



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:15 AM UTC

PDB ID : 4KC3 / pdb_00004kc3
Title : Cytokine/receptor binary complex
Authors : Liu, X.; Wang, X.Q.
Deposited on : 2013-04-24
Resolution : 3.27 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

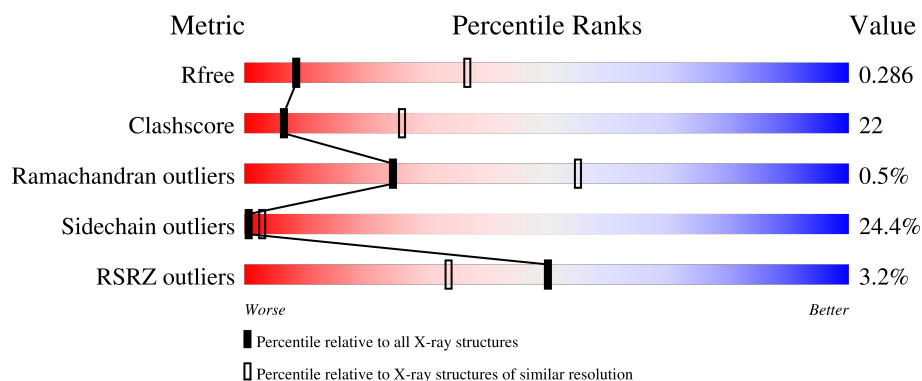
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.27 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}	180053	1303 (3.30-3.26)
Clashscore	190562	1354 (3.30-3.26)
Ramachandran outliers	187476	1334 (3.30-3.26)
Sidechain outliers	187428	1333 (3.30-3.26)
RSRZ outliers	180081	1303 (3.30-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	159	48% 25% 13% 14%
2	B	309	4% 42% 35% 11% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3354 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-33.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	137	Total	C	N	O	S	Se	0	0	0
			1110	712	177	215	3	3			

- Molecule 2 is a protein called Interleukin-1 receptor-like 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	278	Total	C	N	O	S	0	0	0
			2202	1395	378	416	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	322	HIS	-	expression tag	UNP Q01638
B	323	HIS	-	expression tag	UNP Q01638
B	324	HIS	-	expression tag	UNP Q01638
B	325	HIS	-	expression tag	UNP Q01638
B	326	HIS	-	expression tag	UNP Q01638
B	327	HIS	-	expression tag	UNP Q01638

