Full wwPDB X-ray Structure Validation Report ⓘ

Dec 19, 2023 – 07:21 AM EST

PDB ID	:	1IQA
Title	:	CRYSTAL STRUCTURE OF THE EXTRACELLULAR DOMAIN OF MOUSE RANK LIGAND
Authors	:	Ito, S.; Wakabayashi, K.; Ubukata, O.; Hayashi, S.; Okada, F.; Hata, T.
Deposited on	:	2001-07-11
Resolution	:	2.20 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:

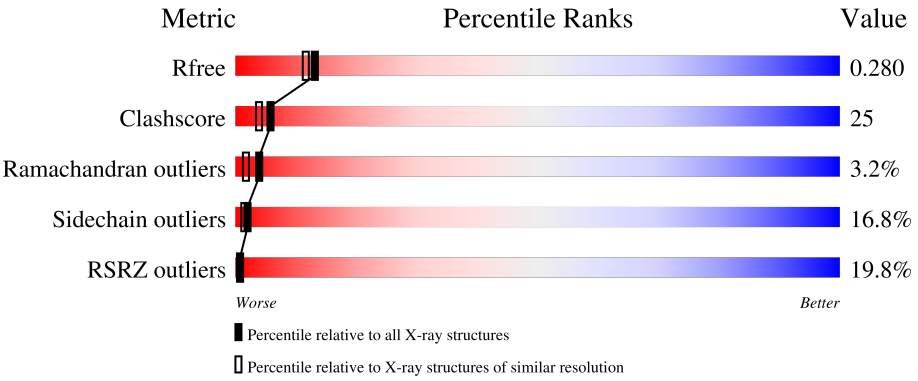
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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 <=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	160	12% 68% 25%
1	B	160	27% 42% 44% 11%
1	C	160	18% 54% 31% 11%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3768 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 RECEPTOR ACTIVATOR OF NUCLEAR FACTOR KAPPA B LIGAND.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	Se	0	0	0
			1233	787	210	232	1	3			
1	B	156	Total	C	N	O	S	Se	0	0	0
			1233	787	210	232	1	3			
1	C	156	Total	C	N	O	S	Se	0	0	0
			1233	787	210	232	1	3			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	198	MSE	MET	modified residue	UNP O35235
A	238	MSE	MET	modified residue	UNP O35235
A	255	MSE	MET	modified residue	UNP O35235
B	198	MSE	MET	modified residue	UNP O35235
B	238	MSE	MET	modified residue	UNP O35235
B	255	MSE	MET	modified residue	UNP O35235
C	198	MSE	MET	modified residue	UNP O35235
C	238	MSE	MET	modified residue	UNP O35235
C	255	MSE	MET	modified residue	UNP O35235

- Molecule 2 is water.

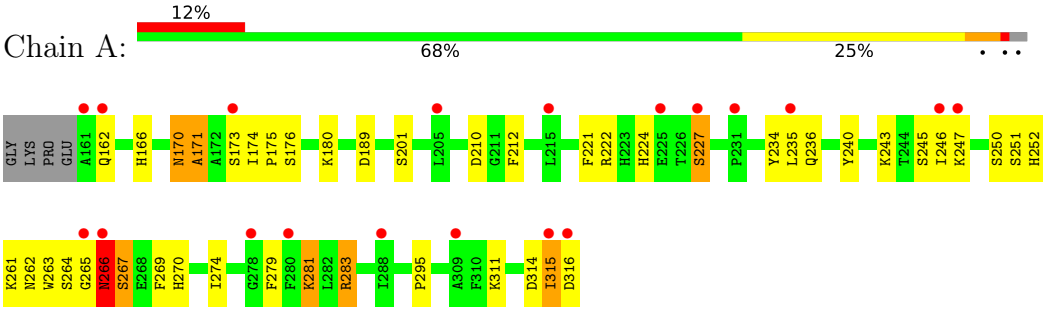
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	38	Total	O	0	0
			38	38		
2	B	14	Total	O	0	0
			14	14		
2	C	17	Total	O	0	0
			17	17		

