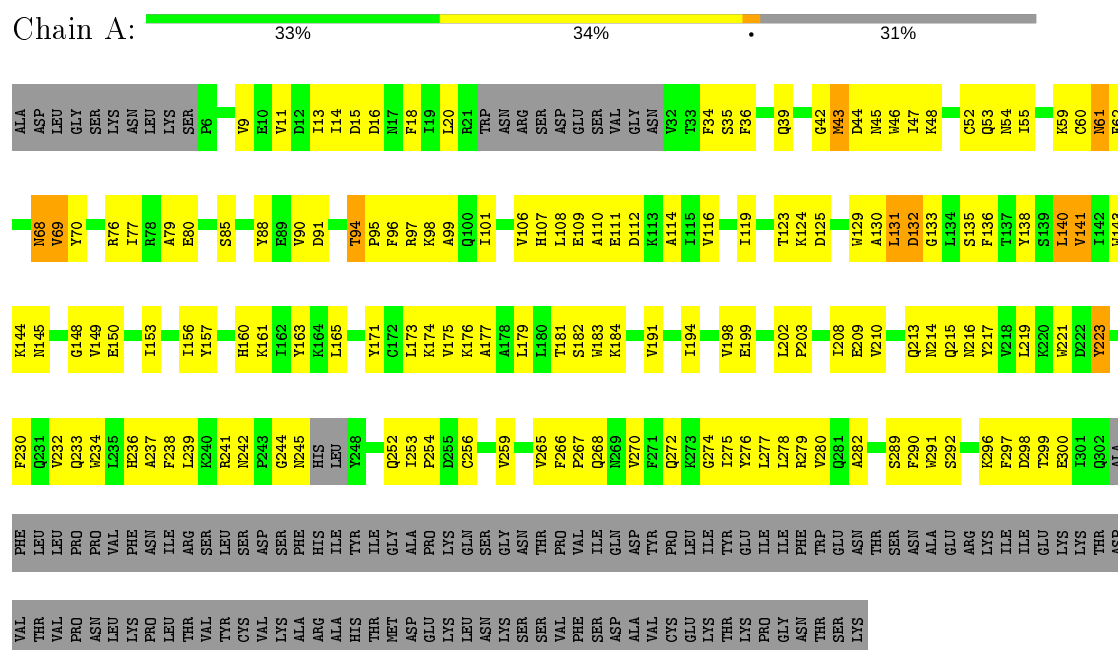


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	14	8	1	5	0	0

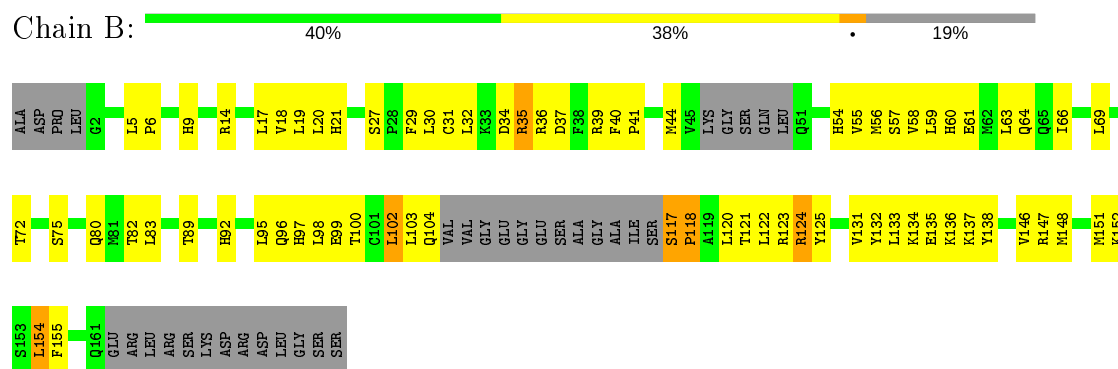
### 3 Residue-property plots

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: Interferon alpha/beta receptor 1



#### • Molecule 2: Interferon omega-1



#### • Molecule 3: Interferon alpha/beta receptor 2



Y184	L185	E186	H187	A192	S196	P197	L203	L204	P205	I103	D104	M105	F107	F112	V115	G116	F117	T118	M119	H120	I121	M122	F127	P128	S129	I130	V131	G132	G133	G134	L135	L141	V142	E148	G149	I150	V151	H154	K155	P156	E157	I158	L159	G160	A161	M162	Y168	I169	I170	L173	I174	T177	M178	Y179	V181	S182	H183																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.49 Å 93.49 Å 403.13 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.84 – 3.50 19.84 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.84-3.50) 99.9 (19.84-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.26	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 3.52 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.213 , 0.288 0.209 , 0.287	Depositor DCC
$R_{free}$ test set	700 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	81.4	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 61.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4784	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	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.*