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

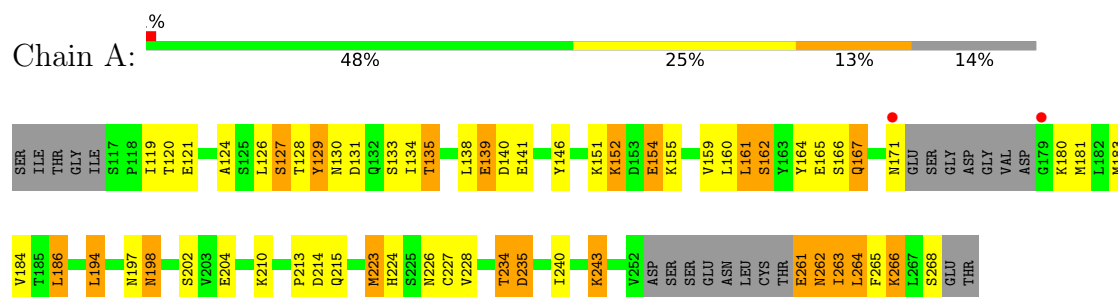


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

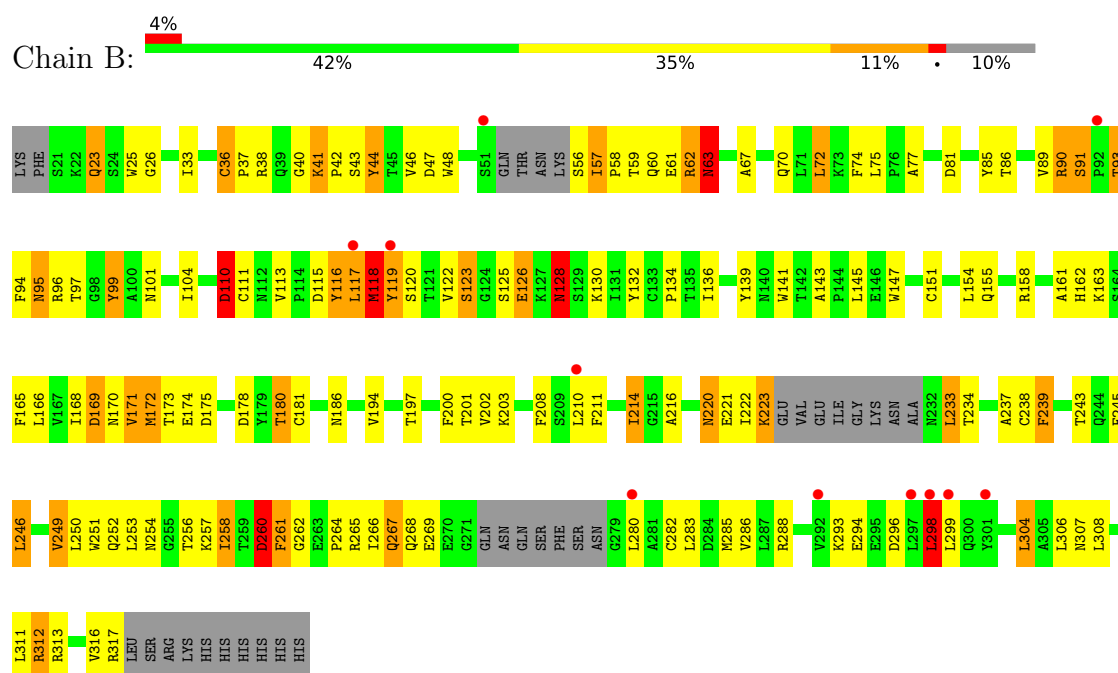
3 Residue-property plots

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: Interleukin-33



• Molecule 2: Interleukin-1 receptor-like 1



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	329.92Å 329.92Å 43.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.01 – 3.27 32.01 – 3.27	Depositor EDS
% Data completeness (in resolution range)	99.8 (32.01-3.27) 99.5 (32.01-3.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.238 , 0.283 0.240 , 0.286	Depositor DCC
R_{free} test set	749 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	110.5	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 100.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3354	wwPDB-VP
Average B, all atoms (Å ²)	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.72	1/1132 (0.1%)	1.12	1/1523 (0.1%)
2	B	0.66	0/2249	1.23	23/3047 (0.8%)
All	All	0.68	1/3381 (0.0%)	1.20	24/4570 (0.5%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	263	ILE	CA-CB	-5.07	1.47	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	258	ILE	N-CA-C	12.70	125.09	112.90
2	B	61	GLU	N-CA-C	10.18	125.00	112.58
2	B	62	ARG	N-CA-C	-9.07	96.44	109.96
2	B	126	GLU	N-CA-C	-8.02	103.06	113.17
1	A	139	GLU	N-CA-C	-7.65	104.04	113.15
2	B	44	TYR	N-CA-C	-7.05	100.04	110.48
2	B	130	LYS	N-CA-C	6.95	119.85	108.52
2	B	119	TYR	N-CA-C	6.94	119.79	108.55
2	B	239	PHE	N-CA-C	6.85	121.80	113.17
2	B	143	ALA	CA-C-N	6.71	127.08	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	143	ALA	C-N-CA	6.71	127.08	119.83
2	B	91	SER	N-CA-C	6.63	121.24	112.35
2	B	220	ASN	N-CA-C	6.33	117.83	108.60
2	B	93	THR	N-CA-C	-6.08	105.87	113.28
2	B	36	CYS	CA-C-N	6.05	126.22	119.32
2	B	36	CYS	C-N-CA	6.05	126.22	119.32
2	B	63	ASN	N-CA-C	6.05	120.12	112.87
2	B	260	ASP	N-CA-C	5.79	118.54	108.76
2	B	110	ASP	N-CA-C	-5.70	105.21	111.82
2	B	172	MET	N-CA-C	-5.66	101.01	109.96
2	B	115	ASP	CA-C-N	-5.32	114.90	122.77
2	B	115	ASP	C-N-CA	-5.32	114.90	122.77
2	B	238	CYS	N-CA-C	5.23	116.95	108.26
2	B	128	ASN	N-CA-C	5.14	116.80	108.26

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	116	TYR	Peptide
2	B	260	ASP	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	1110	0	1083	46	0
2	B	2202	0	2137	106	0
3	B	42	0	39	3	0
All	All	3354	0	3259	144	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 22.