3 Residue-property plots (i)

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

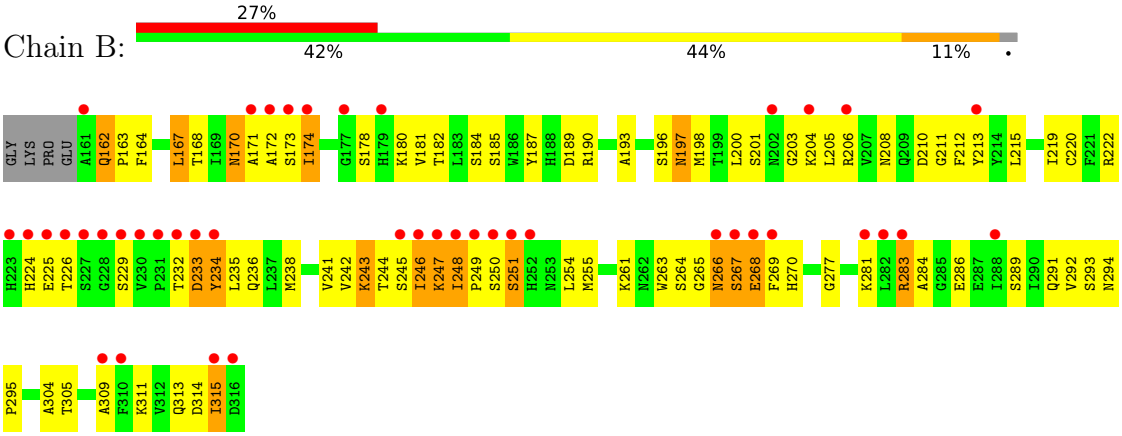
• Molecule 1: RECEPTOR ACTIVATOR OF NUCLEAR FACTOR KAPPA B LIGAND

Chain A:



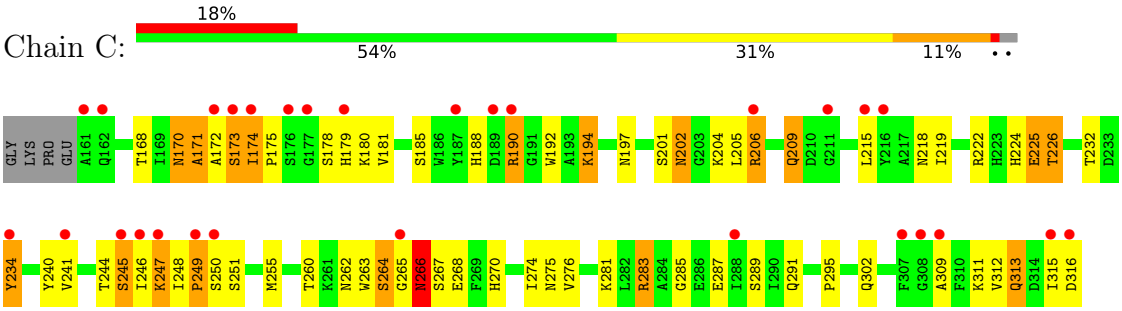
• Molecule 1: RECEPTOR ACTIVATOR OF NUCLEAR FACTOR KAPPA B LIGAND

Chain B:



• Molecule 1: RECEPTOR ACTIVATOR OF NUCLEAR FACTOR KAPPA B LIGAND

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.68Å 78.98Å 100.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20 24.48 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.7 (15.00-2.20) 96.5 (24.48-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.05 (at 2.19Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.226 , 0.274 0.234 , 0.280	Depositor DCC
R_{free} test set	2036 reflections (7.84%)	wwPDB-VP
Wilson B-factor (Å^2)	39.3	Xtriage
Anisotropy	0.616	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 70.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3768	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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

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	0.99	0/1265	0.98	1/1709 (0.1%)
1	B	0.71	0/1265	0.82	0/1709
1	C	0.77	0/1265	0.89	0/1709
All	All	0.83	0/3795	0.90	1/5127 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	166	HIS	N-CA-C	-5.14	97.13	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1233	0	1182	46	0
1	B	1233	0	1182	90	0
1	C	1233	0	1182	55	0
2	A	38	0	0	2	0
2	B	14	0	0	2	0
2	C	17	0	0	3	0
All	All	3768	0	3546	183	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 25.