<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, 0.333 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	A	0.57	0/2227	0.89	10/3050 (0.3%)
2	B	0.51	0/1156	0.82	2/1560 (0.1%)
3	C	0.54	0/1507	0.76	1/2057 (0.0%)
All	All	0.55	0/4890	0.83	13/6667 (0.2%)

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
2	B	0	2

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	LEU	N-CA-C	7.73	131.87	111.00
2	B	117	SER	N-CA-CB	6.88	120.82	110.50
3	C	155	LYS	C-N-CD	-6.21	106.94	120.60
1	A	43	MET	N-CA-C	6.20	127.75	111.00
1	A	69	VAL	N-CA-C	-5.94	94.96	111.00
1	A	61	ASN	N-CA-CB	5.89	121.21	110.60
1	A	42	GLY	N-CA-C	-5.88	98.41	113.10
1	A	94	THR	N-CA-C	-5.87	95.16	111.00
1	A	43	MET	CB-CA-C	-5.85	98.71	110.40
1	A	44	ASP	N-CA-CB	5.61	120.70	110.60
2	B	131	VAL	CB-CA-C	-5.35	101.24	111.40
1	A	141	VAL	N-CA-CB	5.13	122.78	111.50
1	A	160	HIS	N-CA-C	-5.10	97.23	111.00



There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	124	ARG	Sidechain
2	B	35	ARG	Sidechain

## 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	2168	0	1920	163	0
2	B	1133	0	1081	78	0
3	C	1469	0	1363	82	0
4	A	14	0	13	6	0
All	All	4784	0	4377	312	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 34.

