Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2016 – 11:06 PM EDT

PDB ID	:	4NKQ
Title	:	Structure of a Cytokine Receptor Complex
Authors	:	Parker, M.W.; Broughton, S.E.
Deposited on	:	2013-11-13
Resolution	:	3.30 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

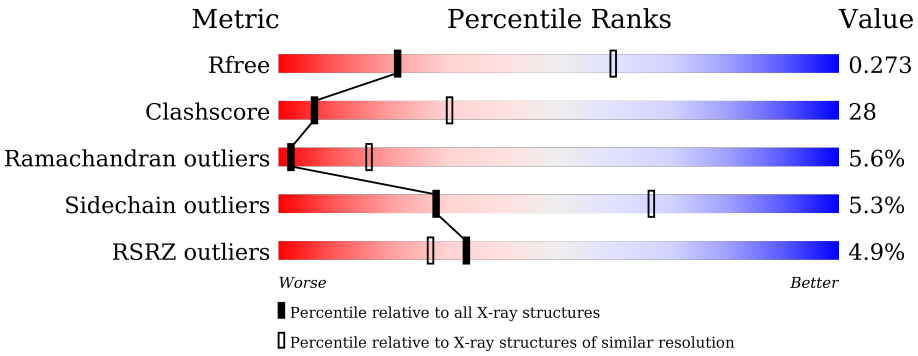
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

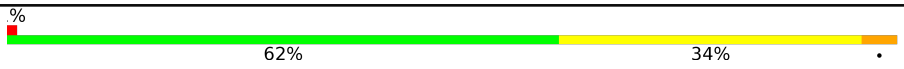
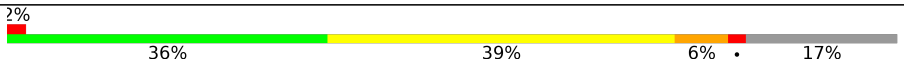
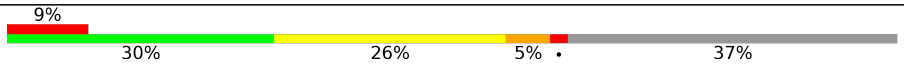
The reported resolution of this entry is 3.30 Å.

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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	C	127	
3	B	305	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5706 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 Cytokine receptor common subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	0	0
			3306	2068	588	632	18			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	346	GLN	ASN	ENGINEERED MUTATION	UNP P32927

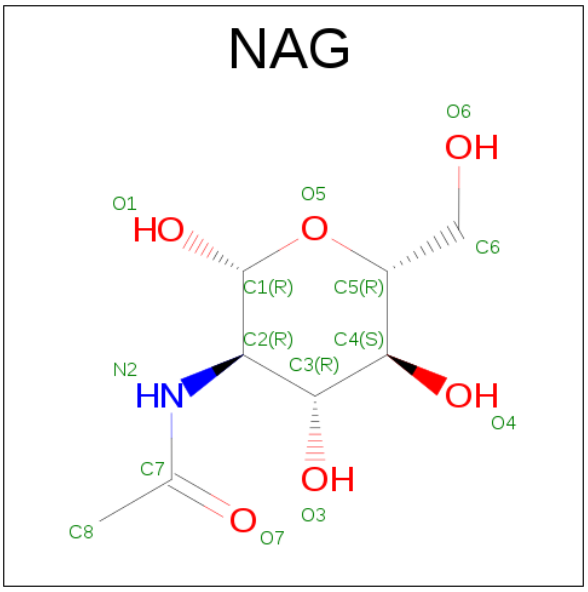
- Molecule 2 is a protein called Granulocyte-macrophage colony-stimulating factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	105	Total	C	N	O	S	0	0	0
			836	526	142	161	7			

- Molecule 3 is a protein called Granulocyte-macrophage colony-stimulating factor receptor subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	191	Total	C	N	O	S	0	0	0
			1508	945	274	282	7			

