



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:10 AM UTC

PDB ID : 2V4H / pdb_00002v4h
Title : NEMO CC2-LZ domain - 1D5 DARPin complex
Authors : Grubisha, O.; Duquerroy, S.; Cordier, F.; Haouz, A.; Delepierre, M.; Veron, M.; Agou, F.
Deposited on : 2008-09-22
Resolution : 2.90 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

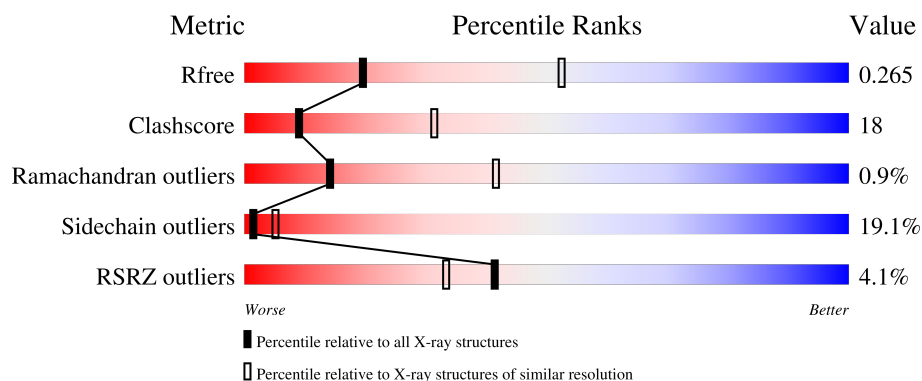
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	110	
1	B	110	
2	C	136	
2	D	136	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3542 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 NF-KAPPA-B ESSENTIAL MODULATOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	98	Total	C	N	O	S	0	0	0
			808	505	144	156	3			
1	B	91	Total	C	N	O	S	0	0	0
			761	476	134	148	3			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	MET	-	expression tag	UNP O88522
A	229	GLY	-	expression tag	UNP O88522
A	230	SER	-	expression tag	UNP O88522
A	231	SER	-	expression tag	UNP O88522
A	232	HIS	-	expression tag	UNP O88522
A	233	HIS	-	expression tag	UNP O88522
A	234	HIS	-	expression tag	UNP O88522
A	235	HIS	-	expression tag	UNP O88522
A	236	HIS	-	expression tag	UNP O88522
A	237	HIS	-	expression tag	UNP O88522
A	238	SER	-	expression tag	UNP O88522
A	239	SER	-	expression tag	UNP O88522
A	240	GLY	-	expression tag	UNP O88522
A	241	LEU	-	expression tag	UNP O88522
A	242	VAL	-	expression tag	UNP O88522
A	243	PRO	-	expression tag	UNP O88522
A	244	ARG	-	expression tag	UNP O88522
A	245	GLY	-	expression tag	UNP O88522
A	246	SER	-	expression tag	UNP O88522
A	247	HIS	-	expression tag	UNP O88522
A	248	MET	-	expression tag	UNP O88522
A	249	ALA	-	expression tag	UNP O88522
A	250	SER	-	expression tag	UNP O88522
B	228	MET	-	expression tag	UNP O88522
B	229	GLY	-	expression tag	UNP O88522

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Chain	Residue	Modelled	Actual	Comment	Reference
B	230	SER	-	expression tag	UNP O88522
B	231	SER	-	expression tag	UNP O88522
B	232	HIS	-	expression tag	UNP O88522
B	233	HIS	-	expression tag	UNP O88522
B	234	HIS	-	expression tag	UNP O88522
B	235	HIS	-	expression tag	UNP O88522
B	236	HIS	-	expression tag	UNP O88522
B	237	HIS	-	expression tag	UNP O88522
B	238	SER	-	expression tag	UNP O88522
B	239	SER	-	expression tag	UNP O88522
B	240	GLY	-	expression tag	UNP O88522
B	241	LEU	-	expression tag	UNP O88522
B	242	VAL	-	expression tag	UNP O88522
B	243	PRO	-	expression tag	UNP O88522
B	244	ARG	-	expression tag	UNP O88522
B	245	GLY	-	expression tag	UNP O88522
B	246	SER	-	expression tag	UNP O88522
B	247	HIS	-	expression tag	UNP O88522
B	248	MET	-	expression tag	UNP O88522
B	249	ALA	-	expression tag	UNP O88522
B	250	SER	-	expression tag	UNP O88522

