



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 09:55 PM EDT

PDB ID : 1ETE / pdb_00001ete
Title : CRYSTAL STRUCTURE OF THE FLT3 LIGAND
Authors : Savvides, S.N.; Boone, T.; Karplus, P.A.
Deposited on : 2000-04-12
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	:	4-5-2 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

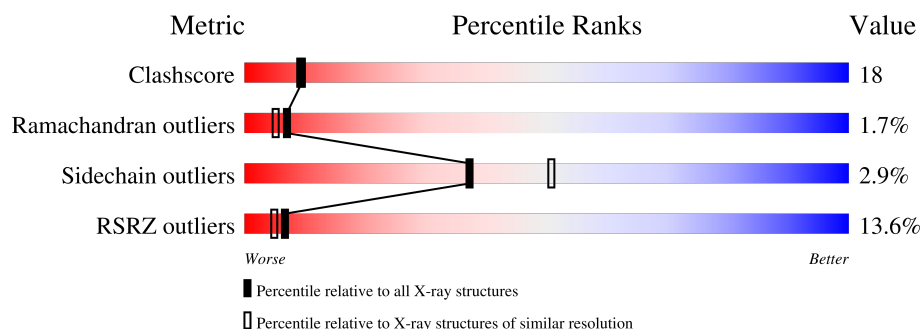
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 $\leq 5\%$. 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	134	65% 31% .
1	B	134	66% 33% .
1	C	134	4% 65% 31% ..
1	D	134	47% 46% 47% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4494 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 FLT3 LIGAND.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	134	Total	C	N	O	S	0	0	0
			1082	683	190	201	8			
1	B	134	Total	C	N	O	S	0	0	0
			1082	683	190	201	8			
1	C	131	Total	C	N	O	S	0	0	0
			1058	669	186	195	8			
1	D	130	Total	C	N	O	S	0	0	0
			1049	664	184	193	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	ASP	GLU	conflict	UNP P49771
B	41	ASP	GLU	conflict	UNP P49771
C	41	ASP	GLU	conflict	UNP P49771
D	41	ASP	GLU	conflict	UNP P49771

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	3	Total	Zn	0	0
			3	3		
2	C	2	Total	Zn	0	0
			2	2		
2	D	1	Total	Zn	0	0
			1	1		

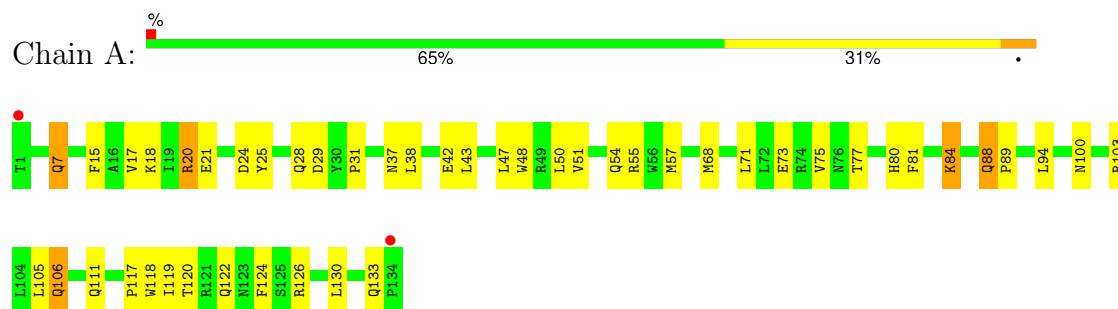
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	85	Total 85	O 85	0	0
3	B	81	Total 81	O 81	0	0
3	C	44	Total 44	O 44	0	0
3	D	4	Total 4	O 4	0	0