All (144) 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:129:TYR:H	1:A:264:LEU:HG	1.38	0.86
2:B:117:LEU:HD23	2:B:197:THR:H	1.45	0.81
2:B:155:GLN:O	2:B:158:ARG:NH1	2.16	0.79
1:A:161:LEU:HD12	1:A:186:LEU:HD12	1.66	0.77
2:B:214:ILE:H	2:B:312:ARG:HH12	1.32	0.77
1:A:166:SER:OG	1:A:181:MSE:O	2.04	0.74
2:B:125:SER:HA	2:B:171:VAL:HG12	1.69	0.72
2:B:46:VAL:HG22	2:B:89:VAL:HG22	1.72	0.70
2:B:123:SER:OG	2:B:128:ASN:O	2.09	0.70
2:B:47:ASP:OD1	2:B:90:ARG:NH1	2.24	0.69
2:B:298:LEU:HD22	2:B:299:LEU:HG	1.73	0.69
2:B:267:GLN:HE22	2:B:288:ARG:HH21	1.41	0.69
2:B:117:LEU:HD23	2:B:197:THR:N	2.07	0.68
2:B:36:CYS:HB3	2:B:70:GLN:HG2	1.77	0.67
2:B:91:SER:OG	2:B:93:THR:N	2.28	0.66
2:B:91:SER:OG	2:B:94:PHE:N	2.29	0.66
2:B:63:ASN:N	2:B:63:ASN:OD1	2.29	0.64
2:B:25:TRP:HE1	2:B:117:LEU:HA	1.62	0.64
1:A:152:LYS:N	2:B:118:MET:O	2.30	0.64
2:B:23:GLN:HG3	2:B:101:ASN:HB3	1.80	0.64
2:B:280:LEU:H	2:B:280:LEU:HD23	1.63	0.63
2:B:77:ALA:HB1	2:B:104:ILE:HG12	1.80	0.62
2:B:25:TRP:HE1	2:B:117:LEU:HD12	1.64	0.60
2:B:253:LEU:HD21	2:B:264:PRO:HG2	1.83	0.60
2:B:25:TRP:NE1	2:B:117:LEU:HD12	2.17	0.59
2:B:123:SER:HB3	2:B:200:PHE:CE1	2.38	0.59
2:B:67:ALA:HB2	2:B:72:LEU:HD23	1.85	0.58
2:B:91:SER:HB3	2:B:94:PHE:CZ	2.38	0.58
1:A:235:ASP:N	1:A:235:ASP:OD1	2.38	0.57
1:A:262:ASN:HA	1:A:264:LEU:HD13	1.87	0.56
2:B:158:ARG:HG3	2:B:170:ASN:HD22	1.70	0.56
2:B:118:MET:HG2	2:B:134:PRO:CB	2.35	0.56
2:B:214:ILE:H	2:B:312:ARG:NH1	2.01	0.55
2:B:125:SER:O	2:B:171:VAL:HB	2.07	0.55
1:A:166:SER:HA	1:A:183:MSE:HE2	1.89	0.55
1:A:130:ASN:HA	2:B:132:TYR:CE2	2.41	0.55
1:A:119:ILE:HD13	1:A:164:TYR:HA	1.89	0.55
2:B:94:PHE:CD2	2:B:96:ARG:HD3	2.42	0.54
2:B:25:TRP:CD1	2:B:117:LEU:HD12	2.42	0.54
1:A:240:ILE:O	1:A:263:ILE:HG23	2.08	0.54
2:B:33:ILE:HG12	2:B:139:TYR:CE1	2.43	0.53
2:B:123:SER:HB3	2:B:200:PHE:CZ	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:298:LEU:HD13	2:B:299:LEU:HD12	1.91	0.52
1:A:152:LYS:CG	2:B:119:TYR:HA	2.39	0.52
2:B:180:THR:HB	2:B:197:THR:OG1	2.08	0.52
2:B:25:TRP:HZ2	2:B:118:MET:H	1.57	0.52
2:B:210:LEU:HG	2:B:211:PHE:H	1.75	0.52
1:A:124:ALA:HB2	2:B:245:PHE:HZ	1.75	0.52
1:A:261:GLU:OE1	1:A:261:GLU:N	2.43	0.51