All (312) 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:A:145:ASN:HD21	4:A:410:NAG:C1	1.35	1.36
1:A:237:ALA:HB2	1:A:275:ILE:HG22	1.41	0.98
1:A:20:LEU:HD21	1:A:77:ILE:CD1	1.99	0.92
3:C:36:PRO:HA	3:C:87:SER:HB2	1.52	0.91
1:A:145:ASN:HD21	4:A:410:NAG:C2	1.82	0.91
1:A:131:LEU:HD12	1:A:132:ASP:H	1.35	0.90
2:B:60:HIS:HD2	2:B:95:LEU:HD22	1.35	0.90
1:A:101:ILE:HG21	1:A:177:ALA:HB3	1.53	0.88
1:A:20:LEU:HD21	1:A:77:ILE:HD12	1.57	0.86
2:B:9:HIS:HD2	2:B:97:HIS:NE2	1.73	0.85
2:B:60:HIS:CD2	2:B:95:LEU:HD22	2.14	0.81
1:A:20:LEU:CD2	1:A:77:ILE:CD1	2.61	0.79
1:A:244:GLY:O	1:A:245:ASN:CB	2.32	0.77
1:A:69:VAL:O	1:A:95:PRO:HD2	1.85	0.76
1:A:140:LEU:HD12	1:A:141:VAL:H	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LEU:HD12	1:A:132:ASP:N	2.01	0.75
3:C:183:VAL:O	3:C:196:SER:HB3	1.87	0.74
1:A:274:GLY:O	1:A:299:THR:HG23	1.86	0.74
1:A:182:SER:O	1:A:183:TRP:HB2	1.85	0.74
1:A:106:VAL:HG12	1:A:108:LEU:CD1	2.18	0.74
1:A:272:GLN:O	1:A:299:THR:HG21	1.87	0.74
2:B:9:HIS:CD2	2:B:97:HIS:NE2	2.56	0.73
1:A:237:ALA:HB2	1:A:275:ILE:CG2	2.16	0.73
2:B:56:MET:HE2	2:B:98:LEU:HD12	1.70	0.72
2:B:58:VAL:HG13	2:B:59:LEU:N	2.05	0.72
3:C:121:ILE:HG13	3:C:173:LEU:CD1	2.20	0.72
1:A:165:LEU:HD22	1:A:171:TYR:CE1	2.25	0.72
3:C:78:ALA:HB2	3:C:100:TRP:CZ2	2.25	0.72
1:A:136:PHE:CD1	1:A:179:LEU:HD21	2.25	0.71
2:B:80:GLN:NE2	2:B:83:LEU:HD23	2.05	0.71
2:B:17:LEU:HD21	2:B:154:LEU:HB3	1.73	0.71
1:A:46:TRP:CZ3	1:A:76:ARG:HB2	2.25	0.71
2:B:6:PRO:HD2	2:B:9:HIS:HB2	1.74	0.70
1:A:101:ILE:CG2	1:A:177:ALA:HB3	2.21	0.70
1:A:20:LEU:HD21	1:A:77:ILE:HD13	1.74	0.70
3:C:174:ILE:O	3:C:177:THR:HB	1.92	0.70
1:A:181:THR:O	1:A:183:TRP:HD1	1.73	0.70
1:A:13:ILE:HD11	1:A:18:PHE:CE1	2.27	0.69
1:A:13:ILE:O	1:A:99:ALA:HA	1.92	0.69
1:A:77:ILE:CG2	1:A:88:TYR:HB2	2.23	0.68
2:B:20:LEU:O	2:B:147:ARG:HD2	1.92	0.68
1:A:232:VAL:HG22	1:A:280:VAL:HG22	1.76	0.68
1:A:238:PHE:HA	2:B:92:HIS:ND1	2.09	0.68
3:C:23:SER:O	3:C:24:ILE:HD13	1.92	0.68
3:C:78:ALA:HB2	3:C:100:TRP:CH2	2.30	0.67
2:B:102:LEU:C	2:B:102:LEU:HD12	2.14	0.66
1:A:35:SER:HA	1:A:53:GLN:HA	1.78	0.66
1:A:215:GLN:C	1:A:268:GLN:NE2	2.49	0.66
1:A:45:ASN:OD1	1:A:46:TRP:N	2.30	0.65
1:A:215:GLN:C	1:A:268:GLN:HE21	2.00	0.65
2:B:63:LEU:HB2	2:B:95:LEU:HD21	1.79	0.65
3:C:127:PHE:CD2	3:C:162:MET:HA	2.31	0.65
1:A:13:ILE:HD11	1:A:18:PHE:HE1	1.61	0.65
1:A:279:ARG:HG3	1:A:291:TRP:CE3	2.32	0.65
1:A:80:GLU:HG2	1:A:85:SER:HA	1.78	0.65
2:B:133:LEU:HD21	2:B:146:VAL:HG21	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:151:VAL:O	3:C:151:VAL:HG13	1.96	0.64
1:A:141:VAL:HG12	1:A:143:TRP:CZ3	2.33	0.64
3:C:52:LEU:H	3:C:52:LEU:HD22	1.63	0.64
1:A:9:VAL:O	1:A:90:VAL:HG22	1.97	0.63
2:B:100:THR:O	2:B:100:THR:HG22	1.98	0.63
1:A:20:LEU:CD2	1:A:77:ILE:HD13	2.27	0.62