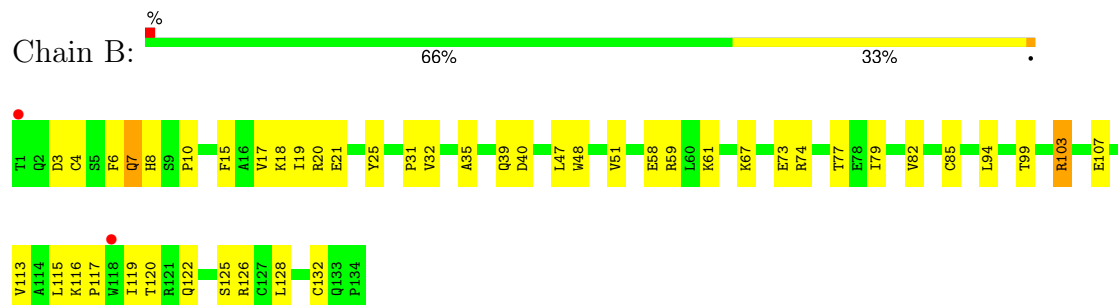
3 Residue-property plots [i](#)

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.

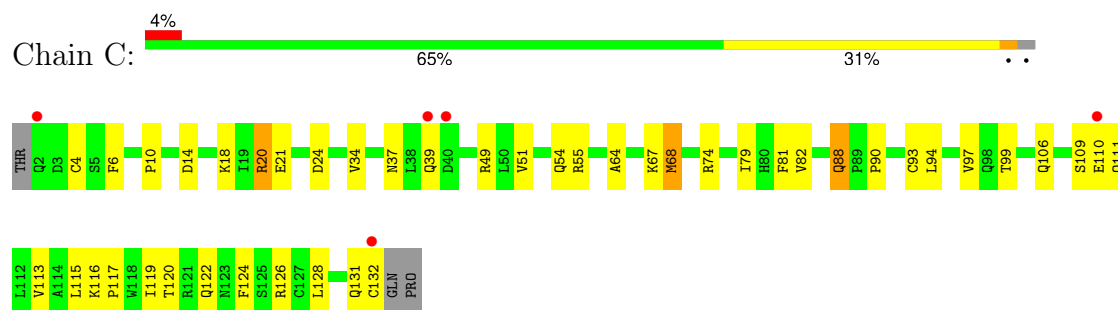
• Molecule 1: FLT3 LIGAND



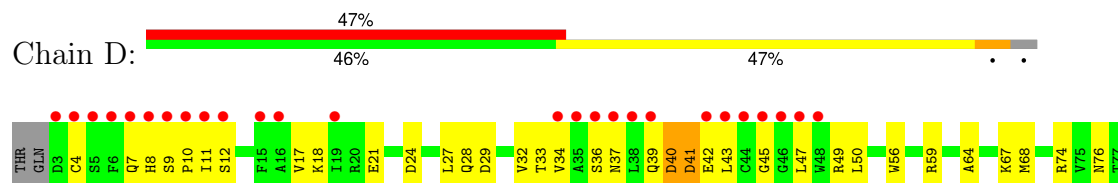
• Molecule 1: FLT3 LIGAND

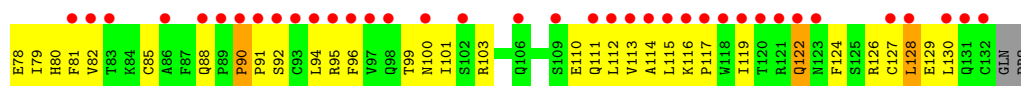


• Molecule 1: FLT3 LIGAND



• Molecule 1: FLT3 LIGAND





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	137.08Å 159.41Å 26.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.20) 94.3 (20.00-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.51 (at 2.20Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.239 , 0.287 0.248 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.659	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 67.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4494	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.49	0/1104	0.96	4/1496 (0.3%)
1	B	0.38	0/1104	0.87	1/1496 (0.1%)
1	C	0.40	0/1079	0.89	1/1462 (0.1%)
1	D	0.42	0/1070	0.93	1/1450 (0.1%)
All	All	0.42	0/4357	0.91	7/5904 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	PRO	N-CA-C	5.67	119.41	110.50
1	A	31	PRO	N-CA-C	5.52	119.27	110.21
1	A	75	VAL	N-CA-C	-5.28	104.90	112.35
1	A	133	GLN	CA-C-O	-5.19	115.31	120.66
1	D	90	PRO	N-CA-C	5.14	116.97	110.70
1	C	68	MET	N-CA-C	-5.07	105.83	111.36
1	A	84	LYS	N-CA-C	-5.04	106.40	112.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1082	0	1078	36	0
1	B	1082	0	1078	34	0
1	C	1058	0	1053	37	0
1	D	1049	0	1045	51	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
3	A	85	0	0	2	0
3	B	81	0	0	2	0
3	C	44	0	0	2	0
3	D	4	0	0	0	0
All	All	4494	0	4254	153	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 18.