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

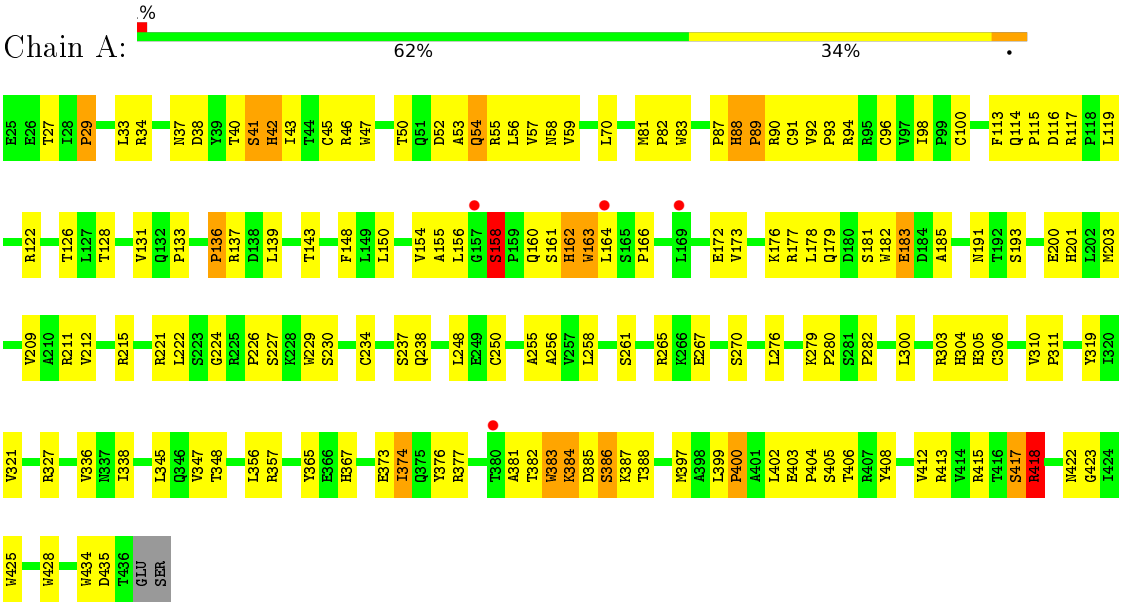


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0

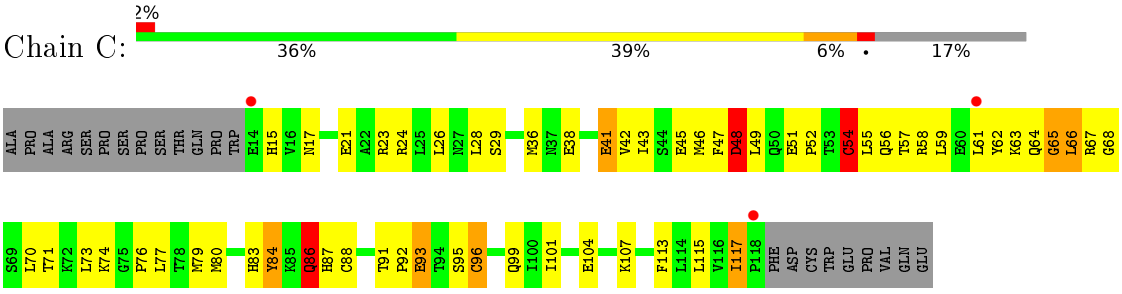
3 Residue-property plots (i)

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.

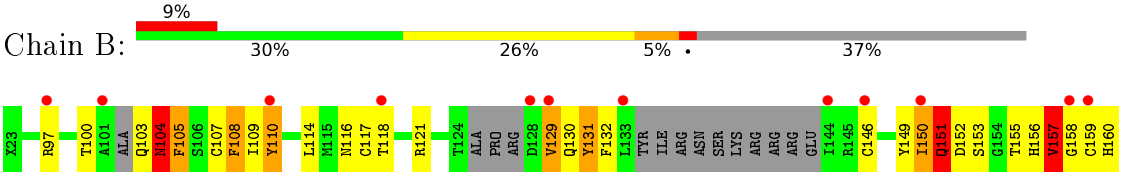
- Molecule 1: Cytokine receptor common subunit beta

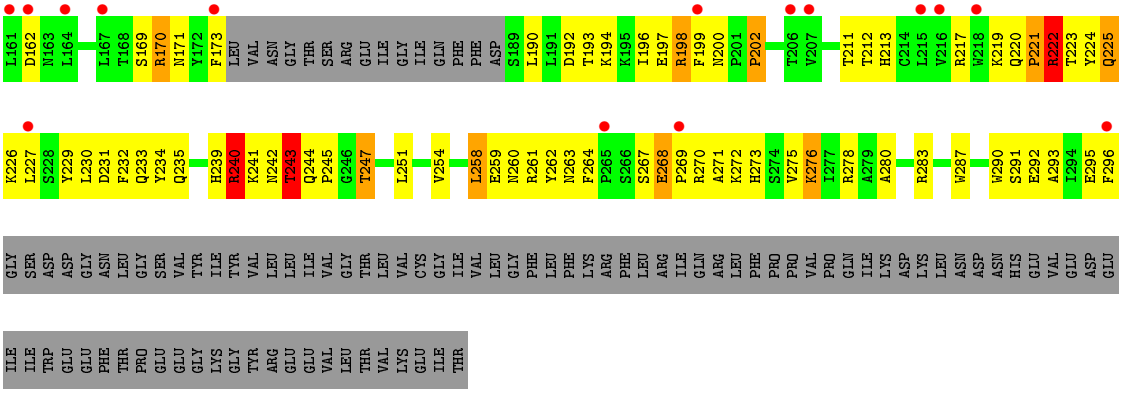


- Molecule 2: Granulocyte-macrophage colony-stimulating factor



- Molecule 3: Granulocyte-macrophage colony-stimulating factor receptor subunit alpha




L161 D162 N163 L164 L167 T168 S169 R170 N171 Y172 F173 LEU VAL ASN GLY THR SER ARG GLU ILE GLY ILE GLN PHE PHE ASP S189 L190 L191 D192 T193 K194 K195 I196 E197 R198 F199 N200 P201 P202 T206 V207 T211 T212 H213 C214 L215 V216 R217 W218 K219 Q220 P221 R222 T223 Y224 Q225
K226 L227 S228 Y229 L230 D231 F232 Q233 Y234 Q235 H239 R240 K241 N242 T243 Q244 P245 G246 T247 L251 V254 L258 E259 N260 R261 Y262 N263 F264 P265 S266 S267 E268 P269 R270 A271 K272 H273 S274 V275 K276 I277 R278 A279 A280 R283 W287 W290 S291 E292 A293 I294 E295 F296
GLY SER ASP ASP GLY ASN LEU GLY SER VAL TYR ILE TYR VAL LEU LEU ILE VAL GLY THR LEU VAL CYS GLY ILE VAL LEU GLY PHE LEU PHE LYS ARG PHE LEU ARG ILE GLN ARG LEU PHE PRO PRO VAL PRO GLN ILE LYS ASP LYS LEU ASN ASP ASN HIS GLU VAL GLU ASP GLU
ILE ILE TRP GLU GLU PHE THR PRO GLU GLU GLY LYS GLY TYR ARG GLU GLU VAL LEU THR VAL LYS GLU ILE THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α, β, γ	166.66Å 166.66Å 213.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.08 – 3.30 36.08 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (36.08-3.30) 99.6 (36.08-3.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.229 , 0.273 0.231 , 0.273	Depositor DCC
R_{free} test set	1348 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	117.6	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 88.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5706	wwPDB-VP
Average B, all atoms (Å^2)	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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	A	0.64	0/3401	0.79	2/4645 (0.0%)
2	C	0.53	0/850	0.83	1/1149 (0.1%)
3	B	0.66	0/1456	1.06	9/1971 (0.5%)
All	All	0.63	0/5707	0.87	12/7765 (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
1	A	0	3
2	C	0	2
3	B	0	3
All	All	0	8