All (183) 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:B:283:ARG:HH11	1:B:283:ARG:HG3	1.16	1.07
1:C:283:ARG:HG3	1:C:283:ARG:HH11	1.21	1.04
1:B:219:ILE:HD13	1:B:305:THR:HG23	1.45	0.98
1:C:224:HIS:CD2	1:C:226:THR:HB	2.03	0.93
1:A:281:LYS:HD2	1:A:315:ILE:HD13	1.51	0.92
1:C:202:ASN:HB2	2:C:53:HOH:O	1.68	0.92
1:C:247:LYS:O	1:C:249:PRO:HD3	1.72	0.89
1:C:171:ALA:HA	1:C:174:ILE:HD11	1.56	0.88
1:B:224:HIS:HA	1:B:268:GLU:O	1.76	0.85
1:A:283:ARG:HH11	1:A:283:ARG:HG3	1.41	0.85
1:A:174:ILE:HG21	2:A:49:HOH:O	1.78	0.84
1:B:162:GLN:NE2	1:B:162:GLN:HA	1.95	0.81
1:B:283:ARG:HH11	1:B:283:ARG:CG	1.94	0.81
1:C:262:ASN:OD1	1:C:264:SER:HB2	1.84	0.78
1:B:167:LEU:HD22	1:B:200:LEU:HD12	1.66	0.77
1:C:224:HIS:HD2	1:C:226:THR:H	1.30	0.77
1:C:190:ARG:HB3	1:C:190:ARG:CZ	2.14	0.77
1:B:248:ILE:O	1:B:248:ILE:HG13	1.84	0.77
1:A:261:LYS:NZ	1:B:261:LYS:NZ	2.34	0.75
1:C:283:ARG:HG3	1:C:283:ARG:NH1	1.93	0.75
1:A:283:ARG:HH11	1:A:283:ARG:CG	2.00	0.74
1:B:210:ASP:OD1	1:B:284:ALA:N	2.19	0.74
1:A:261:LYS:HZ3	1:B:261:LYS:NZ	1.87	0.73
1:C:209:GLN:OE1	1:C:311:LYS:HE3	1.88	0.72
1:A:173:SER:O	1:A:174:ILE:HG12	1.89	0.72
1:B:163:PRO:HB3	1:B:197:ASN:HB3	1.71	0.71
1:C:192:TRP:O	1:C:194:LYS:HE2	1.89	0.71
1:B:248:ILE:N	1:B:249:PRO:HD3	2.06	0.70
1:B:247:LYS:C	1:B:249:PRO:HD3	2.12	0.70
1:B:246:ILE:HG13	1:B:247:LYS:N	2.05	0.70
1:B:225:GLU:HB2	1:B:268:GLU:CB	2.22	0.69
1:C:234:TYR:HE2	1:C:260:THR:HB	1.58	0.68
1:C:225:GLU:OE1	1:C:268:GLU:HG2	1.94	0.68
1:A:170:ASN:HD22	1:A:170:ASN:C	1.96	0.67
1:B:283:ARG:HG3	1:B:283:ARG:NH1	1.98	0.67
1:B:248:ILE:O	1:B:248:ILE:CG1	2.44	0.66
1:B:162:GLN:HA	1:B:162:GLN:HE21	1.60	0.65
1:B:173:SER:O	1:B:174:ILE:HD13	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:GLN:HE21	1:B:163:PRO:CD	2.09	0.65
1:B:242:VAL:HG21	1:B:291:GLN:NE2	2.11	0.65
1:B:283:ARG:NH1	1:B:315:ILE:HD12	2.12	0.64
1:A:234:TYR:OH	1:B:270:HIS:HD2	1.80	0.64
1:B:210:ASP:OD1	1:B:283:ARG:HA	1.98	0.64
1:B:212:PHE:CE2	1:B:281:LYS:HD3	2.33	0.64
1:C:224:HIS:HD2	1:C:226:THR:HB	1.55	0.63
1:C:281:LYS:NZ	2:C:41:HOH:O	2.25	0.63
1:C:263:TRP:CE2	1:C:270:HIS:HB3	2.34	0.62
1:B:212:PHE:HD1	1:B:313:GLN:HG3	1.65	0.61
1:B:225:GLU:HB2	1:B:268:GLU:HA	1.82	0.61
1:B:212:PHE:CE2	1:B:281:LYS:HB2	2.36	0.61
1:A:212:PHE:HB3	1:A:279:PHE:CZ	2.35	0.61
1:A:266:ASN:HD22	1:A:267:SER:H	1.48	0.61
1:A:264:SER:O	1:A:266:ASN:CG	2.39	0.60
1:B:283:ARG:CZ	1:B:315:ILE:HD12	2.31	0.60
1:B:162:GLN:HE21	1:B:163:PRO:HD3	1.67	0.59
1:C:174:ILE:HG22	1:C:295:PRO:O	2.02	0.59
1:B:248:ILE:N	1:B:249:PRO:CD	2.65	0.59
1:C:248:ILE:O	1:C:250:SER:N	2.28	0.59
1:B:251:SER:HB2	2:B:61:HOH:O	2.02	0.58
1:B:281:LYS:HD2	1:B:315:ILE:HD13	1.86	0.58
1:C:215:LEU:HD23	1:C:309:ALA:CB	2.32	0.58
1:C:234:TYR:CE2	1:C:260:THR:HB	2.38	0.58