All (153) 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:C:20:ARG:HH11	1:C:20:ARG:HG3	1.29	0.98
1:C:88:GLN:HE21	1:C:88:GLN:HA	1.37	0.88
1:A:106:GLN:HE21	1:A:106:GLN:HA	1.39	0.86
1:A:88:GLN:HE21	1:A:88:GLN:HA	1.38	0.86
1:C:88:GLN:HA	1:C:88:GLN:NE2	1.95	0.80
1:B:73:GLU:O	1:B:77:THR:HG23	1.84	0.77
1:C:20:ARG:HH11	1:C:20:ARG:CG	1.98	0.76
1:D:36:SER:OG	1:D:95:ARG:HB2	1.85	0.76
1:D:34:VAL:HG23	1:D:99:THR:HG21	1.69	0.74
1:B:8:HIS:O	1:B:10:PRO:HD3	1.88	0.73
1:D:100:ASN:OD1	1:D:103:ARG:HG2	1.89	0.71
1:D:79:ILE:HG22	1:D:112:LEU:HD21	1.72	0.71
1:D:122:GLN:HE21	1:D:122:GLN:HA	1.55	0.71
1:D:114:ALA:O	1:D:117:PRO:HD2	1.91	0.69
1:A:17:VAL:O	1:A:20:ARG:HG3	1.93	0.68
1:A:122:GLN:HB2	1:A:124:PHE:CZ	2.30	0.67
1:D:100:ASN:OD1	1:D:103:ARG:CG	2.42	0.67
1:A:20:ARG:HD2	1:A:21:GLU:HG3	1.77	0.66
1:A:119:ILE:HG23	1:A:120:THR:HG23	1.76	0.66
1:D:8:HIS:O	1:D:10:PRO:HD3	1.96	0.65
1:D:85:CYS:HB3	1:D:128:LEU:HD21	1.81	0.62
1:D:79:ILE:O	1:D:82:VAL:HG22	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:ILE:HG23	1:C:120:THR:HG23	1.83	0.61
1:B:18:LYS:HD3	1:B:74:ARG:HB3	1.81	0.61
1:A:88:GLN:HA	1:A:88:GLN:NE2	2.13	0.60
1:C:116:LYS:HB3	1:C:117:PRO:HD3	1.82	0.60
1:D:41:ASP:C	1:D:43:LEU:H	2.10	0.59
1:B:103:ARG:O	1:B:107:GLU:HG3	2.02	0.58
1:D:110:GLU:O	1:D:113:VAL:HG12	2.04	0.58
1:C:49:ARG:HD2	1:C:111:GLN:NE2	2.19	0.57
1:D:29:ASP:HA	1:D:100:ASN:HB2	1.87	0.57
1:D:90:PRO:HB3	1:D:94:LEU:HD23	1.86	0.56
1:A:57:MET:HE1	1:A:105:LEU:CD2	2.36	0.56
1:B:10:PRO:HG2	1:B:119:ILE:HG23	1.88	0.56
1:D:126:ARG:HD2	1:D:126:ARG:N	2.21	0.56
1:D:124:PHE:HB3	1:D:127:CYS:SG	2.46	0.55
1:A:117:PRO:HG2	1:A:118:TRP:CD1	2.41	0.54
1:B:6:PHE:O	1:B:120:THR:HA	2.07	0.54