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	B	258	LEU	CA-CB-CG	8.07	133.85	115.30
3	B	110	TYR	CA-CB-CG	8.05	128.69	113.40
3	B	240	ARG	CG-CD-NE	7.63	127.83	111.80
3	B	151	GLN	CA-CB-CG	7.11	129.04	113.40
2	C	86	GLN	CA-CB-CG	6.75	128.25	113.40
3	B	222	ARG	NE-CZ-NH2	-6.32	117.14	120.30
3	B	198	ARG	NE-CZ-NH1	5.70	123.15	120.30
3	B	170	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	A	54	GLN	CA-CB-CG	5.29	125.04	113.40
3	B	157	VAL	CA-CB-CG2	-5.23	103.06	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	345	LEU	CA-CB-CG	5.10	127.03	115.30
3	B	170	ARG	NE-CZ-NH2	5.06	122.83	120.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	SER	Peptide
1	A	383	TRP	Peptide
1	A	418	ARG	Peptide
3	B	157	VAL	Peptide
3	B	222	ARG	Peptide
3	B	243	THR	Peptide
2	C	48	ASP	Peptide
2	C	84	TYR	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	3306	0	3158	114	0
2	C	836	0	842	53	0
3	B	1508	0	1390	147	0
4	A	42	0	39	5	0
4	B	14	0	13	2	0
All	All	5706	0	5442	309	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 28.