1:C:234:TYR:CE1	1:C:262:ASN:HB2	2.39	0.58
1:C:180:LYS:HE3	1:C:240:TYR:CE1	2.39	0.58
1:B:198:MSE:HE2	1:B:205:LEU:HG	1.86	0.58
1:C:245:SER:HB2	1:C:248:ILE:O	2.03	0.58
1:B:283:ARG:NH2	1:B:315:ILE:HG21	2.19	0.57
1:C:241:VAL:HG21	1:C:255:MSE:HE3	1.85	0.57
1:B:246:ILE:HG13	1:B:247:LYS:H	1.69	0.57
1:A:266:ASN:HD22	1:A:267:SER:N	2.01	0.57
1:B:264:SER:O	1:B:266:ASN:N	2.38	0.57
1:C:204:LYS:HD2	1:C:289:SER:HB3	1.87	0.57
1:A:262:ASN:OD1	1:A:264:SER:OG	2.22	0.56
1:C:283:ARG:NH1	1:C:283:ARG:CG	2.65	0.56
1:C:215:LEU:CD2	1:C:309:ALA:HB2	2.36	0.56
1:A:224:HIS:HB2	1:A:227:SER:OG	2.05	0.56
1:A:170:ASN:HD22	1:A:171:ALA:N	2.04	0.56
1:C:245:SER:HB2	1:C:248:ILE:C	2.26	0.56
1:C:218:ASN:O	1:C:219:ILE:HD13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:SER:C	1:A:252:HIS:HD2	2.09	0.55
1:C:247:LYS:C	1:C:249:PRO:HD3	2.26	0.55
1:B:181:VAL:HG13	1:B:295:PRO:HG3	1.88	0.55
1:B:210:ASP:HB3	1:B:315:ILE:HG13	1.89	0.55
1:C:312:VAL:HG12	1:C:313:GLN:HE21	1.72	0.55
1:A:261:LYS:NZ	1:B:261:LYS:HZ1	2.04	0.55
1:B:247:LYS:HA	1:B:247:LYS:HE2	1.89	0.54
1:A:281:LYS:CD	1:A:315:ILE:HD13	2.30	0.54
1:C:173:SER:C	1:C:174:ILE:HG12	2.27	0.54
1:A:189:ASP:OD1	1:A:189:ASP:N	2.38	0.54
1:B:283:ARG:CG	1:B:283:ARG:NH1	2.62	0.54
1:B:246:ILE:HG23	1:B:247:LYS:H	1.72	0.54
1:C:171:ALA:CA	1:C:174:ILE:HD11	2.35	0.54
1:C:244:THR:HG22	1:C:251:SER:HB2	1.89	0.54
1:A:212:PHE:HE1	1:A:316:ASP:H	1.55	0.53
1:B:212:PHE:HE2	1:B:281:LYS:HB2	1.70	0.53
1:B:173:SER:C	1:B:174:ILE:HG12	2.28	0.53
1:A:264:SER:O	1:A:266:ASN:OD1	2.27	0.53
1:B:267:SER:C	1:B:269:PHE:H	2.11	0.53
1:B:267:SER:O	1:B:269:PHE:N	2.42	0.53
1:C:215:LEU:HD23	1:C:309:ALA:HB2	1.90	0.53
1:B:181:VAL:CG1	1:B:295:PRO:HG3	2.39	0.52
1:A:264:SER:O	1:A:266:ASN:ND2	2.42	0.52
1:C:316:ASP:O	2:C:29:HOH:O	2.19	0.52
1:A:251:SER:C	1:A:252:HIS:CD2	2.84	0.51
1:B:225:GLU:HB2	1:B:268:GLU:CA	2.39	0.51
1:C:180:LYS:HE2	1:C:291:GLN:OE1	2.10	0.51
1:B:292:VAL:HG23	1:B:293:SER:O	2.11	0.51
1:C:168:THR:HG21	1:C:302:GLN:HB2	1.93	0.50
1:B:215:LEU:HD22	1:B:309:ALA:HB2	1.94	0.50
1:B:281:LYS:HD2	1:B:315:ILE:HG23	1.94	0.50
1:B:244:THR:HG22	1:B:245:SER:N	2.27	0.49
1:A:173:SER:C	1:A:174:ILE:HG12	2.33	0.49
1:A:224:HIS:CE1	1:A:269:PHE:HE1	2.30	0.49
1:A:243:LYS:HD3	1:A:254:LEU:HD21	1.94	0.49
1:A:170:ASN:C	1:A:170:ASN:ND2	2.65	0.49
1:C:265:GLY:O	1:C:266:ASN:HB2	2.12	0.49
1:C:283:ARG:HH12	1:C:315:ILE:HG13	1.77	0.49
1:B:170:ASN:O	1:B:172:ALA:N	2.46	0.49
1:A:261:LYS:HZ3	1:B:261:LYS:HZ2	1.58	0.49
1:B:181:VAL:HG23	1:B:182:THR:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:TRP:CE2	1:B:270:HIS:HB3	2.49	0.48
1:C:225:GLU:HG2	1:C:226:THR:N	2.28	0.48
1:B:164:PHE:CD1	1:B:164:PHE:C	2.87	0.48
1:B:241:VAL:HG21	1:B:255:MSE:HE3	1.96	0.48
1:B:211:GLY:HA3	1:B:311:LYS:HE2	1.96	0.48
1:C:206:ARG:HH11	1:C:246:ILE:CD1	2.27	0.48