3:C:117:PHE:HD1	3:C:120:HIS:NE2	1.97	0.62
1:A:61:ASN:OD1	1:A:61:ASN:C	2.38	0.62
3:C:43:TYR:HB2	3:C:81:THR:HG22	1.82	0.62
1:A:68:ASN:C	1:A:70:TYR:N	2.44	0.61
3:C:112:PHE:CE1	3:C:181:VAL:HG12	2.35	0.61
1:A:217:TYR:CZ	1:A:297:PHE:HZ	2.19	0.61
3:C:121:ILE:HG22	3:C:122:ASN:N	2.15	0.61
1:A:70:TYR:HB2	2:B:124:ARG:HG3	1.82	0.61
2:B:155:PHE:HE2	3:C:100:TRP:CE3	2.19	0.61
3:C:17:SER:HB3	3:C:106:SER:OG	2.00	0.61
1:A:141:VAL:HG12	1:A:143:TRP:HZ3	1.66	0.60
2:B:80:GLN:NE2	2:B:83:LEU:CD2	2.64	0.60
3:C:121:ILE:HG13	3:C:173:LEU:HD13	1.83	0.60
3:C:112:PHE:CG	3:C:183:VAL:HG21	2.37	0.60
1:A:112:ASP:HB2	1:A:199:GLU:HA	1.84	0.59
2:B:5:LEU:CB	2:B:6:PRO:HD2	2.32	0.59
1:A:110:ALA:HB2	1:A:194:ILE:HD11	1.85	0.59
1:A:241:ARG:HH21	2:B:92:HIS:CD2	2.21	0.59
2:B:147:ARG:NH1	2:B:151:MET:HE1	2.17	0.59
1:A:230:PHE:HD1	1:A:282:ALA:HA	1.68	0.59
2:B:58:VAL:CG1	2:B:59:LEU:N	2.65	0.59
1:A:237:ALA:CB	1:A:275:ILE:CG2	2.81	0.58
1:A:217:TYR:CD1	1:A:268:GLN:HA	2.39	0.58
2:B:72:THR:OG1	2:B:75:SER:N	2.30	0.58
1:A:111:GLU:HB2	1:A:114:ALA:O	2.04	0.58
1:A:14:ILE:HG13	1:A:14:ILE:O	2.00	0.58
1:A:106:VAL:CG1	1:A:108:LEU:HD11	2.33	0.57
1:A:34:PHE:O	1:A:54:ASN:N	2.37	0.57
1:A:77:ILE:HG23	1:A:88:TYR:HB2	1.85	0.57
1:A:136:PHE:HB3	1:A:138:TYR:CE2	2.39	0.57
2:B:117:SER:O	2:B:121:THR:HG22	2.05	0.57
1:A:275:ILE:HG22	1:A:276:TYR:N	2.18	0.57
1:A:181:THR:O	1:A:183:TRP:CD1	2.56	0.57
1:A:99:ALA:O	1:A:184:LYS:HD3	2.04	0.57
1:A:279:ARG:HG3	1:A:291:TRP:CZ3	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:127:PHE:HB3	3:C:128:PRO:HD2	1.87	0.57
3:C:117:PHE:O	3:C:203:LEU:HD22	2.04	0.56
3:C:178:ASN:HD21	3:C:202:LEU:HB2	1.70	0.56
1:A:61:ASN:OD1	1:A:62:PHE:N	2.38	0.56
1:A:18:PHE:O	1:A:59:LYS:HA	2.05	0.56
1:A:238:PHE:HA	2:B:92:HIS:CE1	2.40	0.56
2:B:5:LEU:CB	2:B:6:PRO:CD	2.83	0.56
1:A:173:LEU:C	1:A:173:LEU:HD12	2.26	0.56
2:B:122:LEU:O	2:B:125:TYR:HB3	2.05	0.56
3:C:162:MET:SD	3:C:162:MET:N	2.79	0.56
2:B:57:SER:O	2:B:61:GLU:HB2	2.04	0.56
1:A:232:VAL:O	1:A:252:GLN:HG3	2.06	0.56
1:A:80:GLU:HG2	1:A:85:SER:CA	2.36	0.56
1:A:275:ILE:CG2	1:A:276:TYR:N	2.67	0.56
3:C:25:LEU:HD23	3:C:41:LEU:HD21	1.88	0.56
3:C:202:LEU:HD12	3:C:203:LEU:N	2.20	0.56
2:B:133:LEU:HD21	2:B:146:VAL:CG2	2.35	0.55
1:A:48:LYS:HB3	1:A:53:GLN:NE2	2.21	0.55
1:A:20:LEU:CD2	1:A:77:ILE:HD12	2.31	0.55
1:A:221:TRP:HZ2	1:A:230:PHE:CD2	2.25	0.55
1:A:145:ASN:ND2	4:A:410:NAG:C2	2.58	0.54
1:A:215:GLN:HA	1:A:268:GLN:HE22	1.72	0.54
3:C:91:THR:HG22	3:C:91:THR:O	2.05	0.54
1:A:106:VAL:HG12	1:A:108:LEU:HD11	1.87	0.54
1:A:101:ILE:HG21	1:A:177:ALA:CB	2.31	0.54
2:B:102:LEU:CD1	2:B:102:LEU:C	2.76	0.54
1:A:144:LYS:O	1:A:145:ASN:C	2.43	0.54
3:C:42:LEU:HB3	3:C:52:LEU:HB3	1.89	0.54
1:A:174:LYS:HB3	1:A:191:VAL:HG22	1.89	0.53