All (309) 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)
3:B:150:ILE:HG13	3:B:157:VAL:HG21	1.25	1.19
3:B:240:ARG:HD2	3:B:273:HIS:CD2	1.95	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:239:HIS:O	3:B:244:GLN:NE2	2.02	0.92
3:B:240:ARG:HH21	3:B:242:ASN:HB3	1.32	0.90
3:B:150:ILE:HG13	3:B:157:VAL:CG2	2.04	0.88
1:A:58:ASN:ND2	4:A:501:NAG:O5	2.09	0.85
2:C:41:GLU:OE2	2:C:61:LEU:HB3	1.76	0.84
3:B:152:ASP:O	3:B:155:THR:OG1	1.95	0.83
3:B:239:HIS:O	3:B:240:ARG:HG2	1.79	0.82
3:B:110:TYR:HB3	3:B:198:ARG:HD2	1.62	0.81
1:A:163:TRP:O	1:A:221:ARG:NH2	2.16	0.79
2:C:115:LEU:O	3:B:194:LYS:NZ	2.16	0.79
2:C:43:ILE:HG13	2:C:58:ARG:HG2	1.67	0.76
3:B:212:THR:H	4:B:401:NAG:H82	1.50	0.76
3:B:240:ARG:CD	3:B:273:HIS:CD2	2.69	0.75
3:B:110:TYR:CB	3:B:198:ARG:HH11	1.99	0.74
3:B:259:GLU:HG3	3:B:261:ARG:NE	2.03	0.74
3:B:240:ARG:HD2	3:B:273:HIS:HD2	1.53	0.74
3:B:159:CYS:SG	3:B:160:HIS:N	2.60	0.74
3:B:110:TYR:N	3:B:198:ARG:NH1	2.36	0.74
3:B:240:ARG:NH2	3:B:272:LYS:O	2.21	0.74
2:C:45:GLU:O	2:C:58:ARG:NH2	2.18	0.74
3:B:240:ARG:CD	3:B:273:HIS:HD2	2.01	0.74
3:B:110:TYR:N	3:B:198:ARG:HH11	1.86	0.73
3:B:240:ARG:HH11	3:B:273:HIS:HD2	1.37	0.73
1:A:136:PRO:HB2	1:A:230:SER:HB3	1.70	0.73
1:A:356:LEU:HD12	1:A:399:LEU:HD21	1.69	0.73
3:B:103:GLN:HG2	3:B:104:ASN:H	1.53	0.72
3:B:110:TYR:CD2	3:B:198:ARG:NH1	2.57	0.72
3:B:197:GLU:HG3	3:B:225:GLN:HE21	1.55	0.72
1:A:373:GLU:OE1	1:A:413:ARG:NH2	2.22	0.71
3:B:121:ARG:NH1	3:B:152:ASP:O	2.24	0.71
3:B:227:LEU:HD11	3:B:232:PHE:CE2	2.26	0.71
3:B:276:LYS:CD	3:B:290:TRP:HB3	2.20	0.71
1:A:384:LYS:HE2	1:A:385:ASP:OD2	1.89	0.70
3:B:240:ARG:HD2	3:B:273:HIS:CG	2.25	0.70
3:B:276:LYS:HD3	3:B:290:TRP:HB3	1.73	0.70
1:A:279:LYS:NZ	1:A:282:PRO:O	2.25	0.70
1:A:215:ARG:HG2	1:A:226:PRO:HB3	1.73	0.70
3:B:217:ARG:HG3	3:B:261:ARG:HD2	1.73	0.69
1:A:191:ASN:ND2	4:A:503:NAG:O5	2.26	0.69
1:A:162:HIS:O	1:A:164:LEU:N	2.26	0.68
1:A:238:GLN:N	1:A:238:GLN:OE1	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ILE:H	1:A:423:GLY:HA3	1.57	0.68
3:B:222:ARG:HG2	3:B:223:THR:N	2.09	0.68
3:B:240:ARG:NE	3:B:273:HIS:HA	2.10	0.67
1:A:54:GLN:HA	1:A:57:VAL:O	1.95	0.67
1:A:37:ASN:ND2	1:A:38:ASP:O	2.28	0.67
2:C:66:LEU:HD11	2:C:77:LEU:HD12	1.75	0.67
1:A:374:ILE:HD11	1:A:397:MET:SD	2.35	0.66
2:C:77:LEU:HA	2:C:80:MET:HG2	1.76	0.66
2:C:58:ARG:O	2:C:62:TYR:N	2.29	0.66
1:A:267:GLU:O	1:A:270:SER:OG	2.12	0.65
3:B:276:LYS:HD3	3:B:291:SER:N	2.12	0.65
1:A:176:LYS:HG3	1:A:177:ARG:O	1.97	0.65
3:B:108:PHE:HA	3:B:196:ILE:HB	1.79	0.65
3:B:242:ASN:HA	3:B:244:GLN:HG3	1.79	0.64
1:A:41:SER:O	1:A:42:HIS:HB2	1.97	0.64
3:B:278:ARG:HD2	3:B:287:TRP:HB3	1.78	0.64
1:A:403:GLU:O	1:A:406:THR:OG1	2.11	0.64
2:C:84:TYR:HD1	2:C:88:CYS:HB3	1.63	0.63
3:B:194:LYS:HA	3:B:225:GLN:HE22	1.63	0.63
3:B:110:TYR:HB3	3:B:198:ARG:CD	2.28	0.63
3:B:291:SER:OG	3:B:292:GLU:N	2.32	0.63
3:B:157:VAL:HG23	3:B:158:GLY:N	2.14	0.63
3:B:240:ARG:NH1	3:B:273:HIS:HD2	1.95	0.63
2:C:61:LEU:HA	2:C:64:GLN:HG2	1.80	0.63
1:A:374:ILE:HG22	1:A:412:VAL:HG23	1.79	0.62
1:A:303:ARG:HD3	1:A:305:HIS:CE1	2.34	0.62
3:B:240:ARG:HA	3:B:244:GLN:HE21	1.65	0.62
1:A:221:ARG:HG3	1:A:222:LEU:HG	1.82	0.61
3:B:194:LYS:HA	3:B:225:GLN:NE2	2.15	0.61
3:B:259:GLU:HG3	3:B:261:ARG:HE	1.63	0.61
1:A:417:SER:OG	1:A:417:SER:O	2.17	0.61
3:B:240:ARG:HH11	3:B:273:HIS:CD2	2.18	0.60
3:B:240:ARG:NE	3:B:242:ASN:H	1.98	0.60
2:C:117:ILE:H	2:C:117:ILE:HD12	1.66	0.60
3:B:108:PHE:CD2	3:B:198:ARG:NE	2.67	0.60
3:B:171:ASN:HB2	3:B:173:PHE:CE1	2.38	0.59
3:B:219:LYS:NZ	3:B:261:ARG:HH22	1.99	0.59
2:C:64:GLN:O	2:C:66:LEU:N	2.35	0.59
1:A:40:THR:O	1:A:40:THR:OG1	2.21	0.59
3:B:108:PHE:O	3:B:198:ARG:NH2	2.37	0.58
3:B:130:GLN:NE2	3:B:155:THR:HB	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:223:THR:HB	3:B:226:LYS:HA	1.85	0.58
2:C:47:PHE:HB2	2:C:58:ARG:CZ	2.33	0.58
3:B:150:ILE:CG1	3:B:157:VAL:HG21	2.16	0.58
3:B:198:ARG:O	3:B:222:ARG:NH1	2.37	0.58
3:B:240:ARG:HB3	3:B:241:LYS:HA	1.84	0.58
3:B:227:LEU:HD11	3:B:232:PHE:CD2	2.39	0.58
3:B:146:CYS:HB2	3:B:149:TYR:CZ	2.39	0.57
1:A:57:VAL:HG11	1:A:119:LEU:HD11	1.85	0.57
2:C:42:VAL:HG11	2:C:101:ILE:HD11	1.87	0.56
1:A:52:ASP:OD2	1:A:90:ARG:NH1	2.37	0.56
2:C:54:CYS:HB3	2:C:93:GLU:HA	1.86	0.56
1:A:367:HIS:O	1:A:418:ARG:NH1	2.38	0.56
3:B:130:GLN:HE22	3:B:155:THR:HB	1.69	0.56
3:B:131:TYR:HD2	3:B:132:PHE:N	2.03	0.56
3:B:242:ASN:CA	3:B:244:GLN:HG3	2.35	0.56
3:B:251:LEU:HD23	3:B:251:LEU:H	1.71	0.56
1:A:336:VAL:HG23	1:A:422:ASN:HB3	1.88	0.56
4:A:502:NAG:H3	4:A:502:NAG:H83	1.88	0.56
2:C:57:THR:O	2:C:61:LEU:HB2	2.05	0.56