- Molecule 2 is a protein called 1D5 DARPIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	125	Total	C	N	O	S	0	0	0
			949	587	169	192	1			
2	D	128	Total	C	N	O	S	0	0	0
			973	601	176	195	1			

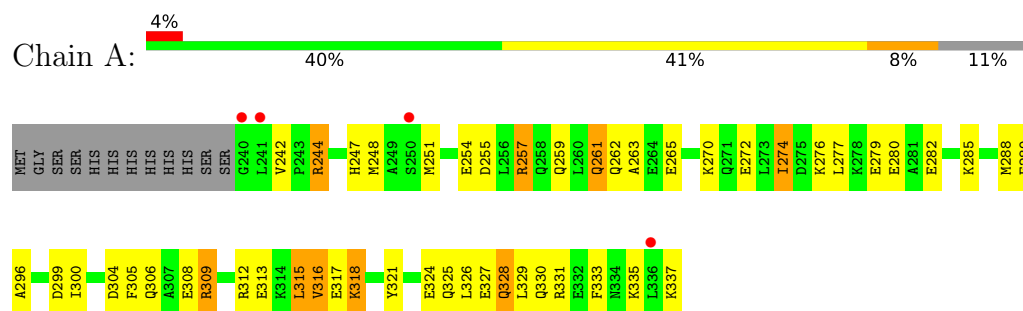
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	8	Total	O	0	0
			8	8		
3	C	14	Total	O	0	0
			14	14		
3	D	19	Total	O	0	0
			19	19		

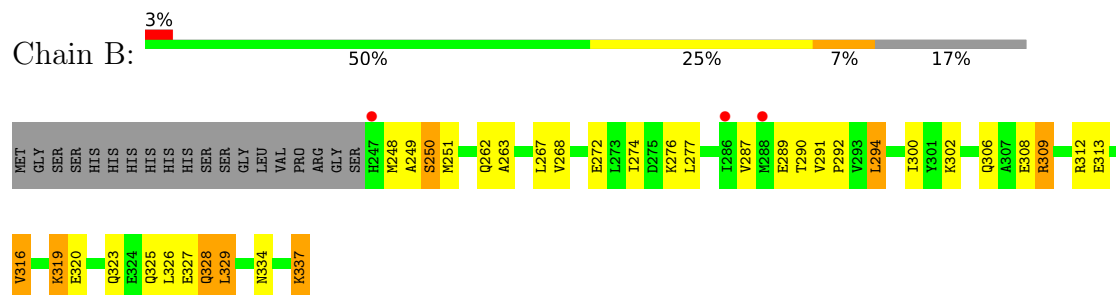
3 Residue-property plots

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.

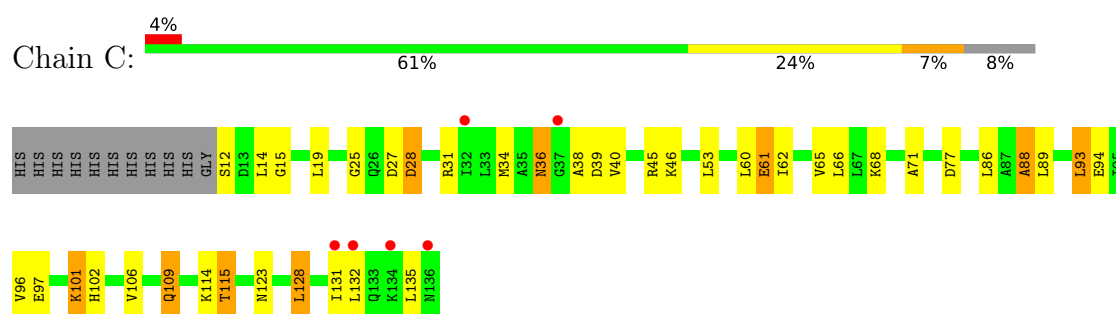
• Molecule 1: NF-KAPPA-B ESSENTIAL MODULATOR