3:C:118:THR:HA	3:C:204:PRO:O	2.08	0.53
3:C:86:PHE:HB3	3:C:90:THR:O	2.07	0.53
1:A:106:VAL:HG12	1:A:108:LEU:HD12	1.90	0.53
3:C:179:TYR:HE2	3:C:203:LEU:CD1	2.21	0.53
1:A:256:CYS:O	1:A:259:VAL:HG13	2.08	0.53
1:A:96:PHE:CE2	2:B:123:ARG:NH1	2.76	0.53
1:A:14:ILE:O	1:A:14:ILE:CG1	2.57	0.53
3:C:67:ASP:C	3:C:67:ASP:OD2	2.47	0.53
2:B:32:LEU:HB3	2:B:35:ARG:HH21	1.72	0.53
3:C:142:VAL:HG11	3:C:184:TYR:CZ	2.44	0.52
1:A:106:VAL:CG1	1:A:108:LEU:CD1	2.86	0.52
3:C:117:PHE:O	3:C:204:PRO:HD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:SER:O	1:A:183:TRP:CB	2.56	0.52
2:B:137:LYS:O	2:B:137:LYS:HG2	2.10	0.52
2:B:55:VAL:O	2:B:58:VAL:HG12	2.09	0.52
3:C:20:ASN:O	3:C:21:PHE:HB2	2.10	0.52
1:A:236:HIS:HB2	1:A:239:LEU:HD12	1.91	0.52
3:C:142:VAL:HG11	3:C:184:TYR:OH	2.09	0.52
3:C:43:TYR:CB	3:C:81:THR:HG22	2.39	0.52
1:A:55:ILE:HG13	1:A:55:ILE:O	2.09	0.52
1:A:107:HIS:C	1:A:108:LEU:HD12	2.31	0.51
2:B:117:SER:N	2:B:118:PRO:HD2	2.25	0.51
2:B:135:GLU:C	2:B:137:LYS:H	2.14	0.51
1:A:216:ASN:HA	1:A:267:PRO:HA	1.93	0.51
3:C:121:ILE:HG12	3:C:203:LEU:HD21	1.91	0.51
1:A:70:TYR:OH	1:A:131:LEU:HD11	2.11	0.51
1:A:217:TYR:N	1:A:266:PHE:O	2.38	0.51
1:A:70:TYR:CB	2:B:124:ARG:HG3	2.41	0.51
2:B:37:ASP:OD1	2:B:39:ARG:N	2.40	0.51
2:B:36:ARG:CZ	2:B:132:TYR:HD1	2.24	0.51
2:B:61:GLU:O	2:B:64:GLN:HG2	2.10	0.51
3:C:127:PHE:HB3	3:C:128:PRO:CD	2.41	0.50
3:C:127:PHE:HD2	3:C:162:MET:HA	1.73	0.50
1:A:108:LEU:N	1:A:108:LEU:HD12	2.26	0.50
1:A:136:PHE:CE1	1:A:179:LEU:HD21	2.46	0.50
3:C:93:PHE:CD1	3:C:93:PHE:C	2.84	0.50
1:A:242:ASN:O	1:A:242:ASN:OD1	2.30	0.50
1:A:267:PRO:O	1:A:270:VAL:HG23	2.11	0.50
2:B:64:GLN:HA	2:B:95:LEU:HD11	1.93	0.50
3:C:36:PRO:HG2	3:C:39:TYR:CE1	2.46	0.50
3:C:107:PHE:CE2	3:C:187:HIS:HB2	2.46	0.50
3:C:35:VAL:HG13	3:C:36:PRO:HD2	1.94	0.50
1:A:62:PHE:CD1	1:A:62:PHE:O	2.65	0.50
3:C:42:LEU:HD12	3:C:42:LEU:N	2.26	0.50
1:A:140:LEU:HD11	1:A:173:LEU:HB2	1.94	0.50
2:B:83:LEU:HD22	2:B:83:LEU:N	2.27	0.50
3:C:88:GLY:C	3:C:90:THR:H	2.15	0.50
1:A:131:LEU:C	1:A:133:GLY:H	2.14	0.49
1:A:149:VAL:O	1:A:149:VAL:HG13	2.12	0.49
2:B:103:LEU:O	2:B:104:GLN:HG3	2.12	0.49
1:A:253:ILE:HG23	1:A:256:CYS:HB2	1.95	0.49
1:A:123:THR:O	1:A:123:THR:OG1	2.30	0.49
1:A:138:TYR:N	1:A:138:TYR:CD2	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ILE:HG13	1:A:157:TYR:O	2.13	0.49
2:B:14:ARG:O	2:B:18:VAL:HG23	2.12	0.49
2:B:40:PHE:CD2	2:B:41:PRO:HD2	2.48	0.49
3:C:150:ILE:CG2	3:C:151:VAL:N	2.75	0.49
3:C:72:TRP:CZ2	3:C:81:THR:HG21	2.47	0.49
2:B:58:VAL:HG23	2:B:122:LEU:HD11	1.93	0.49
2:B:60:HIS:CE1	2:B:99:GLU:HB3	2.47	0.49
1:A:110:ALA:HB2	1:A:194:ILE:CD1	2.41	0.49
1:A:145:ASN:ND2	4:A:410:NAG:C7	2.76	0.49
3:C:121:ILE:CG2	3:C:122:ASN:N	2.74	0.48
3:C:16:ILE:O	3:C:105:MET:HA	2.13	0.48
2:B:151:MET:HE3	3:C:100:TRP:NE1	2.29	0.48