3:B:240:ARG:NH1	3:B:273:HIS:CD2	2.73	0.56
3:B:240:ARG:NH2	3:B:242:ASN:HB3	2.14	0.55
2:C:84:TYR:CD1	2:C:88:CYS:HB3	2.41	0.55
3:B:150:ILE:O	3:B:157:VAL:HG22	2.06	0.55
1:A:415:ARG:NH1	1:A:423:GLY:O	2.38	0.55
3:B:110:TYR:CA	3:B:198:ARG:HH11	2.20	0.55
1:A:404:PRO:O	1:A:406:THR:N	2.39	0.55
1:A:413:ARG:HG3	1:A:428:TRP:CZ3	2.41	0.55
3:B:202:PRO:HA	3:B:221:PRO:HB3	1.89	0.54
1:A:381:ALA:HB1	1:A:385:ASP:OD2	2.08	0.54
1:A:382:THR:HG22	1:A:384:LYS:NZ	2.22	0.54
1:A:173:VAL:HG22	1:A:212:VAL:HG22	1.88	0.54
3:B:108:PHE:C	3:B:198:ARG:NH2	2.61	0.54
3:B:276:LYS:HD2	3:B:290:TRP:HB3	1.88	0.54
3:B:239:HIS:C	3:B:240:ARG:HG2	2.28	0.54
3:B:239:HIS:C	3:B:244:GLN:NE2	2.61	0.54
1:A:250:CYS:HB3	1:A:258:LEU:HD11	1.90	0.54
2:C:84:TYR:HA	2:C:86:GLN:H	1.74	0.53
1:A:143:THR:HG22	1:A:148:PHE:HD2	1.73	0.53
1:A:385:ASP:O	1:A:387:LYS:HD2	2.08	0.53
3:B:199:PHE:HD2	3:B:280:ALA:HA	1.72	0.53
1:A:92:VAL:O	1:A:92:VAL:HG12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:254:VAL:HG21	3:B:262:TYR:CD2	2.44	0.53
2:C:93:GLU:O	2:C:95:SER:N	2.41	0.53
1:A:117:ARG:HH11	1:A:117:ARG:HG3	1.74	0.53
1:A:382:THR:OG1	1:A:383:TRP:N	2.41	0.53
1:A:418:ARG:NH2	2:C:17:ASN:OD1	2.39	0.53
1:A:52:ASP:OD1	1:A:90:ARG:HD2	2.09	0.52
3:B:213:HIS:CD2	3:B:213:HIS:H	2.25	0.52
3:B:273:HIS:HB2	3:B:296:PHE:CZ	2.45	0.52
3:B:110:TYR:CB	3:B:198:ARG:HD2	2.38	0.51
2:C:61:LEU:HD23	2:C:64:GLN:HE21	1.74	0.51
3:B:110:TYR:HD2	3:B:198:ARG:NH1	2.04	0.51
3:B:222:ARG:HG2	3:B:223:THR:CA	2.41	0.51
1:A:137:ARG:CZ	1:A:155:ALA:HB2	2.41	0.51
3:B:254:VAL:HG21	3:B:262:TYR:HD2	1.74	0.51
2:C:56:GLN:O	2:C:59:LEU:N	2.42	0.51
1:A:413:ARG:HG3	1:A:428:TRP:CE3	2.46	0.51
3:B:110:TYR:CE1	3:B:114:LEU:HD22	2.46	0.51
1:A:237:SER:HB2	1:A:238:GLN:OE1	2.11	0.50
3:B:217:ARG:HG3	3:B:261:ARG:CD	2.40	0.50
3:B:151:GLN:C	3:B:151:GLN:OE1	2.50	0.50
3:B:242:ASN:N	3:B:244:GLN:HG3	2.26	0.50
1:A:58:ASN:O	1:A:115:PRO:HA	2.11	0.50
1:A:133:PRO:O	1:A:227:SER:HB3	2.12	0.50
1:A:177:ARG:NH1	1:A:203:MET:SD	2.84	0.50
1:A:256:ALA:HA	1:A:310:VAL:HG22	1.93	0.50
3:B:200:ASN:N	3:B:222:ARG:NH2	2.59	0.50
3:B:240:ARG:NH2	3:B:242:ASN:O	2.45	0.50
3:B:242:ASN:ND2	3:B:244:GLN:OE1	2.45	0.50
3:B:197:GLU:CG	3:B:225:GLN:HE21	2.23	0.49
3:B:240:ARG:CZ	3:B:273:HIS:HA	2.42	0.49
1:A:367:HIS:HB2	1:A:418:ARG:HH12	1.77	0.49
2:C:68:GLY:O	2:C:71:THR:OG1	2.30	0.49
3:B:272:LYS:HA	3:B:296:PHE:C	2.32	0.49
1:A:415:ARG:HB3	1:A:425:TRP:CE3	2.48	0.49
2:C:83:HIS:CE1	2:C:84:TYR:CD2	3.00	0.49
3:B:110:TYR:HB3	3:B:198:ARG:HH11	1.75	0.49
1:A:131:VAL:O	1:A:224:GLY:HA3	2.13	0.49
1:A:384:LYS:O	1:A:387:LYS:NZ	2.46	0.48
2:C:65:GLY:O	2:C:67:ARG:N	2.46	0.48
3:B:240:ARG:CB	3:B:241:LYS:HA	2.43	0.48
3:B:211:THR:HG21	3:B:268:GLU:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ASN:HB3	1:A:43:ILE:HG12	1.95	0.48
1:A:382:THR:N	1:A:385:ASP:OD2	2.44	0.48
3:B:272:LYS:N	3:B:272:LYS:HD2	2.29	0.48
3:B:110:TYR:HE1	3:B:114:LEU:HD22	1.78	0.48
3:B:152:ASP:HA	3:B:153:SER:HA	1.68	0.48
1:A:382:THR:HG23	1:A:384:LYS:HG3	1.95	0.48
2:C:84:TYR:CZ	2:C:86:GLN:HG3	2.48	0.48
3:B:212:THR:OG1	3:B:213:HIS:HD2	1.97	0.48
3:B:233:GLN:NE2	3:B:234:TYR:O	2.47	0.48
2:C:113:PHE:CE1	2:C:117:ILE:HD11	2.49	0.48
1:A:211:ARG:HD2	1:A:229:TRP:CG	2.49	0.47
3:B:149:TYR:HB3	3:B:156:HIS:ND1	2.28	0.47
3:B:239:HIS:CE1	3:B:247:THR:HG23	2.48	0.47
1:A:50:THR:HG23	1:A:53:ALA:H	1.78	0.47
1:A:377:ARG:HB3	1:A:386:SER:OG	2.15	0.47
2:C:26:LEU:O	2:C:29:SER:HB3	2.14	0.47
1:A:402:LEU:HG	1:A:408:TYR:CZ	2.50	0.47
3:B:193:THR:O	3:B:197:GLU:HB2	2.14	0.47
3:B:212:THR:N	4:B:401:NAG:H82	2.25	0.47
1:A:139:LEU:HD11	1:A:150:LEU:HD11	1.96	0.47
1:A:200:GLU:HG2	1:A:201:HIS:CD2	2.49	0.47
1:A:33:LEU:O	1:A:34:ARG:HD3	2.15	0.47
3:B:97:ARG:HB3	3:B:100:THR:HG23	1.95	0.47
2:C:65:GLY:HA2	2:C:67:ARG:CZ	2.44	0.47
2:C:84:TYR:HD1	2:C:88:CYS:CB	2.26	0.47
1:A:143:THR:HG22	1:A:148:PHE:CD2	2.50	0.46
3:B:109:ILE:HB	3:B:197:GLU:HA	1.96	0.46
1:A:365:TYR:CE1	2:C:21:GLU:HA	2.51	0.46
3:B:131:TYR:HD2	3:B:132:PHE:H	1.62	0.46
2:C:36:MET:HB3	2:C:104:GLU:HB2	1.96	0.46
3:B:275:VAL:O	3:B:293:ALA:HA	2.15	0.46
2:C:56:GLN:N	2:C:93:GLU:OE2	2.44	0.46
3:B:213:HIS:CD2	3:B:213:HIS:N	2.84	0.46
2:C:24:ARG:O	2:C:28:LEU:HD23	2.16	0.46
1:A:209:VAL:HB	1:A:234:CYS:SG	2.56	0.46
1:A:117:ARG:NH1	4:A:501:NAG:H81	2.31	0.46
1:A:158:SER:O	1:A:161:SER:OG	2.33	0.46
3:B:108:PHE:CD1	3:B:198:ARG:NH2	2.79	0.46
3:B:220:GLN:NE2	3:B:260:ASN:HD21	2.14	0.46
2:C:63:LYS:HB3	2:C:63:LYS:HE3	1.69	0.46
3:B:105:PHE:HB3	3:B:118:THR:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:ARG:HD3	1:A:428:TRP:CE2	2.50	0.46
3:B:240:ARG:HD2	3:B:273:HIS:CB	2.46	0.46