1:B:267:SER:C	1:B:269:PHE:N	2.66	0.47
1:A:210:ASP:HB3	1:A:315:ILE:HG13	1.96	0.47
1:B:243:LYS:HG2	1:B:244:THR:N	2.30	0.47
1:B:184:SER:HA	1:B:203:GLY:HA3	1.97	0.47
1:C:170:ASN:O	1:C:172:ALA:N	2.47	0.47
1:B:243:LYS:HB2	1:B:254:LEU:HD11	1.96	0.46
1:B:173:SER:HB2	1:B:185:SER:HB2	1.95	0.46
1:A:252:HIS:CD2	1:A:252:HIS:N	2.81	0.46
1:A:266:ASN:ND2	1:A:267:SER:H	2.11	0.46
1:A:262:ASN:OD1	1:A:264:SER:CB	2.63	0.46
1:B:234:TYR:OH	1:C:270:HIS:HE1	1.98	0.46
1:B:219:ILE:HD13	1:B:305:THR:CG2	2.32	0.45
1:B:247:LYS:C	1:B:248:ILE:HG23	2.37	0.45
1:A:235:LEU:O	1:A:260:THR:HA	2.16	0.45
1:B:162:GLN:HE21	1:B:163:PRO:HD2	1.79	0.45
1:C:215:LEU:CD2	1:C:309:ALA:CB	2.94	0.45
1:A:261:LYS:HZ1	1:B:261:LYS:NZ	2.15	0.45
1:C:206:ARG:HH11	1:C:246:ILE:HD13	1.81	0.45
1:C:247:LYS:HE3	1:C:285:GLY:HA3	1.99	0.45
1:A:266:ASN:ND2	1:A:266:ASN:N	2.64	0.45
1:B:215:LEU:O	1:B:277:GLY:HA2	2.17	0.45
1:C:190:ARG:HB3	1:C:190:ARG:NH1	2.31	0.44
1:C:248:ILE:C	1:C:250:SER:H	2.16	0.44
1:C:316:ASP:OD2	1:C:316:ASP:OXT	2.34	0.44
1:A:175:PRO:HA	2:A:25:HOH:O	2.17	0.44
1:B:197:ASN:O	1:B:208:ASN:HB2	2.17	0.44
1:B:243:LYS:HE3	1:B:286:GLU:OE2	2.18	0.44
1:A:263:TRP:CE2	1:A:270:HIS:HB3	2.53	0.43
1:B:220:CYS:HB2	1:B:304:ALA:HB1	2.00	0.43
1:A:174:ILE:HG23	1:A:295:PRO:O	2.18	0.43
1:B:213:TYR:CD1	1:B:311:LYS:HA	2.53	0.43
1:B:167:LEU:HD22	1:B:200:LEU:CD1	2.42	0.43
1:A:221:PHE:HE1	1:A:274:ILE:HD11	1.84	0.43
1:A:316:ASP:OD2	1:A:316:ASP:OXT	2.37	0.42
1:C:188:HIS:CD2	1:C:188:HIS:C	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:PRO:HA	1:B:196:SER:O	2.19	0.42
1:B:236:GLN:O	1:B:293:SER:OG	2.30	0.42
1:B:235:LEU:CD2	1:B:294:ASN:ND2	2.83	0.42
1:B:238:MSE:HE3	1:B:238:MSE:HB3	1.89	0.42
1:B:225:GLU:HB2	1:B:268:GLU:HB3	2.01	0.42
1:B:246:ILE:HG23	1:B:247:LYS:N	2.35	0.42
1:A:251:SER:H	1:A:252:HIS:HD2	1.68	0.41
1:A:210:ASP:O	1:A:311:LYS:HE2	2.19	0.41
1:B:170:ASN:C	1:B:170:ASN:HD22	2.23	0.41
1:A:173:SER:C	1:A:174:ILE:CG1	2.89	0.41
1:A:261:LYS:HZ3	1:B:261:LYS:HZ1	1.62	0.41
1:C:173:SER:HB2	1:C:185:SER:H	1.86	0.41
1:C:274:ILE:HG22	1:C:275:ASN:N	2.35	0.41
1:A:180:LYS:HD2	1:A:240:TYR:CE1	2.56	0.41
1:B:187:TYR:HA	2:B:24:HOH:O	2.21	0.41
1:B:189:ASP:N	1:B:189:ASP:OD1	2.54	0.41
1:B:281:LYS:CE	1:B:315:ILE:HG23	2.51	0.41
1:B:247:LYS:CA	1:B:249:PRO:HD3	2.51	0.40
1:B:168:THR:OG1	1:B:193:ALA:HB2	2.20	0.40
1:B:233:ASP:OD2	1:B:233:ASP:N	2.54	0.40
1:C:173:SER:HB2	1:C:185:SER:N	2.36	0.40
1:C:181:VAL:HG22	1:C:295:PRO:HG3	2.04	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	154/160 (96%)	142 (92%)	8 (5%)	4 (3%)	5	3
1	B	154/160 (96%)	140 (91%)	8 (5%)	6 (4%)	3	1
1	C	154/160 (96%)	141 (92%)	8 (5%)	5 (3%)	4	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	462/480 (96%)	423 (92%)	24 (5%)	15 (3%)	4 2

