



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:49 PM UTC

PDB ID : 1S55 / pdb_00001s55
Title : Mouse RANKL Structure at 1.9A Resolution
Authors : Teale, M.J.; Feug, X.; Chen, L.; Bice, T.; Meehan, E.J.
Deposited on : 2004-01-19
Resolution : 1.90 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
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

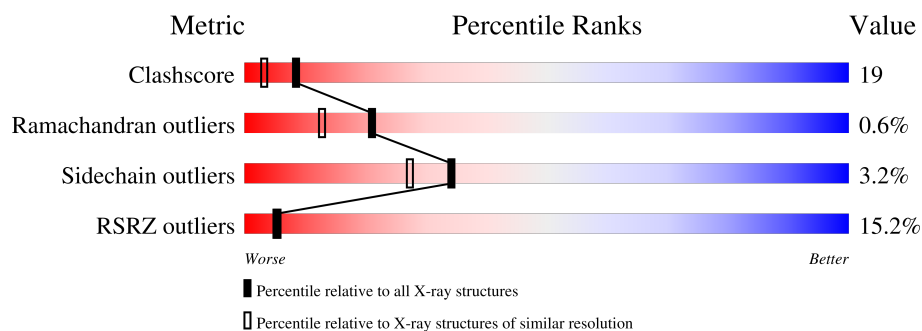
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	156	
1	B	156	
1	C	156	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3917 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 Tumor necrosis factor ligand superfamily member 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	0	0
			1233	787	210	232	4			
1	B	156	Total	C	N	O	S	0	0	0
			1233	787	210	232	4			
1	C	156	Total	C	N	O	S	0	0	0
			1233	787	210	232	4			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cl	0	0
			2	2		
2	B	1	Total	Cl	0	0
			1	1		

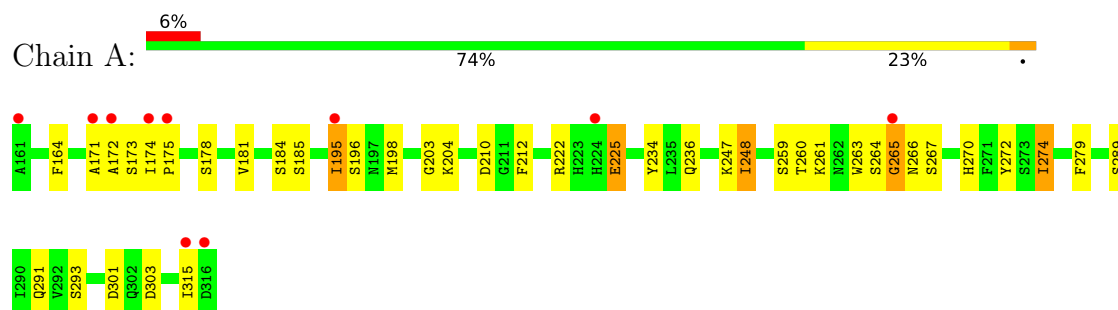
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	110	Total	O	0	0
			110	110		
3	B	45	Total	O	0	0
			45	45		
3	C	60	Total	O	0	0
			60	60		

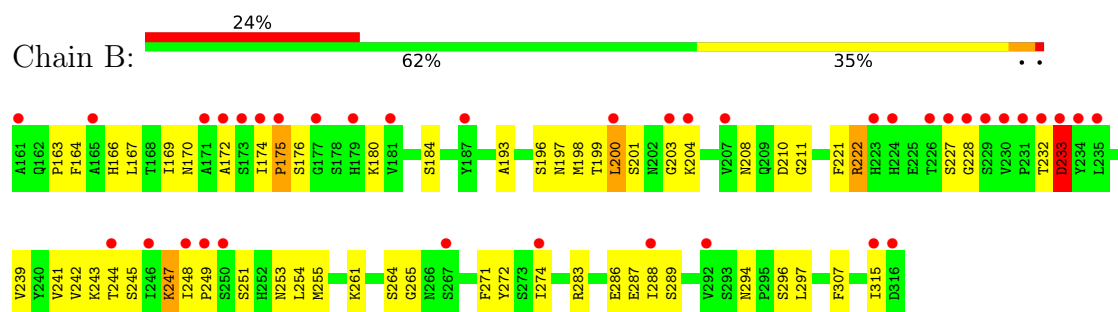
3 Residue-property plots [i](#)

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.