1:A:156:LEU:CD1	1:A:166:PRO:HD3	2.46	0.45
2:C:91:THR:HA	2:C:92:PRO:HD2	1.43	0.45
3:B:259:GLU:HG3	3:B:261:ARG:CZ	2.46	0.45
1:A:33:LEU:HD12	1:A:47:TRP:HB3	1.98	0.45
2:C:38:GLU:OE1	2:C:67:ARG:NE	2.49	0.45
3:B:129:VAL:HG23	3:B:129:VAL:O	2.16	0.45
1:A:45:CYS:HB2	1:A:96:CYS:HB2	1.99	0.45
1:A:156:LEU:HD11	1:A:166:PRO:HD3	1.98	0.45
3:B:151:GLN:OE1	3:B:152:ASP:N	2.48	0.45
2:C:77:LEU:HA	2:C:77:LEU:HD23	1.75	0.45
1:A:41:SER:HA	1:A:100:CYS:O	2.16	0.45
1:A:56:LEU:O	1:A:117:ARG:NH2	2.48	0.45
1:A:336:VAL:HA	1:A:422:ASN:H	1.82	0.45
1:A:376:TYR:O	1:A:386:SER:HB3	2.17	0.45
3:B:150:ILE:O	3:B:151:GLN:HB2	2.16	0.45
3:B:213:HIS:HB3	3:B:263:ASN:OD1	2.16	0.45
2:C:83:HIS:O	2:C:86:GLN:HB3	2.16	0.44
3:B:240:ARG:HH21	3:B:242:ASN:CB	2.18	0.44
1:A:46:ARG:HD3	1:A:82:PRO:HD2	2.00	0.44
1:A:55:ARG:HB3	1:A:55:ARG:HE	1.55	0.44
1:A:176:LYS:HD3	1:A:182:TRP:CE3	2.53	0.44
3:B:243:THR:HA	3:B:244:GLN:HB2	2.00	0.44
1:A:280:PRO:HB3	1:A:319:TYR:CZ	2.52	0.44
1:A:37:ASN:HB2	1:A:42:HIS:O	2.18	0.44
3:B:259:GLU:HA	3:B:261:ARG:CZ	2.48	0.44
1:A:172:GLU:OE1	1:A:215:ARG:HD3	2.17	0.44
1:A:403:GLU:HG3	1:A:406:THR:HG21	2.00	0.43
3:B:273:HIS:HB2	3:B:296:PHE:CE1	2.52	0.43
1:A:43:ILE:HB	1:A:98:ILE:HB	2.01	0.43
3:B:242:ASN:HA	3:B:244:GLN:CG	2.48	0.43
3:B:197:GLU:OE2	3:B:224:TYR:HB3	2.18	0.43
1:A:128:THR:HG22	1:A:163:TRP:HZ2	1.83	0.43
1:A:279:LYS:HE2	1:A:279:LYS:HB3	1.64	0.43
3:B:260:ASN:C	3:B:261:ARG:HD3	2.39	0.43
2:C:24:ARG:CZ	2:C:28:LEU:HD21	2.48	0.43
1:A:265:ARG:CZ	1:A:300:LEU:HD23	2.49	0.43
3:B:220:GLN:OE1	3:B:232:PHE:CE2	2.72	0.43
3:B:107:CYS:HA	3:B:117:CYS:HA	2.00	0.43
1:A:400:PRO:HB3	3:B:267:SER:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:HIS:CG	1:A:89:PRO:HD2	2.54	0.43
2:C:15:HIS:CE1	2:C:83:HIS:CE1	3.07	0.43
1:A:137:ARG:NH2	1:A:154:VAL:O	2.49	0.43
1:A:365:TYR:HB3	1:A:367:HIS:CE1	2.54	0.43
3:B:244:GLN:HA	3:B:245:PRO:HD3	1.60	0.43
3:B:263:ASN:OD1	3:B:264:PHE:N	2.52	0.43
2:C:42:VAL:HG23	2:C:99:GLN:HB3	2.00	0.43
1:A:387:LYS:HE3	1:A:387:LYS:HA	2.01	0.42
3:B:149:TYR:C	3:B:150:ILE:O	2.56	0.42
1:A:29:PRO:HB3	1:A:113:PHE:CZ	2.54	0.42
3:B:260:ASN:O	3:B:261:ARG:HD3	2.19	0.42
1:A:261:SER:HA	1:A:304:HIS:O	2.19	0.42
3:B:110:TYR:H	3:B:198:ARG:NH1	2.14	0.42
3:B:219:LYS:HZ3	3:B:261:ARG:HH22	1.68	0.42
3:B:269:PRO:O	3:B:271:ALA:N	2.47	0.42
3:B:235:GLN:HB2	3:B:287:TRP:CZ3	2.53	0.42
1:A:356:LEU:CD1	1:A:399:LEU:HD21	2.45	0.42
2:C:57:THR:HG22	2:C:61:LEU:HG	2.01	0.42
2:C:70:LEU:HB3	2:C:73:LEU:HD12	2.02	0.42
1:A:404:PRO:O	1:A:406:THR:HG23	2.20	0.42
1:A:155:ALA:O	1:A:156:LEU:HD23	2.20	0.42
1:A:265:ARG:HD2	1:A:265:ARG:HA	1.88	0.42
1:A:92:VAL:HG12	1:A:94:ARG:HE	1.85	0.42
3:B:272:LYS:HB3	3:B:295:GLU:HB3	2.02	0.42
1:A:38:ASP:OD1	1:A:42:HIS:HB3	2.20	0.42
3:B:104:ASN:O	3:B:105:PHE:HB2	2.20	0.42
1:A:178:LEU:HD12	1:A:178:LEU:HA	1.58	0.41
1:A:347:VAL:HG11	1:A:434:TRP:CE3	2.55	0.41
2:C:84:TYR:HE1	2:C:87:HIS:O	2.02	0.41
1:A:177:ARG:HH11	1:A:203:MET:CE	2.33	0.41
1:A:81:MET:HG2	1:A:93:PRO:HB3	2.01	0.41
3:B:170:ARG:HG2	3:B:192:ASP:OD1	2.20	0.41
2:C:63:LYS:HD2	2:C:74:LYS:HG3	2.02	0.41
2:C:79:MET:O	2:C:83:HIS:HB2	2.20	0.41
2:C:76:PRO:O	2:C:80:MET:HG2	2.20	0.41
1:A:114:GLN:HG3	1:A:115:PRO:HD2	2.02	0.41
1:A:58:ASN:ND2	4:A:501:NAG:C1	2.83	0.41
3:B:240:ARG:CZ	3:B:242:ASN:H	2.34	0.41
2:C:70:LEU:HD21	2:C:107:LYS:HE2	2.02	0.41
1:A:46:ARG:HD2	1:A:83:TRP:CD2	2.55	0.41
3:B:229:TYR:C	3:B:231:ASP:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:116:ASN:N	3:B:198:ARG:HH22	2.18	0.41
1:A:276:LEU:HD22	1:A:306:CYS:HB3	2.01	0.41
1:A:59:VAL:HA	1:A:114:GLN:O	2.21	0.41
3:B:157:VAL:CG2	3:B:158:GLY:N	2.74	0.41
3:B:278:ARG:HG3	3:B:287:TRP:CE3	2.55	0.41
2:C:46:MET:SD	2:C:46:MET:N	2.93	0.41
3:B:103:GLN:CG	3:B:104:ASN:H	2.30	0.41
3:B:150:ILE:HG21	3:B:150:ILE:HD13	1.91	0.41
1:A:348:THR:HG21	1:A:357:ARG:NH1	2.36	0.40
2:C:59:LEU:HA	2:C:62:TYR:HB2	2.02	0.40
2:C:67:ARG:HG3	2:C:68:GLY:H	1.86	0.40
1:A:70:LEU:O	1:A:70:LEU:HD12	2.21	0.40
3:B:131:TYR:CD2	3:B:132:PHE:N	2.88	0.40
3:B:251:LEU:HD12	3:B:290:TRP:HH2	1.86	0.40
1:A:248:LEU:HD21	1:A:321:VAL:HG12	2.04	0.40
2:C:48:ASP:HB2	3:B:169:SER:HB2	2.03	0.40
3:B:198:ARG:O	3:B:199:PHE:HD1	2.04	0.40
2:C:23:ARG:NH1	3:B:283:ARG:HG2	2.36	0.40
1:A:181:SER:C	1:A:183:GLU:H	2.25	0.40
3:B:278:ARG:HG2	3:B:290:TRP:CZ3	2.56	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	410/414 (99%)	343 (84%)	48 (12%)	19 (5%)	3 21
2	C	103/127 (81%)	77 (75%)	20 (19%)	6 (6%)	2 15
3	B	164/305 (54%)	121 (74%)	30 (18%)	13 (8%)	1 8
All	All	677/846 (80%)	541 (80%)	98 (14%)	38 (6%)	2 16