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	171	ALA
1	B	246	ILE
1	B	265	GLY
1	B	266	ASN
1	C	171	ALA
1	C	249	PRO
1	A	250	SER
1	A	265	GLY
1	A	171	ALA
1	B	250	SER
1	B	268	GLU
1	C	173	SER
1	C	266	ASN
1	A	266	ASN
1	C	175	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	135/135 (100%)	119 (88%)	16 (12%)	5 4
1	B	135/135 (100%)	109 (81%)	26 (19%)	1 1
1	C	135/135 (100%)	109 (81%)	26 (19%)	1 1
All	All	405/405 (100%)	337 (83%)	68 (17%)	2 1

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	GLN

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Mol	Chain	Res	Type
1	A	170	ASN
1	A	176	SER
1	A	201	SER
1	A	222	ARG
1	A	227	SER
1	A	236	GLN
1	A	245	SER
1	A	246	ILE
1	A	247	LYS
1	A	266	ASN
1	A	267	SER
1	A	281	LYS
1	A	283	ARG
1	A	314	ASP
1	A	315	ILE
1	B	162	GLN
1	B	167	LEU
1	B	170	ASN
1	B	174	ILE
1	B	178	SER
1	B	180	LYS
1	B	190	ARG
1	B	197	ASN
1	B	201	SER
1	B	204	LYS
1	B	206	ARG
1	B	222	ARG
1	B	226	THR
1	B	229	SER
1	B	232	THR
1	B	233	ASP
1	B	234	TYR
1	B	243	LYS
1	B	247	LYS
1	B	248	ILE
1	B	251	SER
1	B	267	SER
1	B	283	ARG
1	B	289	SER
1	B	314	ASP
1	B	315	ILE
1	C	170	ASN