1:C:64:ALA:HB1	1:C:68:MET:HB3	1.89	0.54
1:B:17:VAL:O	1:B:21:GLU:HG3	2.06	0.54
1:C:37:ASN:O	1:C:132:CYS:HA	2.08	0.54
1:C:90:PRO:HB3	1:C:94:LEU:HD23	1.90	0.54
1:D:56:TRP:CZ3	1:D:59:ARG:HD2	2.42	0.54
1:A:50:LEU:HG	1:A:111:GLN:HE21	1.74	0.53
1:A:57:MET:HE1	1:A:105:LEU:HD21	1.91	0.53
1:C:20:ARG:CG	1:C:20:ARG:NH1	2.66	0.52
1:C:88:GLN:HE21	1:C:88:GLN:CA	2.18	0.52
1:B:4:CYS:HB2	1:B:128:LEU:HD21	1.91	0.52
1:A:7:GLN:N	1:A:7:GLN:CD	2.68	0.52
1:C:126:ARG:HG2	3:C:6025:HOH:O	2.09	0.52
1:A:106:GLN:HA	1:A:106:GLN:NE2	2.18	0.52
1:A:47:LEU:O	1:A:51:VAL:HG23	2.10	0.51
1:D:49:ARG:HB2	1:D:111:GLN:NE2	2.25	0.51
1:A:18:LYS:N	1:A:18:LYS:HD2	2.25	0.51
1:A:54:GLN:NE2	1:A:80:HIS:CD2	2.79	0.51
1:D:122:GLN:HE21	1:D:122:GLN:CA	2.22	0.51
1:B:39:GLN:HG2	1:B:40:ASP:N	2.26	0.50
1:D:127:CYS:C	1:D:129:GLU:H	2.19	0.50
1:B:59:ARG:HG3	3:B:5051:HOH:O	2.11	0.50
1:B:32:VAL:HG23	1:B:99:THR:HG23	1.93	0.50
1:C:34:VAL:HG23	1:C:97:VAL:HG12	1.93	0.50
1:D:4:CYS:HB2	1:D:128:LEU:HD21	1.94	0.50
1:A:7:GLN:N	1:A:7:GLN:NE2	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:VAL:O	1:D:21:GLU:HG3	2.12	0.50
1:D:64:ALA:HB1	1:D:68:MET:HB3	1.93	0.50
1:C:106:GLN:O	1:C:110:GLU:HG3	2.12	0.49
1:B:126:ARG:HG2	3:B:5037:HOH:O	2.11	0.49
1:D:116:LYS:HB3	1:D:117:PRO:HD3	1.94	0.49
1:B:6:PHE:HD2	1:B:8:HIS:HE1	1.60	0.49
1:A:37:ASN:OD1	1:A:94:LEU:HD12	2.13	0.49
1:C:51:VAL:O	1:C:55:ARG:HG2	2.13	0.49
1:D:41:ASP:O	1:D:43:LEU:N	2.46	0.48
1:C:39:GLN:NE2	1:C:131:GLN:HB2	2.28	0.48
1:D:40:ASP:CG	1:D:41:ASP:H	2.21	0.48
1:B:8:HIS:C	1:B:10:PRO:HD3	2.37	0.48
1:D:8:HIS:O	1:D:8:HIS:CD2	2.66	0.48
1:B:15:PHE:O	1:B:19:ILE:HG13	2.14	0.48
1:B:58:GLU:O	1:B:61:LYS:HB2	2.13	0.47
1:A:48:TRP:CD1	1:A:130:LEU:HG	2.50	0.47