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	163	TRP
1	A	185	ALA
1	A	311	PRO
1	A	384	LYS
1	A	405	SER
3	B	104	ASN
3	B	105	PHE
3	B	162	ASP
3	B	247	THR
3	B	270	ARG
1	A	87	PRO
1	A	116	ASP
2	C	65	GLY
2	C	86	GLN
3	B	222	ARG
3	B	225	GLN
3	B	230	LEU
1	A	158	SER
1	A	183	GLU
1	A	255	ALA
1	A	327	ARG
3	B	221	PRO
1	A	29	PRO
1	A	89	PRO
1	A	160	GLN
1	A	179	GLN
2	C	66	LEU
3	B	157	VAL
3	B	190	LEU
1	A	41	SER
1	A	193	SER
2	C	54	CYS
2	C	96	CYS
1	A	88	HIS
3	B	150	ILE
3	B	202	PRO
2	C	52	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	373/375 (100%)	360 (96%)	13 (4%)	43 77
2	C	96/116 (83%)	87 (91%)	9 (9%)	11 39
3	B	159/261 (61%)	148 (93%)	11 (7%)	19 57
All	All	628/752 (84%)	595 (95%)	33 (5%)	28 66

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	91	CYS
1	A	122	ARG
1	A	126	THR
1	A	136	PRO
1	A	162	HIS
1	A	374	ILE
1	A	386	SER
1	A	388	THR
1	A	400	PRO
1	A	417	SER
1	A	418	ARG
1	A	435	ASP
2	C	41	GLU
2	C	48	ASP
2	C	49	LEU
2	C	51	GLU
2	C	54	CYS
2	C	55	LEU
2	C	93	GLU
2	C	96	CYS
2	C	117	ILE
3	B	104	ASN
3	B	108	PHE
3	B	129	VAL
3	B	131	TYR