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Mol	Chain	Res	Type
1	C	174	ILE
1	C	178	SER
1	C	179	HIS
1	C	190	ARG
1	C	194	LYS
1	C	197	ASN
1	C	201	SER
1	C	202	ASN
1	C	205	LEU
1	C	206	ARG
1	C	209	GLN
1	C	222	ARG
1	C	225	GLU
1	C	226	THR
1	C	232	THR
1	C	234	TYR
1	C	245	SER
1	C	247	LYS
1	C	264	SER
1	C	266	ASN
1	C	267	SER
1	C	276	VAL
1	C	283	ARG
1	C	287	GLU
1	C	313	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	A	252	HIS
1	A	266	ASN
1	A	294	ASN
1	B	162	GLN
1	B	170	ASN
1	B	197	ASN
1	B	209	GLN
1	B	270	HIS
1	B	294	ASN
1	C	170	ASN
1	C	202	ASN
1	C	208	ASN

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Mol	Chain	Res	Type
1	C	224	HIS
1	C	236	GLN
1	C	270	HIS
1	C	313	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	153/160 (95%)	0.33	19 (12%)	4	3	21, 35, 67, 87	0
1	B	153/160 (95%)	1.74	43 (28%)	0	0	32, 64, 104, 121	0
1	C	153/160 (95%)	1.16	29 (18%)	1	1	29, 51, 86, 100	0
All	All	459/480 (95%)	1.08	91 (19%)	1	1	21, 49, 95, 121	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	226	THR	13.6
1	B	231	PRO	10.4
1	B	229	SER	8.9
1	B	230	VAL	8.3
1	B	228	GLY	7.9
1	B	246	ILE	7.9
1	B	232	THR	7.8
1	B	173	SER	7.3
1	C	161	ALA	7.3
1	C	249	PRO	7.1
1	B	172	ALA	6.9
1	B	161	ALA	6.9
1	C	173	SER	6.8
1	B	177	GLY	6.8
1	B	227	SER	6.5
1	A	316	ASP	6.4
1	B	179	HIS	6.2
1	B	233	ASP	5.8
1	B	250	SER	5.6
1	B	316	ASP	5.6
1	C	172	ALA	5.4
1	C	179	HIS	5.4
1	B	252	HIS	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	266	ASN	5.1
1	C	189	ASP	5.0
1	C	215	LEU	5.0
1	B	224	HIS	5.0
1	A	265	GLY	4.9
1	C	246	ILE	4.9
1	B	245	SER	4.8
1	B	225	GLU	4.6
1	B	174	ILE	4.5
1	C	316	ASP	4.5
1	C	265	GLY	4.3
1	C	190	ARG	4.3
1	C	309	ALA	4.3
1	C	174	ILE	4.1
1	B	234	TYR	4.1
1	C	245	SER	4.0
1	B	249	PRO	3.9
1	C	177	GLY	3.9
1	A	246	ILE	3.9
1	C	250	SER	3.8
1	C	308	GLY	3.8
1	B	247	LYS	3.7
1	B	268	GLU	3.6
1	A	161	ALA	3.6
1	C	162	GLN	3.4
1	C	234	TYR	3.3
1	C	288	ILE	3.1
1	A	225	GLU	3.1
1	B	202	ASN	3.0
1	A	315	ILE	3.0
1	B	269	PHE	2.9
1	B	310	PHE	2.9
1	A	247	LYS	2.8
1	C	307	PHE	2.8
1	B	315	ILE	2.8
1	A	280	PHE	2.8
1	B	281	LYS	2.8
1	A	173	SER	2.7
1	B	267	SER	2.7
1	C	247	LYS	2.6
1	A	205	LEU	2.6
1	B	248	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	288	ILE	2.5
1	B	204	LYS	2.5
1	A	215	LEU	2.4
1	A	266	ASN	2.4
1	B	206	ARG	2.4
1	B	223	HIS	2.4
1	C	315	ILE	2.3
1	C	206	ARG	2.3
1	A	162	GLN	2.3
1	B	171	ALA	2.2
1	B	282	LEU	2.1
1	C	187	TYR	2.1
1	C	211	GLY	2.1
1	A	231	PRO	2.1
1	C	176	SER	2.1
1	B	251	SER	2.1
1	C	241	VAL	2.1
1	B	283	ARG	2.0
1	B	288	ILE	2.0
1	A	227	SER	2.0
1	A	278	GLY	2.0
1	B	213	TYR	2.0
1	C	216	TYR	2.0
1	A	235	LEU	2.0
1	B	309	ALA	2.0
1	A	309	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.