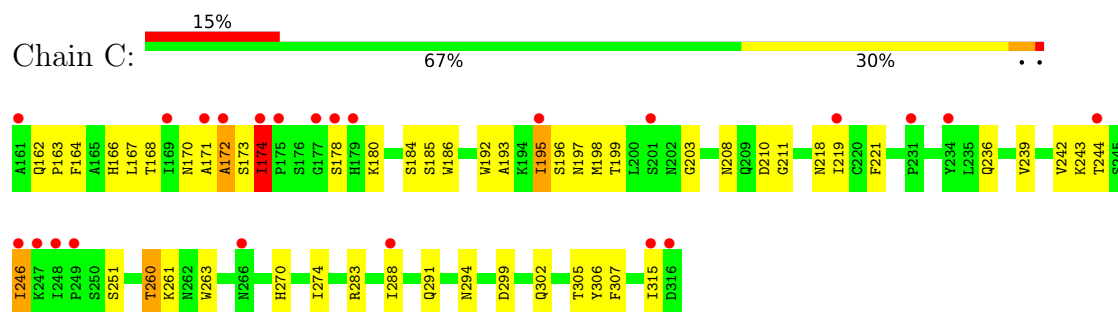
- Molecule 1: Tumor necrosis factor ligand superfamily member 11



- Molecule 1: Tumor necrosis factor ligand superfamily member 11



- Molecule 1: Tumor necrosis factor ligand superfamily member 11



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.53Å 81.32Å 99.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.43 – 1.90 45.43 – 1.90	Depositor EDS
% Data completeness (in resolution range)	83.9 (45.43-1.90) 91.6 (45.43-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 1.89Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.230 , 0.252 0.222 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3917	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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:
CL

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	0.45	0/1268	0.92	1/1718 (0.1%)
1	B	0.40	0/1268	0.87	5/1718 (0.3%)
1	C	0.37	0/1268	0.84	3/1718 (0.2%)
All	All	0.41	0/3804	0.88	9/5154 (0.2%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	LYS	N-CA-C	-9.39	98.42	110.53
1	B	228	GLY	N-CA-C	7.74	123.50	112.81
1	B	233	ASP	N-CA-C	-7.43	103.05	112.93
1	A	293	SER	N-CA-C	-5.72	101.99	110.46
1	B	227	SER	N-CA-C	-5.58	98.82	108.52
1	C	260	THR	N-CA-C	-5.54	101.44	110.20
1	C	299	ASP	N-CA-C	-5.18	103.13	109.65
1	B	232	THR	N-CA-C	-5.16	99.81	110.80
1	C	174	ILE	CB-CG1-CD1	5.14	124.61	113.80

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	53	0
1	C	1233	0	1182	54	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	110	0	0	4	0
3	B	45	0	0	2	0
3	C	60	0	0	1	0
All	All	3917	0	3546	138	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 19.