3:C:120:HIS:HB2	3:C:170:ILE:O	2.13	0.48
1:A:145:ASN:CG	4:A:410:NAG:C1	2.78	0.48
2:B:92:HIS:O	2:B:96:GLN:HB2	2.14	0.48
1:A:47:ILE:N	1:A:47:ILE:HD12	2.28	0.48
1:A:140:LEU:HD12	1:A:141:VAL:N	2.24	0.47
1:A:234:TRP:HB3	1:A:278:LEU:CD2	2.45	0.47
1:A:161:LYS:HE3	1:A:163:TYR:CE1	2.49	0.47
1:A:36:PHE:HD2	1:A:52:CYS:O	1.97	0.47
1:A:217:TYR:O	1:A:265:VAL:HA	2.14	0.47
1:A:208:ILE:HD11	1:A:292:SER:HB2	1.97	0.47
2:B:20:LEU:HA	2:B:20:LEU:HD23	1.75	0.47
3:C:151:VAL:O	3:C:151:VAL:HG22	2.14	0.47
1:A:210:VAL:HG22	1:A:219:LEU:HD13	1.96	0.46
2:B:135:GLU:O	2:B:137:LYS:N	2.48	0.46
2:B:83:LEU:HD22	2:B:83:LEU:H	1.81	0.46
3:C:65:PHE:CD2	3:C:65:PHE:C	2.88	0.46
1:A:98:LYS:HG2	1:A:98:LYS:O	2.14	0.46
2:B:155:PHE:CE2	3:C:100:TRP:CE3	3.03	0.46
3:C:115:VAL:HG12	3:C:115:VAL:O	2.15	0.46
1:A:111:GLU:HG2	1:A:290:PHE:CE1	2.51	0.46
3:C:148:GLU:O	3:C:150:ILE:HD13	2.15	0.46
3:C:197:PRO:CD	3:C:197:PRO:O	2.64	0.46
3:C:186:GLU:O	3:C:186:GLU:HG3	2.15	0.46
2:B:121:THR:HG23	2:B:122:LEU:N	2.30	0.46
2:B:132:TYR:CD2	2:B:132:TYR:C	2.89	0.46
1:A:96:PHE:O	1:A:184:LYS:HE3	2.16	0.46
2:B:137:LYS:O	2:B:138:TYR:C	2.54	0.45
1:A:144:LYS:O	1:A:145:ASN:O	2.34	0.45
1:A:18:PHE:HD2	1:A:60:CYS:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLN:CB	1:A:43:MET:SD	3.04	0.45
1:A:277:LEU:HD23	1:A:296:LYS:HA	1.99	0.45
1:A:68:ASN:C	1:A:70:TYR:H	2.13	0.45
2:B:147:ARG:HH11	2:B:151:MET:HE1	1.80	0.45
1:A:109:GLU:HB3	1:A:116:VAL:HB	1.98	0.45
1:A:15:ASP:HB3	1:A:16:ASP:H	1.60	0.45
3:C:154:HIS:ND1	3:C:168:TYR:OH	2.36	0.45
1:A:238:PHE:CE1	1:A:239:LEU:CD2	3.00	0.45
3:C:62:THR:HG23	3:C:63:ARG:N	2.32	0.45
1:A:279:ARG:CG	1:A:291:TRP:CE3	3.00	0.45
1:A:90:VAL:HG12	1:A:91:ASP:O	2.17	0.45
1:A:213:GLN:O	1:A:214:ASN:C	2.54	0.44
1:A:203:PRO:O	1:A:223:TYR:HE2	2.00	0.44
1:A:175:VAL:HG22	1:A:176:LYS:N	2.32	0.44
1:A:253:ILE:HG13	1:A:254:PRO:HD2	1.98	0.44
3:C:117:PHE:HB2	3:C:120:HIS:O	2.17	0.44
3:C:141:LEU:HD23	3:C:156:PRO:HG2	1.98	0.44
3:C:29:LEU:HD22	3:C:32:HIS:CE1	2.52	0.44
2:B:63:LEU:HB2	2:B:95:LEU:CD2	2.46	0.44
3:C:72:TRP:HZ2	3:C:81:THR:CG2	2.31	0.44
2:B:154:LEU:HD12	2:B:154:LEU:HA	1.70	0.44
3:C:204:PRO:HA	3:C:205:PRO:HD3	1.58	0.44
1:A:108:LEU:CD1	1:A:108:LEU:N	2.81	0.44
2:B:29:PHE:O	2:B:31:CYS:N	2.51	0.44
2:B:19:LEU:CD2	2:B:83:LEU:HD12	2.47	0.44
3:C:120:HIS:HA	3:C:173:LEU:HD12	1.98	0.44
1:A:90:VAL:HG12	1:A:91:ASP:N	2.32	0.44
1:A:277:LEU:O	1:A:278:LEU:HD23	2.18	0.43
1:A:145:ASN:ND2	4:A:410:NAG:N2	2.64	0.43
2:B:135:GLU:C	2:B:137:LYS:N	2.70	0.43
2:B:44:MET:CE	2:B:58:VAL:HG23	2.49	0.43
2:B:97:HIS:HA	2:B:100:THR:OG1	2.19	0.43
2:B:148:MET:CE	3:C:46:MET:HG3	2.48	0.43
1:A:202:LEU:N	1:A:202:LEU:HD12	2.34	0.43
3:C:16:ILE:HG23	3:C:16:ILE:O	2.17	0.43
1:A:140:LEU:O	1:A:153:ILE:N	2.40	0.43