1:D:74:ARG:O	1:D:78:GLU:HG2	2.14	0.47
1:C:14:ASP:O	1:C:18:LYS:HD3	2.14	0.47
1:D:11:ILE:HG22	1:D:12:SER:N	2.30	0.47
1:D:36:SER:HG	1:D:95:ARG:HB2	1.79	0.47
1:D:91:PRO:HG3	1:D:130:LEU:O	2.15	0.47
1:B:116:LYS:HB3	1:B:117:PRO:HD3	1.97	0.47
1:A:126:ARG:HG2	3:A:4032:HOH:O	2.13	0.47
1:A:73:GLU:O	1:A:77:THR:HG23	2.15	0.46
1:B:79:ILE:O	1:B:82:VAL:HG22	2.15	0.46
1:C:39:GLN:HE21	1:C:131:GLN:HB2	1.79	0.46
1:A:24:ASP:O	1:B:67:LYS:HB2	2.15	0.46
1:C:10:PRO:HD2	1:C:119:ILE:HG21	1.96	0.46
1:D:91:PRO:HD2	1:D:94:LEU:HD22	1.97	0.46
1:B:77:THR:HG21	1:D:95:ARG:NH2	2.31	0.46
1:C:79:ILE:O	1:C:82:VAL:HG22	2.15	0.46
1:B:6:PHE:HB3	1:B:8:HIS:CE1	2.50	0.46
1:D:50:LEU:HG	1:D:111:GLN:HE21	1.79	0.46
1:B:39:GLN:HB2	1:B:132:CYS:C	2.41	0.46
1:A:51:VAL:O	1:A:55:ARG:HG2	2.17	0.45
1:A:38:LEU:HB2	3:A:4009:HOH:O	2.17	0.45
1:D:8:HIS:CD2	1:D:8:HIS:C	2.94	0.45
1:D:32:VAL:HG11	1:D:101:ILE:HD13	1.98	0.45
1:D:33:THR:HB	1:D:96:PHE:HB3	1.99	0.45
1:A:103:ARG:HA	1:A:103:ARG:HD2	1.61	0.45
1:B:48:TRP:O	1:B:51:VAL:HB	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:PRO:HB2	1:C:81:PHE:CB	2.47	0.45
1:D:47:LEU:N	1:D:115:LEU:HD11	2.32	0.45
1:B:113:VAL:O	1:B:117:PRO:HD3	2.17	0.44
1:B:3:ASP:HA	1:B:125:SER:OG	2.17	0.44
1:C:93:CYS:C	1:C:132:CYS:SG	3.00	0.44
1:D:27:LEU:O	1:D:29:ASP:N	2.51	0.44
1:A:122:GLN:HB2	1:A:124:PHE:CE1	2.52	0.44
1:D:18:LYS:HE3	1:D:74:ARG:NH2	2.32	0.44
1:D:37:ASN:ND2	1:D:95:ARG:HG3	2.33	0.44
1:B:35:ALA:HB1	1:B:94:LEU:HD11	1.99	0.44
1:C:122:GLN:HB2	1:C:124:PHE:CZ	2.53	0.44
1:C:20:ARG:HG3	1:C:20:ARG:NH1	2.11	0.44
1:A:29:ASP:HA	1:A:100:ASN:CG	2.43	0.43
1:D:81:PHE:CE1	1:D:82:VAL:HG13	2.53	0.43
1:C:109:SER:O	1:C:113:VAL:HG23	2.18	0.43