All (138) 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:261:LYS:NZ	1:C:261:LYS:HZ3	1.46	1.12
1:A:195:ILE:HD11	1:A:198:MET:HB2	1.39	1.04
1:A:261:LYS:HZ1	1:C:261:LYS:HZ3	1.15	0.93
1:C:246:ILE:HD13	1:C:246:ILE:H	1.36	0.86
1:C:210:ASP:HB3	1:C:315:ILE:HD12	1.59	0.84
1:A:195:ILE:HD13	1:A:196:SER:N	1.94	0.82
1:C:174:ILE:HD13	1:C:174:ILE:O	1.81	0.81
1:C:171:ALA:HA	1:C:174:ILE:HG23	1.63	0.81
1:B:163:PRO:HB3	1:B:197:ASN:HB3	1.65	0.79
1:C:195:ILE:HD11	1:C:198:MET:HB2	1.65	0.77
1:A:195:ILE:HD11	1:A:198:MET:CB	2.17	0.73
1:B:176:SER:HA	1:B:296:SER:HB3	1.69	0.73
1:A:248:ILE:H	1:A:248:ILE:HD13	1.54	0.71
1:A:261:LYS:NZ	1:C:261:LYS:NZ	2.34	0.71
1:C:199:THR:HG23	1:C:208:ASN:HD21	1.55	0.71
1:A:247:LYS:HE2	3:A:409:HOH:O	1.90	0.70
1:C:195:ILE:HD13	1:C:196:SER:H	1.56	0.69
1:C:174:ILE:HD12	1:C:174:ILE:H	1.58	0.69
1:A:261:LYS:HZ3	1:C:261:LYS:HZ3	1.40	0.68
1:B:233:ASP:HA	1:B:264:SER:HB3	1.77	0.65
1:A:195:ILE:CD1	1:A:198:MET:HB2	2.23	0.65
1:A:195:ILE:HD13	1:A:196:SER:H	1.61	0.65
1:C:174:ILE:HD12	1:C:174:ILE:N	2.12	0.65
1:C:242:VAL:HG11	1:C:251:SER:HB3	1.79	0.65
1:B:170:ASN:HD21	1:B:172:ALA:HB2	1.61	0.64
1:C:195:ILE:CD1	1:C:198:MET:HB2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ASP:OD2	1:B:283:ARG:HG3	2.00	0.61
1:C:219:ILE:HD13	1:C:239:VAL:HG21	1.82	0.61
1:C:246:ILE:H	1:C:246:ILE:CD1	2.01	0.61
1:B:211:GLY:HA2	1:B:315:ILE:HG13	1.83	0.60
1:A:261:LYS:HZ1	1:B:261:LYS:HZ1	1.47	0.60
1:B:199:THR:HG23	1:B:208:ASN:HD21	1.66	0.60
1:C:184:SER:HA	1:C:203:GLY:HA3	1.83	0.60
1:C:170:ASN:HB3	1:C:185:SER:OG	2.01	0.60
1:B:174:ILE:N	1:B:175:PRO:HD3	2.17	0.59
1:B:242:VAL:HG11	1:B:251:SER:HB3	1.85	0.59
1:A:210:ASP:HB3	1:A:315:ILE:HD12	1.84	0.59
1:A:261:LYS:NZ	1:B:261:LYS:NZ	2.50	0.58
1:C:236:GLN:HG2	1:C:260:THR:HG22	1.85	0.58
1:C:195:ILE:HD13	1:C:196:SER:N	2.19	0.57
1:B:294:ASN:HB3	1:B:297:LEU:HD12	1.87	0.57
1:C:174:ILE:N	1:C:174:ILE:CD1	2.67	0.57
1:A:181:VAL:HG12	3:A:388:HOH:O	2.05	0.55
1:C:180:LYS:HE2	1:C:291:GLN:OE1	2.06	0.55
1:A:204:LYS:HG2	1:A:289:SER:HB3	1.89	0.55
1:B:210:ASP:HB3	1:B:315:ILE:HD12	1.89	0.55