2:B:125:SER:OG	2:B:171:VAL:O	2.15	0.51
1:A:131:ASP:OD1	1:A:266:LYS:NZ	2.40	0.51
2:B:254:ASN:OD1	2:B:299:LEU:HB3	2.11	0.51
1:A:152:LYS:HG2	2:B:119:TYR:HA	1.91	0.50
2:B:95:ASN:OD1	3:B:401:NAG:O5	2.24	0.50
2:B:186:ASN:HD21	3:B:402:NAG:H4	1.76	0.50
2:B:169:ASP:OD2	2:B:169:ASP:N	2.38	0.50
2:B:172:MET:HB2	2:B:174:GLU:HB2	1.93	0.50
2:B:246:LEU:HD12	2:B:308:LEU:HD23	1.94	0.49
1:A:165:GLU:OE1	2:B:313:ARG:NH1	2.44	0.49
1:A:121:GLU:HB2	1:A:160:LEU:HD11	1.95	0.49
2:B:172:MET:O	2:B:202:VAL:HG21	2.12	0.49
1:A:135:THR:HG22	1:A:146:TYR:HB2	1.95	0.49
2:B:155:GLN:OE1	2:B:155:GLN:N	2.45	0.48
2:B:91:SER:HG	2:B:94:PHE:N	2.11	0.48
1:A:129:TYR:N	1:A:264:LEU:HG	2.18	0.47
2:B:186:ASN:ND2	3:B:402:NAG:H4	2.29	0.47
2:B:36:CYS:HB2	2:B:48:TRP:CZ2	2.49	0.47
2:B:265:ARG:NH1	2:B:266:ILE:O	2.47	0.47
1:A:128:THR:HG23	1:A:134:ILE:HD11	1.96	0.47
1:A:151:LYS:O	1:A:154:GLU:HB2	2.15	0.47
2:B:158:ARG:HG3	2:B:170:ASN:ND2	2.29	0.47
2:B:214:ILE:HG13	2:B:312:ARG:NH1	2.30	0.46
1:A:162:SER:O	1:A:184:VAL:HA	2.15	0.46
1:A:167:GLN:H	1:A:167:GLN:CD	2.23	0.46
2:B:72:LEU:HD13	2:B:74:PHE:CE2	2.50	0.46
2:B:81:ASP:O	2:B:85:TYR:OH	2.20	0.46
2:B:110:ASP:OD1	2:B:111:CYS:N	2.49	0.46
1:A:262:ASN:C	1:A:264:LEU:HD13	2.40	0.46
1:A:262:ASN:CA	1:A:264:LEU:HD13	2.46	0.45
2:B:168:ILE:CG2	2:B:171:VAL:HG23	2.46	0.45
2:B:91:SER:CB	2:B:93:THR:H	2.28	0.45
2:B:239:PHE:HZ	2:B:249:VAL:HG12	1.80	0.45
2:B:38:ARG:CZ	2:B:96:ARG:HG3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:GLY:C	2:B:41:LYS:HD2	2.42	0.45
2:B:74:PHE:O	2:B:75:LEU:HD23	2.16	0.45
1:A:129:TYR:HB3	1:A:264:LEU:HB2	1.98	0.45
2:B:261:PHE:CD2	2:B:262:GLY:N	2.85	0.45
2:B:47:ASP:OD1	2:B:90:ARG:HD2	2.17	0.45
1:A:152:LYS:HB3	1:A:152:LYS:HE3	1.73	0.45
2:B:155:GLN:CD	2:B:158:ARG:HH22	2.25	0.45
1:A:129:TYR:CG	1:A:264:LEU:HD12	2.52	0.45
1:A:186:LEU:N	1:A:186:LEU:HD13	2.32	0.45
2:B:214:ILE:HG22	2:B:216:ALA:O	2.17	0.45
2:B:38:ARG:NH1	2:B:96:ARG:HG3	2.32	0.44
2:B:122:VAL:HG11	2:B:203:LYS:HZ2	1.83	0.44
2:B:136:ILE:HG12	2:B:141:TRP:NE1	2.32	0.44
2:B:254:ASN:OD1	2:B:299:LEU:HD13	2.17	0.44
1:A:130:ASN:HA	2:B:132:TYR:CD2	2.53	0.44
2:B:33:ILE:HG12	2:B:139:TYR:CD1	2.52	0.44
2:B:214:ILE:HA	2:B:237:ALA:HA	1.98	0.44