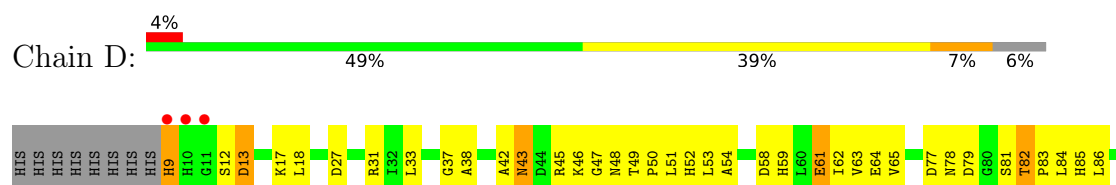
• Molecule 1: NF-KAPPA-B ESSENTIAL MODULATOR

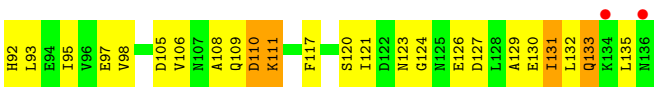


• Molecule 2: 1D5 DARPIN



• Molecule 2: 1D5 DARPIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	63.02Å 63.02Å 436.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.67 – 2.90 47.67 – 2.90	Depositor EDS
% Data completeness (in resolution range)	86.5 (47.67-2.90) 86.4 (47.67-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.208 , 0.268 0.206 , 0.265	Depositor DCC
R_{free} test set	883 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3542	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 4.01% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.95	1/816 (0.1%)	1.10	2/1088 (0.2%)
1	B	0.83	0/768	1.04	1/1023 (0.1%)
2	C	0.91	0/961	1.05	1/1299 (0.1%)
2	D	1.00	0/987	1.18	4/1334 (0.3%)
All	All	0.93	1/3532 (0.0%)	1.10	8/4744 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	315	LEU	CA-C	-5.14	1.46	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	13	ASP	N-CA-C	-8.19	100.95	113.89
2	C	88	ALA	N-CA-C	-7.45	102.76	111.03
1	A	247	HIS	N-CA-C	6.83	120.13	110.23
1	A	315	LEU	N-CA-C	-6.81	103.78	111.14
1	B	316	VAL	CB-CA-C	-6.73	103.26	111.88
2	D	82	THR	N-CA-C	-5.76	101.60	110.58
2	D	43	ASN	N-CA-C	5.61	117.55	108.34
2	D	78	ASN	N-CA-C	5.28	117.78	111.71