1:A:171:ALA:HA	1:A:174:ILE:CD1	2.37	0.55
1:C:163:PRO:HG3	1:C:197:ASN:CG	2.32	0.54
1:C:246:ILE:HD13	1:C:246:ILE:N	2.16	0.54
1:A:184:SER:HA	1:A:203:GLY:HA3	1.89	0.54
1:A:274:ILE:N	1:A:274:ILE:HD12	2.23	0.53
1:C:171:ALA:C	1:C:173:SER:H	2.17	0.53
1:B:245:SER:HB3	1:B:248:ILE:HG23	1.90	0.53
1:A:261:LYS:HZ1	1:C:261:LYS:NZ	1.99	0.53
1:B:243:LYS:HB2	1:B:254:LEU:HD11	1.92	0.52
1:B:261:LYS:NZ	1:C:261:LYS:NZ	2.58	0.52
1:A:259:SER:HB3	1:B:272:TYR:HA	1.92	0.52
1:B:222:ARG:HH11	1:B:222:ARG:HG3	1.76	0.51
1:B:204:LYS:HD3	1:B:289:SER:HB3	1.92	0.51
1:C:174:ILE:H	1:C:174:ILE:CD1	2.24	0.51
1:A:171:ALA:HA	1:A:174:ILE:HD12	1.93	0.50
1:C:178:SER:HA	1:C:294:ASN:HA	1.93	0.50
1:C:211:GLY:HA2	1:C:315:ILE:HG13	1.94	0.50
1:C:244:THR:HG22	3:C:331:HOH:O	2.12	0.50
1:B:174:ILE:HG13	1:B:174:ILE:O	2.11	0.50
1:B:170:ASN:ND2	1:B:172:ALA:HB2	2.26	0.50
1:C:166:HIS:O	1:C:193:ALA:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:LYS:O	1:B:248:ILE:C	2.55	0.49
1:B:199:THR:HG23	1:B:208:ASN:ND2	2.28	0.49
1:B:167:LEU:HD12	1:B:307:PHE:CZ	2.48	0.49
1:B:241:VAL:HG21	1:B:255:MET:HE3	1.95	0.49
1:B:265:GLY:HA3	3:B:329:HOH:O	2.13	0.49
1:B:283:ARG:HG3	1:B:283:ARG:HH11	1.78	0.49
1:C:167:LEU:HD12	1:C:307:PHE:CE2	2.48	0.49
1:B:288:ILE:N	1:B:288:ILE:HD12	2.27	0.48
1:A:261:LYS:NZ	1:B:261:LYS:HZ1	2.10	0.48
1:C:288:ILE:HD12	1:C:288:ILE:N	2.28	0.48
1:B:184:SER:HA	1:B:203:GLY:HA3	1.95	0.48
1:A:171:ALA:O	1:A:172:ALA:C	2.55	0.48
1:A:259:SER:HB2	1:B:271:PHE:O	2.14	0.47
1:B:287:GLU:C	1:B:288:ILE:HD12	2.39	0.47
1:A:236:GLN:HG2	1:A:260:THR:HG22	1.96	0.47
1:A:173:SER:HB2	1:A:185:SER:OG	2.14	0.47
1:B:261:LYS:HZ1	1:C:261:LYS:NZ	2.13	0.47
1:C:186:TRP:CD1	1:C:203:GLY:HA2	2.50	0.47
1:C:170:ASN:OD1	1:C:172:ALA:HB3	2.15	0.47
1:B:221:PHE:HE1	1:B:274:ILE:HD12	1.79	0.47
1:C:168:THR:HG21	1:C:302:GLN:HB2	1.98	0.46
1:A:266:ASN:HB3	1:A:267:SER:H	1.59	0.46
1:A:173:SER:O	1:A:174:ILE:HG13	2.15	0.46
1:C:167:LEU:HD12	1:C:307:PHE:CZ	2.51	0.46
1:B:248:ILE:HG12	1:B:248:ILE:O	2.16	0.46
1:C:164:PHE:C	1:C:164:PHE:CD1	2.94	0.46
1:A:234:TYR:CE2	1:A:260:THR:HB	2.51	0.45
1:A:301:ASP:HB3	1:A:303:ASP:OD1	2.16	0.45