1:A:186:LEU:HD23	1:A:194:LEU:HD22	1.99	0.44
2:B:285:MET:HE2	2:B:285:MET:HB2	1.86	0.44
2:B:158:ARG:HB2	2:B:170:ASN:HB3	1.99	0.44
2:B:293:LYS:N	2:B:296:ASP:OD2	2.33	0.44
1:A:127:SER:O	1:A:265:PHE:HA	2.16	0.44
2:B:222:ILE:O	2:B:223:LYS:HD3	2.17	0.44
1:A:197:ASN:ND2	1:A:204:GLU:OE1	2.41	0.44
1:A:213:PRO:HB2	1:A:215:GLN:OE1	2.18	0.44
2:B:132:TYR:CD1	2:B:165:PHE:HB3	2.53	0.43
1:A:129:TYR:HB3	1:A:264:LEU:CB	2.49	0.43
1:A:138:LEU:C	1:A:140:ASP:H	2.24	0.43
1:A:198:ASN:OD1	1:A:198:ASN:N	2.51	0.43
2:B:48:TRP:O	2:B:57:ILE:HB	2.18	0.43
2:B:210:LEU:O	2:B:307:ASN:ND2	2.52	0.43
1:A:243:LYS:HA	1:A:243:LYS:HE2	2.01	0.43
2:B:41:LYS:HB2	2:B:44:TYR:CD2	2.53	0.43
1:A:129:TYR:CD2	1:A:264:LEU:HD12	2.54	0.42
1:A:214:ASP:HB3	1:A:234:THR:HG23	2.01	0.42
2:B:171:VAL:HG22	2:B:175:ASP:HB2	2.00	0.42
2:B:116:TYR:CD2	2:B:116:TYR:N	2.85	0.42
1:A:167:GLN:HA	1:A:180:LYS:HE2	2.02	0.42
2:B:254:ASN:O	2:B:254:ASN:ND2	2.53	0.42
2:B:48:TRP:CE3	2:B:72:LEU:HG	2.55	0.42
2:B:266:ILE:HG12	2:B:285:MET:SD	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:GLY:O	2:B:104:ILE:HA	2.19	0.42
2:B:304:LEU:HB3	2:B:311:LEU:HD11	2.03	0.41
1:A:186:LEU:H	1:A:186:LEU:HD22	1.84	0.41
2:B:253:LEU:N	2:B:256:THR:O	2.37	0.41
2:B:99:TYR:N	2:B:99:TYR:CD2	2.88	0.41
2:B:233:LEU:HD12	2:B:234:THR:H	1.84	0.41
1:A:129:TYR:CD2	1:A:130:ASN:N	2.88	0.41
2:B:162:HIS:CE1	2:B:163:LYS:HG3	2.55	0.41
1:A:226:ASN:HD21	2:B:245:PHE:HB2	1.84	0.41
2:B:233:LEU:HD11	2:B:251:TRP:CH2	2.56	0.41
2:B:252:GLN:HG2	2:B:256:THR:N	2.35	0.41
1:A:223:MSE:SE	1:A:223:MSE:N	3.03	0.41
2:B:161:ALA:HB2	2:B:166:LEU:HD13	2.02	0.41
2:B:172:MET:C	2:B:174:GLU:H	2.30	0.40
1:A:197:ASN:HB3	1:A:202:SER:OG	2.21	0.40
2:B:36:CYS:HA	2:B:37:PRO:HD3	1.88	0.40
2:B:118:MET:HG2	2:B:134:PRO:HB3	2.03	0.40
2:B:147:TRP:CE3	2:B:181:CYS:HB3	2.55	0.40
2:B:58:PRO:HG2	2:B:62:ARG:HB3	2.03	0.40
2:B:42:PRO:O	2:B:43:SER:OG	2.28	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	131/159 (82%)	120 (92%)	11 (8%)	0	100	100
2	B	270/309 (87%)	251 (93%)	17 (6%)	2 (1%)	18	48
All	All	401/468 (86%)	371 (92%)	28 (7%)	2 (0%)	24	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	118	MET
2	B	298	LEU