1:B:115:LEU:HG	1:B:119:ILE:HD13	2.00	0.43
1:C:4:CYS:HB2	1:C:128:LEU:HD21	1.99	0.43
1:A:54:GLN:HE21	1:A:80:HIS:CD2	2.36	0.43
1:A:88:GLN:HE21	1:A:89:PRO:HD2	1.84	0.43
1:C:67:LYS:HB2	1:D:24:ASP:O	2.19	0.43
1:B:39:GLN:HB2	1:B:132:CYS:O	2.18	0.42
1:A:20:ARG:HD3	1:A:20:ARG:C	2.44	0.42
1:D:39:GLN:HE21	1:D:39:GLN:HA	1.85	0.42
1:C:88:GLN:NE2	1:C:88:GLN:CA	2.74	0.42
1:A:106:GLN:HE21	1:A:106:GLN:CA	2.13	0.42
1:C:34:VAL:HG13	1:C:99:THR:HG21	2.00	0.42
1:D:34:VAL:HG23	1:D:99:THR:CG2	2.43	0.42
1:B:7:GLN:HE21	1:B:7:GLN:HB2	1.63	0.42
1:C:6:PHE:O	1:C:120:THR:HA	2.19	0.42
1:C:14:ASP:CG	1:C:18:LYS:NZ	2.78	0.42
1:B:6:PHE:HB3	1:B:10:PRO:HG3	2.02	0.41
1:D:76:ASN:O	1:D:80:HIS:N	2.53	0.41
1:C:14:ASP:OD1	1:C:14:ASP:C	2.63	0.41
1:D:7:GLN:NE2	1:D:7:GLN:HA	2.36	0.41
1:C:24:ASP:HB3	1:D:67:LYS:HG3	2.03	0.41
1:A:28:GLN:O	1:A:100:ASN:HB3	2.20	0.41
1:A:68:MET:HB2	1:B:25:TYR:HA	2.02	0.41
1:C:21:GLU:OE1	1:C:74:ARG:NH1	2.47	0.41
1:A:25:TYR:CD1	1:A:71:LEU:HD11	2.56	0.41
1:B:85:CYS:HB3	1:B:128:LEU:HD21	2.03	0.41
1:D:18:LYS:HE3	1:D:74:ARG:HH21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:LEU:O	1:B:51:VAL:HG23	2.20	0.40
1:D:8:HIS:HD2	1:D:10:PRO:N	2.19	0.40
1:A:81:PHE:O	1:A:84:LYS:HB2	2.21	0.40
1:C:55:ARG:NH1	3:C:6047:HOH:O	2.52	0.40
1:A:15:PHE:CD1	1:A:15:PHE:C	2.99	0.40
1:C:54:GLN:HA	1:C:79:ILE:HD11	2.03	0.40
1:D:81:PHE:CD1	1:D:81:PHE:C	2.98	0.40
1:B:20:ARG:HH11	1:B:20:ARG:HG2	1.86	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	132/134 (98%)	124 (94%)	7 (5%)	1 (1%)	16	16
1	B	132/134 (98%)	121 (92%)	11 (8%)	0	100	100
1	C	129/134 (96%)	123 (95%)	6 (5%)	0	100	100
1	D	128/134 (96%)	114 (89%)	6 (5%)	8 (6%)	1	0
All	All	521/536 (97%)	482 (92%)	30 (6%)	9 (2%)	7	5