1:B:222:ARG:HG3	1:B:222:ARG:NH1	2.31	0.45
1:C:195:ILE:HD12	1:C:198:MET:O	2.15	0.45
1:A:225:GLU:OE1	1:A:225:GLU:HA	2.16	0.45
1:C:196:SER:C	1:C:198:MET:H	2.23	0.45
1:B:244:THR:HG22	3:B:352:HOH:O	2.16	0.45
1:B:170:ASN:C	1:B:172:ALA:H	2.25	0.45
1:A:272:TYR:CE2	1:A:274:ILE:HG13	2.52	0.44
1:B:242:VAL:HG12	1:B:243:LYS:N	2.32	0.44
1:C:221:PHE:HE1	1:C:274:ILE:HD12	1.83	0.44
1:B:248:ILE:N	1:B:249:PRO:CD	2.80	0.44
1:A:181:VAL:O	1:A:291:GLN:HA	2.18	0.44
1:B:174:ILE:O	1:B:174:ILE:HG23	2.18	0.44
1:B:196:SER:C	1:B:198:MET:H	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:TRP:HD1	1:C:203:GLY:HA2	1.82	0.43
1:C:306:TYR:CD1	1:C:306:TYR:C	2.97	0.43
1:A:195:ILE:HD11	1:A:198:MET:C	2.44	0.43
1:B:239:VAL:HG12	1:B:274:ILE:HG21	2.00	0.43
1:A:178:SER:HA	3:A:393:HOH:O	2.19	0.43
1:A:248:ILE:HD13	1:A:248:ILE:N	2.30	0.42
1:A:212:PHE:HE1	1:A:315:ILE:HA	1.84	0.42
1:B:254:LEU:HD23	1:C:192:TRP:CE2	2.54	0.42
1:B:242:VAL:HG22	1:B:253:ASN:OD1	2.19	0.42
1:B:261:LYS:NZ	1:C:261:LYS:HZ3	2.18	0.42
1:A:178:SER:HB2	3:A:350:HOH:O	2.19	0.42
1:A:164:PHE:C	1:A:164:PHE:CD1	2.98	0.42
1:A:212:PHE:CE1	1:A:315:ILE:HA	2.55	0.42
1:A:212:PHE:HB3	1:A:279:PHE:CZ	2.55	0.42
1:B:211:GLY:CA	1:B:315:ILE:HG13	2.50	0.42
1:C:283:ARG:HG3	1:C:283:ARG:HH11	1.85	0.42
1:C:218:ASN:O	1:C:305:THR:HA	2.20	0.42
1:B:245:SER:HB2	1:B:286:GLU:HG2	2.02	0.41
1:C:263:TRP:CE2	1:C:270:HIS:HB3	2.55	0.41
1:C:242:VAL:HG12	1:C:243:LYS:N	2.36	0.41
1:B:166:HIS:O	1:B:193:ALA:HA	2.21	0.41
1:B:170:ASN:ND2	1:B:172:ALA:H	2.18	0.41
1:A:175:PRO:HG2	1:A:181:VAL:HG21	2.03	0.41
1:A:264:SER:O	1:A:265:GLY:C	2.64	0.41
1:B:261:LYS:HZ1	1:C:261:LYS:HZ3	1.66	0.41
1:A:195:ILE:HD11	1:A:198:MET:CA	2.50	0.41
1:A:263:TRP:CD2	1:A:270:HIS:HB3	2.56	0.41
1:B:200:LEU:HD23	1:B:201:SER:N	2.37	0.40
1:B:164:PHE:CD1	1:B:164:PHE:C	2.99	0.40
1:C:162:GLN:HA	1:C:163:PRO:HD3	1.90	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	154/156 (99%)	149 (97%)	4 (3%)	1 (1%)	21	13
1	B	154/156 (99%)	142 (92%)	11 (7%)	1 (1%)	21	13
1	C	154/156 (99%)	144 (94%)	9 (6%)	1 (1%)	21	13
All	All	462/468 (99%)	435 (94%)	24 (5%)	3 (1%)	21	13