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	129/145 (89%)	97 (75%)	32 (25%)	1	3
2	B	240/269 (89%)	182 (76%)	58 (24%)	1	3
All	All	369/414 (89%)	279 (76%)	90 (24%)	1	3

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	THR
1	A	126	LEU
1	A	127	SER
1	A	129	TYR
1	A	133	SER
1	A	135	THR
1	A	139	GLU
1	A	141	GLU
1	A	152	LYS
1	A	154	GLU
1	A	155	LYS
1	A	159	VAL
1	A	161	LEU
1	A	162	SER
1	A	167	GLN
1	A	171	ASN
1	A	186	LEU
1	A	194	LEU
1	A	198	ASN
1	A	210	LYS
1	A	223	MSE
1	A	224	HIS

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Mol	Chain	Res	Type
1	A	227	CYS
1	A	228	VAL
1	A	234	THR
1	A	235	ASP
1	A	243	LYS
1	A	261	GLU
1	A	262	ASN
1	A	264	LEU
1	A	266	LYS
1	A	268	SER
2	B	23	GLN
2	B	41	LYS
2	B	56	SER
2	B	57	ILE
2	B	59	THR
2	B	60	GLN
2	B	63	ASN
2	B	72	LEU
2	B	86	THR
2	B	90	ARG
2	B	95	ASN
2	B	97	THR
2	B	99	TYR
2	B	110	ASP
2	B	113	VAL
2	B	117	LEU
2	B	118	MET
2	B	120	SER
2	B	123	SER
2	B	126	GLU
2	B	128	ASN
2	B	145	LEU
2	B	151	CYS
2	B	154	LEU
2	B	169	ASP
2	B	171	VAL
2	B	173	THR
2	B	178	ASP
2	B	180	THR
2	B	194	VAL
2	B	201	THR
2	B	208	PHE

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Mol	Chain	Res	Type
2	B	214	ILE
2	B	220	ASN
2	B	221	GLU
2	B	223	LYS
2	B	233	LEU
2	B	243	THR
2	B	246	LEU
2	B	249	VAL
2	B	250	LEU
2	B	257	LYS
2	B	258	ILE
2	B	260	ASP
2	B	261	PHE
2	B	267	GLN
2	B	268	GLN
2	B	269	GLU
2	B	282	CYS
2	B	283	LEU
2	B	286	VAL
2	B	294	GLU
2	B	298	LEU
2	B	304	LEU
2	B	306	LEU
2	B	312	ARG
2	B	316	VAL
2	B	317	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	HIS
1	A	246	HIS
2	B	60	GLN
2	B	150	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	B	402	2	14,14,15	0.64	0	17,19,21	1.29	2 (11%)
3	NAG	B	403	2	14,14,15	0.53	0	17,19,21	1.14	1 (5%)
3	NAG	B	401	2	14,14,15	1.10	1 (7%)	17,19,21	1.53	4 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	402	2	-	4/6/23/26	0/1/1/1
3	NAG	B	403	2	-	4/6/23/26	0/1/1/1
3	NAG	B	401	2	-	5/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	NAG	C1-C2	3.20	1.56	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	NAG	O5-C5-C4	-3.51	102.28	110.83
3	B	402	NAG	C1-O5-C5	2.58	115.64	112.19
3	B	401	NAG	C2-N2-C7	2.45	126.18	122.90
3	B	402	NAG	O3-C3-C2	-2.40	104.41	109.40
3	B	401	NAG	C3-C4-C5	-2.14	106.35	110.23
3	B	401	NAG	O5-C5-C6	2.07	111.69	107.66
3	B	403	NAG	O5-C5-C6	2.03	111.61	107.66

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	NAG	C8-C7-N2-C2
3	B	401	NAG	O7-C7-N2-C2
3	B	402	NAG	C8-C7-N2-C2
3	B	402	NAG	O7-C7-N2-C2
3	B	403	NAG	C8-C7-N2-C2
3	B	403	NAG	O7-C7-N2-C2
3	B	402	NAG	O5-C5-C6-O6
3	B	403	NAG	C4-C5-C6-O6
3	B	401	NAG	O5-C5-C6-O6
3	B	402	NAG	C4-C5-C6-O6
3	B	403	NAG	O5-C5-C6-O6
3	B	401	NAG	C4-C5-C6-O6
3	B	401	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	NAG	2	0
3	B	401	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	134/159 (84%)	-0.07	2 (1%) 72 53	93, 123, 178, 216	0
2	B	278/309 (89%)	0.20	11 (3%) 42 28	92, 127, 201, 238	0
All	All	412/468 (88%)	0.11	13 (3%) 50 34	92, 126, 196, 238	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	299	LEU	4.9
2	B	301	TYR	3.8
2	B	297	LEU	3.5
2	B	119	TYR	2.9
2	B	92	PRO	2.8
1	A	171	ASN	2.7
2	B	280	LEU	2.7
2	B	117	LEU	2.4
2	B	292	VAL	2.2
1	A	179	GLY	2.2
2	B	298	LEU	2.2
2	B	210	LEU	2.1
2	B	51	SER	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	B	403	14/15	0.29	0.14	110,110,110,110	0
3	NAG	B	401	14/15	0.38	0.14	110,110,110,110	0
3	NAG	B	402	14/15	0.81	0.10	110,110,110,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.