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Mol	Chain	Res	Type
3	B	151	GLN
3	B	222	ARG
3	B	240	ARG
3	B	243	THR
3	B	258	LEU
3	B	268	GLU
3	B	276	LYS

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	58	ASN
1	A	160	GLN
1	A	305	HIS
2	C	64	GLN
2	C	83	HIS
3	B	130	GLN
3	B	171	ASN
3	B	213	HIS
3	B	220	GLN
3	B	225	GLN
3	B	242	ASN
3	B	244	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 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	$\#\|Z\| > 2$
4	NAG	A	501	-	14,14,15	0.66	1 (7%)	15,19,21	0.46	0
4	NAG	A	502	-	14,14,15	0.51	0	15,19,21	1.28	1 (6%)
4	NAG	A	503	-	14,14,15	0.39	0	15,19,21	0.79	0
4	NAG	B	401	-	14,14,15	0.46	0	15,19,21	0.96	1 (6%)

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	501	-	-	0/6/23/26	0/1/1/1
4	NAG	A	502	-	-	0/6/23/26	0/1/1/1
4	NAG	A	503	-	-	0/6/23/26	0/1/1/1
4	NAG	B	401	-	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	NAG	C1-C2	-2.02	1.49	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	401	NAG	C3-C4-C5	2.10	113.96	110.23
4	A	502	NAG	C2-N2-C7	4.51	128.97	123.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	NAG	3	0
4	A	502	NAG	1	0
4	A	503	NAG	1	0
4	B	401	NAG	2	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

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	A	412/414 (99%)	-0.04	4 (0%) 84 80	65, 105, 154, 203	0
2	C	105/127 (82%)	0.08	3 (2%) 55 49	113, 163, 201, 219	0
3	B	174/305 (57%)	0.76	27 (15%) 3 2	130, 193, 243, 268	0
All	All	691/846 (81%)	0.18	34 (4%) 33 27	65, 131, 220, 268	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	144	ILE	5.4
3	B	206	THR	5.3
3	B	199	PHE	4.3
3	B	207	VAL	3.8
3	B	133	LEU	3.7
3	B	158	GLY	3.6
3	B	162	ASP	3.6
3	B	173	PHE	3.4
3	B	216	VAL	3.3
3	B	129	VAL	3.1
3	B	164	LEU	3.1
3	B	150	ILE	3.0
3	B	118	THR	2.9
2	C	118	PRO	2.9
1	A	380	THR	2.9
3	B	218	TRP	2.8
3	B	159	CYS	2.6
1	A	164	LEU	2.6
3	B	146	CYS	2.6
3	B	161	LEU	2.6
1	A	169	LEU	2.6
3	B	215	LEU	2.5
3	B	265	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
3	B	296	PHE	2.4
3	B	128	ASP	2.4
3	B	269	PRO	2.3
3	B	167	LEU	2.3
3	B	110	TYR	2.2
3	B	101	ALA	2.2
3	B	97	ARG	2.2
3	B	227	LEU	2.2
1	A	157	GLY	2.1
2	C	14	GLU	2.1
2	C	61	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 carbohydrates 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. 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^{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	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	B	401	14/15	0.81	0.30	-0.04	146,183,211,218	0
4	NAG	A	501	14/15	0.92	0.18	-0.73	154,157,164,200	0
4	NAG	A	502	14/15	0.81	0.28	-	155,169,191,192	0
4	NAG	A	503	14/15	0.84	0.24	-	147,161,183,188	0

6.5 Other polymers (i)

There are no such residues in this entry.