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	28	GLN
1	D	42	GLU
1	A	42	GLU
1	D	119	ILE
1	D	128	LEU
1	D	40	ASP
1	D	41	ASP

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Mol	Chain	Res	Type
1	D	45	GLY
1	D	9	SER

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	124/124 (100%)	119 (96%)	5 (4%)	28	38
1	B	124/124 (100%)	121 (98%)	3 (2%)	43	58
1	C	121/124 (98%)	118 (98%)	3 (2%)	42	56
1	D	120/124 (97%)	117 (98%)	3 (2%)	42	56
All	All	489/496 (99%)	475 (97%)	14 (3%)	37	51

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	20	ARG
1	A	43	LEU
1	A	88	GLN
1	A	106	GLN
1	B	7	GLN
1	B	103	ARG
1	B	122	GLN
1	C	20	ARG
1	C	88	GLN
1	C	115	LEU
1	D	88	GLN
1	D	92	SER
1	D	122	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	28	GLN
1	A	39	GLN
1	A	54	GLN
1	A	88	GLN
1	A	106	GLN
1	A	111	GLN
1	A	122	GLN
1	A	133	GLN
1	B	2	GLN
1	B	7	GLN
1	B	8	HIS
1	B	100	ASN
1	B	106	GLN
1	B	122	GLN
1	B	131	GLN
1	B	133	GLN
1	C	7	GLN
1	C	39	GLN
1	C	88	GLN
1	C	98	GLN
1	C	106	GLN
1	C	111	GLN
1	C	131	GLN
1	D	7	GLN
1	D	8	HIS
1	D	39	GLN
1	D	80	HIS
1	D	106	GLN
1	D	111	GLN
1	D	122	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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 [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, 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	134/134 (100%)	0.12	2 (1%) 72 69	21, 36, 60, 71	0
1	B	134/134 (100%)	0.19	2 (1%) 72 69	20, 35, 60, 93	0
1	C	131/134 (97%)	0.20	5 (3%) 44 41	18, 36, 62, 86	0
1	D	130/134 (97%)	1.98	63 (48%) 0 0	31, 75, 99, 100	0
All	All	529/536 (98%)	0.62	72 (13%) 7 5	18, 41, 94, 100	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	35	ALA	6.1
1	D	112	LEU	5.4
1	D	132	CYS	5.1
1	D	38	LEU	4.9
1	D	96	PHE	4.5
1	D	119	ILE	4.4
1	D	118	TRP	4.4
1	D	94	LEU	4.3
1	D	113	VAL	4.1
1	D	130	LEU	4.1
1	D	114	ALA	4.1
1	D	90	PRO	3.8
1	D	34	VAL	3.7
1	D	10	PRO	3.7
1	D	11	ILE	3.6
1	D	6	PHE	3.5
1	D	89	PRO	3.5
1	D	120	THR	3.5
1	D	92	SER	3.4
1	D	8	HIS	3.4
1	D	44	CYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	91	PRO	3.3
1	B	1	THR	3.3
1	D	43	LEU	3.2
1	D	45	GLY	3.2
1	D	97	VAL	3.2
1	D	9	SER	3.1
1	D	81	PHE	3.1
1	D	82	VAL	3.0
1	A	1	THR	2.9
1	C	40	ASP	2.9
1	D	4	CYS	2.9
1	D	93	CYS	2.8
1	D	36	SER	2.8
1	D	5	SER	2.7
1	D	102	SER	2.7
1	D	117	PRO	2.7
1	D	48	TRP	2.7
1	D	109	SER	2.6
1	D	128	LEU	2.6
1	D	12	SER	2.6
1	D	115	LEU	2.6
1	D	15	PHE	2.6
1	A	134	PRO	2.5
1	D	98	GLN	2.5
1	D	39	GLN	2.5
1	D	46	GLY	2.4
1	D	106	GLN	2.4
1	D	111	GLN	2.4
1	D	95	ARG	2.4
1	C	2	GLN	2.4
1	D	3	ASP	2.3
1	D	100	ASN	2.3
1	D	122	GLN	2.3
1	C	132	CYS	2.3
1	D	127	CYS	2.3
1	B	118	TRP	2.3
1	D	86	ALA	2.3
1	C	39	GLN	2.2
1	D	47	LEU	2.2
1	D	88	GLN	2.2
1	C	110	GLU	2.2
1	D	7	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	16	ALA	2.2
1	D	37	ASN	2.1
1	D	83	THR	2.1
1	D	42	GLU	2.1
1	D	116	LYS	2.1
1	D	123	ASN	2.1
1	D	131	GLN	2.0
1	D	19	ILE	2.0
1	D	121	ARG	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($\text{\AA}^2$)	Q<0.9
2	ZN	A	137	1/1	0.84	0.10	100,100,100,100	0
2	ZN	D	3135	1/1	0.85	0.10	82,82,82,82	0
2	ZN	A	136	1/1	0.92	0.06	69,69,69,69	0
2	ZN	C	2135	1/1	0.93	0.09	63,63,63,63	0
2	ZN	B	1136	1/1	0.96	0.05	65,65,65,65	0
2	ZN	A	135	1/1	0.96	0.06	54,54,54,54	0
2	ZN	B	1135	1/1	0.96	0.07	63,63,63,63	0
2	ZN	C	2136	1/1	0.97	0.05	40,40,40,40	0
2	ZN	B	1137	1/1	0.98	0.04	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.