1:A:215:GLN:HA	1:A:268:GLN:NE2	2.32	0.43
1:A:237:ALA:CB	1:A:275:ILE:HG22	2.26	0.43
3:C:73:ARG:HD3	3:C:135:LEU:CB	2.49	0.43
1:A:236:HIS:HB2	1:A:239:LEU:CD1	2.49	0.43
1:A:79:ALA:HB3	1:A:88:TYR:HE2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:GLU:HG2	1:A:290:PHE:HE1	1.84	0.43
1:A:119:ILE:HG21	1:A:138:TYR:CD1	2.54	0.43
1:A:198:VAL:HG13	1:A:198:VAL:O	2.18	0.43
1:A:208:ILE:HG22	1:A:209:GLU:N	2.32	0.43
1:A:94:THR:HG1	1:A:97:ARG:HB3	1.84	0.43
1:A:11:VAL:O	1:A:98:LYS:HD3	2.19	0.42
2:B:69:LEU:O	2:B:72:THR:HG23	2.19	0.42
3:C:44:THR:OG1	3:C:45:ILE:N	2.52	0.42
1:A:18:PHE:HB2	1:A:60:CYS:HB3	2.01	0.42
1:A:215:GLN:O	1:A:215:GLN:CG	2.67	0.42
1:A:223:TYR:HD2	1:A:223:TYR:HA	1.73	0.42
2:B:152:LYS:O	2:B:155:PHE:HB2	2.20	0.42
3:C:88:GLY:C	3:C:90:THR:N	2.72	0.42
1:A:124:LYS:O	1:A:125:ASP:HB2	2.18	0.42
1:A:131:LEU:CD1	1:A:132:ASP:N	2.78	0.42
1:A:202:LEU:O	1:A:289:SER:HB2	2.19	0.42
2:B:82:THR:HB	2:B:83:LEU:HD22	2.02	0.42
3:C:40:THR:HG22	3:C:41:LEU:N	2.35	0.42
2:B:29:PHE:C	2:B:31:CYS:H	2.23	0.42
1:A:298:ASP:C	1:A:300:GLU:N	2.72	0.42
1:A:62:PHE:O	1:A:62:PHE:HD1	2.02	0.42
3:C:23:SER:O	3:C:24:ILE:CD1	2.65	0.42
2:B:57:SER:O	2:B:61:GLU:CB	2.67	0.42
2:B:121:THR:HG23	2:B:122:LEU:H	1.85	0.41
1:A:90:VAL:CG1	1:A:91:ASP:N	2.83	0.41
1:A:210:VAL:HG22	1:A:219:LEU:CD1	2.51	0.41
1:A:208:ILE:CG2	1:A:209:GLU:N	2.82	0.41
2:B:133:LEU:O	2:B:134:LYS:C	2.59	0.41
3:C:66:CYS:SG	3:C:67:ASP:N	2.93	0.41
1:A:129:TRP:O	1:A:130:ALA:C	2.57	0.41
1:A:233:GLN:HA	1:A:252:GLN:HA	2.03	0.41
2:B:146:VAL:O	2:B:147:ARG:C	2.59	0.41
1:A:111:GLU:CD	1:A:290:PHE:HD1	2.24	0.41
2:B:30:LEU:N	2:B:30:LEU:HD23	2.36	0.41
3:C:196:SER:CB	3:C:197:PRO:CD	2.98	0.41
1:A:94:THR:O	1:A:94:THR:OG1	2.38	0.41
2:B:6:PRO:O	2:B:6:PRO:CD	2.69	0.41
3:C:105:MET:HE2	3:C:107:PHE:CE1	2.56	0.41
3:C:90:THR:CG2	3:C:91:THR:N	2.83	0.41
1:A:234:TRP:HA	1:A:277:LEU:O	2.22	0.41
3:C:178:ASN:ND2	3:C:202:LEU:HB2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:HIS:HD2	3:C:103:ILE:HD13	1.85	0.40
1:A:77:ILE:HG22	1:A:88:TYR:HB2	2.01	0.40
2:B:32:LEU:HB3	2:B:35:ARG:NH2	2.36	0.40
3:C:183:VAL:O	3:C:184:TYR:HB3	2.21	0.40
3:C:97:HIS:HD2	3:C:98:ASN:O	2.04	0.40
1:A:221:TRP:CZ2	1:A:230:PHE:CD2	3.07	0.40
3:C:62:THR:CG2	3:C:63:ARG:N	2.83	0.40
1:A:150:GLU:O	1:A:150:GLU:HG3	2.21	0.40
3:C:97:HIS:HD2	3:C:98:ASN:N	2.20	0.40
2:B:29:PHE:HD2	2:B:30:LEU:HD23	1.87	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	279/414 (67%)	254 (91%)	24 (9%)	1 (0%)	34	72
2	B	137/177 (77%)	117 (85%)	18 (13%)	2 (2%)	10	45
3	C	184/199 (92%)	166 (90%)	15 (8%)	3 (2%)	9	43
All	All	600/790 (76%)	537 (90%)	57 (10%)	6 (1%)	15	54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	118	PRO
3	C	151	VAL
2	B	136	LYS
3	C	192	ALA
1	A	148	GLY
3	C	128	PRO