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	265	GLY
1	C	172	ALA
1	B	175	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	135/135 (100%)	130 (96%)	5 (4%)	30	22
1	B	135/135 (100%)	130 (96%)	5 (4%)	30	22
1	C	135/135 (100%)	132 (98%)	3 (2%)	45	42
All	All	405/405 (100%)	392 (97%)	13 (3%)	34	27

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	ILE
1	A	222	ARG
1	A	225	GLU
1	A	248	ILE
1	A	274	ILE
1	B	169	ILE
1	B	180	LYS

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Mol	Chain	Res	Type
1	B	200	LEU
1	B	222	ARG
1	B	233	ASP
1	C	174	ILE
1	C	195	ILE
1	C	246	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	GLN
1	A	236	GLN
1	B	170	ASN
1	B	208	ASN
1	B	209	GLN
1	B	294	ASN
1	B	313	GLN
1	C	197	ASN
1	C	252	HIS
1	C	262	ASN
1	C	275	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	156/156 (100%)	0.44	10 (6%)	25 27	23, 35, 65, 75	0
1	B	156/156 (100%)	1.44	38 (24%)	2 1	31, 57, 90, 102	0
1	C	156/156 (100%)	1.08	23 (14%)	6 6	27, 48, 74, 86	0
All	All	468/468 (100%)	0.99	71 (15%)	5 5	23, 46, 82, 102	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	172	ALA	5.5
1	C	174	ILE	5.5
1	B	248	ILE	5.0
1	B	234	TYR	4.5
1	B	226	THR	4.4
1	A	161	ALA	4.4
1	B	161	ALA	4.3
1	B	230	VAL	4.3
1	C	248	ILE	4.0
1	C	172	ALA	3.8
1	A	174	ILE	3.7
1	B	174	ILE	3.7
1	B	175	PRO	3.6
1	C	266	ASN	3.6
1	B	315	ILE	3.6
1	B	249	PRO	3.5
1	A	316	ASP	3.4
1	C	161	ALA	3.4
1	B	288	ILE	3.4
1	B	171	ALA	3.3
1	C	316	ASP	3.2
1	B	177	GLY	3.2
1	A	175	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	207	VAL	3.1
1	B	165	ALA	3.0
1	B	203	GLY	3.0
1	B	229	SER	2.9
1	B	232	THR	2.9
1	C	175	PRO	2.8
1	B	173	SER	2.8
1	C	177	GLY	2.8
1	B	246	ILE	2.7
1	B	227	SER	2.7
1	B	233	ASP	2.7
1	B	200	LEU	2.7
1	C	178	SER	2.7
1	A	315	ILE	2.7
1	C	246	ILE	2.6
1	B	267	SER	2.6
1	C	201	SER	2.5
1	B	244	THR	2.5
1	B	250	SER	2.5
1	C	195	ILE	2.5
1	C	219	ILE	2.4
1	C	315	ILE	2.4
1	B	235	LEU	2.4
1	B	179	HIS	2.4
1	B	187	TYR	2.3
1	A	195	ILE	2.3
1	B	231	PRO	2.3
1	A	265	GLY	2.3
1	C	171	ALA	2.3
1	C	247	LYS	2.3
1	C	288	ILE	2.3
1	A	224	HIS	2.3
1	B	224	HIS	2.3
1	C	234	TYR	2.2
1	C	169	ILE	2.2
1	B	316	ASP	2.2
1	B	181	VAL	2.2
1	B	228	GLY	2.2
1	C	179	HIS	2.1
1	A	172	ALA	2.1
1	C	244	THR	2.1
1	B	292	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	231	PRO	2.1
1	A	171	ALA	2.1
1	C	249	PRO	2.0
1	B	204	LYS	2.0
1	B	223	HIS	2.0
1	B	274	ILE	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
2	CL	B	317	1/1	0.94	0.09	61,61,61,61	0
2	CL	A	317	1/1	0.98	0.05	33,33,33,33	0
2	CL	A	318	1/1	0.99	0.04	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.