### 5.3.2 Protein sidechains ⓘ

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	212/382 (56%)	207 (98%)	5 (2%)	49	76
2	B	116/160 (72%)	108 (93%)	8 (7%)	15	47
3	C	160/189 (85%)	158 (99%)	2 (1%)	69	86
All	All	488/731 (67%)	473 (97%)	15 (3%)	40	70

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	131	LEU
1	A	132	ASP
1	A	135	SER
1	A	223	TYR
2	B	27	SER
2	B	34	ASP
2	B	54	HIS
2	B	66	ILE
2	B	89	THR
2	B	102	LEU
2	B	120	LEU
2	B	154	LEU
3	C	80	VAL
3	C	86	PHE

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

Mol	Chain	Res	Type
1	A	68	ASN
1	A	145	ASN
1	A	155	ASN
1	A	215	GLN
1	A	268	GLN
2	B	9	HIS

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Mol	Chain	Res	Type
2	B	60	HIS
2	B	80	GLN
3	C	97	HIS
3	C	98	ASN
3	C	176	ASN
3	C	187	HIS

### 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](#)

1 ligand is 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	$\# Z  > 2$
4	NAG	A	410	1	14,14,15	0.62	0	17,19,21	1.05	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
4	NAG	A	410	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	410	NAG	C1-O5-C5	-3.12	107.97	112.19
4	A	410	NAG	O5-C1-C2	-2.03	108.08	111.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	410	NAG	6	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, 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	285/414 (68%)	-0.61	0 100 100	41, 78, 117, 154	0
2	B	143/177 (80%)	-0.72	0 100 100	38, 66, 118, 154	0
3	C	190/199 (95%)	-0.71	0 100 100	39, 70, 114, 134	0
All	All	618/790 (78%)	-0.67	0 100 100	38, 73, 117, 154	0

There are no RSRZ outliers to report.

### 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<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	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	A	410	14/15	0.89	0.31	98,132,143,145	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.