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	808	0	824	44	0
1	B	761	0	773	33	0
2	C	949	0	924	32	0
2	D	973	0	941	35	0
3	A	10	0	0	1	0
3	B	8	0	0	0	0
3	C	14	0	0	3	0
3	D	19	0	0	3	0
All	All	3542	0	3462	128	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 (128) 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:319:LYS:NZ	1:B:323:GLN:HE21	1.46	1.13
1:A:251:MET:O	1:A:255:ASP:HB2	1.65	0.96
1:B:319:LYS:HZ2	1:B:323:GLN:HE21	0.98	0.95
1:A:244:ARG:HA	1:A:259:GLN:HE22	1.35	0.89
2:C:101:LYS:HD2	3:C:2009:HOH:O	1.73	0.88
2:C:14:LEU:HB3	2:C:38:ALA:HB2	1.56	0.85
1:A:327:GLU:O	1:A:331:ARG:HB2	1.78	0.84
1:A:328:GLN:NE2	1:A:328:GLN:HA	1.92	0.83
1:A:308:GLU:OE1	1:B:309:ARG:HD3	1.79	0.82
2:D:61:GLU:CD	2:D:61:GLU:H	1.90	0.79
2:C:101:LYS:HG2	2:C:102:HIS:CD2	2.18	0.79
1:B:302:LYS:HG2	1:B:306:GLN:NE2	1.97	0.78
1:B:319:LYS:HZ2	1:B:323:GLN:NE2	1.80	0.78
2:C:61:GLU:H	2:C:61:GLU:CD	1.92	0.77
2:C:101:LYS:HG2	2:C:102:HIS:HD2	1.49	0.75
1:B:319:LYS:NZ	1:B:323:GLN:NE2	2.30	0.73
1:B:248:MET:HG2	1:B:250:SER:HB2	1.71	0.72
2:D:13:ASP:O	2:D:17:LYS:HG2	1.91	0.70
1:B:248:MET:O	1:B:251:MET:N	2.22	0.69
2:D:51:LEU:HD11	2:D:63:VAL:HG13	1.75	0.69
2:D:61:GLU:O	2:D:65:VAL:HG23	1.93	0.69
1:B:312:ARG:HE	2:D:123:ASN:ND2	1.91	0.68
2:C:34:MET:HE3	2:C:34:MET:HA	1.75	0.67
1:B:316:VAL:O	1:B:320:GLU:HG2	1.95	0.67
2:C:93:LEU:O	2:C:96:VAL:HB	1.95	0.66
1:A:308:GLU:CD	1:B:309:ARG:HH11	2.04	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ARG:HH11	1:A:257:ARG:HB2	1.63	0.64
2:D:130:GLU:HA	2:D:133:GLN:HG3	1.79	0.63
2:D:43:ASN:HA	2:D:48:ASN:O	1.98	0.63
2:D:105:ASP:HB3	2:D:108:ALA:HB2	1.80	0.62
2:D:79:ASP:O	2:D:111:LYS:HG3	2.01	0.61
2:C:96:VAL:HG21	2:C:128:LEU:HD21	1.83	0.60
2:D:9:HIS:N	2:D:12:SER:HG	2.01	0.59
1:A:308:GLU:OE1	1:B:309:ARG:NH1	2.24	0.58
2:C:128:LEU:CD1	2:C:132:LEU:HD12	2.33	0.57
1:A:333:PHE:O	1:A:337:LYS:HB3	2.04	0.57
2:C:14:LEU:HB3	2:C:38:ALA:CB	2.33	0.57
2:D:127:ASP:O	2:D:131:ILE:HG23	2.04	0.57
1:A:270:LYS:O	1:A:274:ILE:HG12	2.04	0.57
1:A:254:GLU:O	1:A:255:ASP:C	2.48	0.56
1:A:312:ARG:HE	2:C:123:ASN:ND2	2.04	0.56
2:D:49:THR:HB	2:D:50:PRO:HD2	1.87	0.55
1:B:334:ASN:O	1:B:337:LYS:HG3	2.06	0.55
1:B:302:LYS:HG2	1:B:306:GLN:HE21	1.71	0.54
2:C:128:LEU:CD1	2:C:132:LEU:CD1	2.85	0.54
2:C:128:LEU:HD12	2:C:132:LEU:HD12	1.88	0.54
1:A:288:MET:HE3	1:B:287:VAL:HG21	1.90	0.54
2:D:43:ASN:ND2	3:D:2006:HOH:O	2.40	0.53
1:A:291:VAL:HB	1:A:292:PRO:HD3	1.90	0.52
2:D:82:THR:HB	2:D:83:PRO:HD2	1.90	0.51
1:A:308:GLU:CD	1:B:309:ARG:NH1	2.68	0.51
1:A:262:GLN:HG3	1:A:263:ALA:N	2.25	0.51
2:D:58:ASP:HA	2:D:95:ILE:HD12	1.93	0.51
2:D:37:GLY:O	2:D:38:ALA:C	2.54	0.50
2:C:115:THR:HB	3:C:2010:HOH:O	2.10	0.50
2:C:28:ASP:OD2	2:C:28:ASP:N	2.45	0.49
1:A:315:LEU:O	1:A:316:VAL:C	2.53	0.49
1:A:327:GLU:HA	1:A:327:GLU:OE1	2.12	0.49
1:A:312:ARG:HD2	1:B:308:GLU:OE1	2.12	0.49
1:B:291:VAL:HB	1:B:292:PRO:HD3	1.95	0.49
2:C:36:ASN:OD1	2:C:36:ASN:N	2.46	0.49
1:B:268:VAL:O	1:B:272:GLU:HB2	2.12	0.49
1:B:302:LYS:HG2	1:B:306:GLN:HE22	1.77	0.48
1:B:312:ARG:HE	2:D:123:ASN:HD22	1.59	0.48
2:C:40:VAL:CG2	2:C:71:ALA:HB2	2.44	0.48
2:D:129:ALA:O	2:D:133:GLN:HG2	2.13	0.48
1:A:280:GLU:C	1:A:282:GLU:N	2.69	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ARG:HH21	2:C:123:ASN:ND2	2.12	0.48
2:D:120:SER:O	2:D:124:GLY:N	2.44	0.47
1:A:293:VAL:O	1:A:296:ALA:HB3	2.15	0.47
1:B:309:ARG:HG3	1:B:313:GLU:OE2	2.14	0.47
1:B:248:MET:O	1:B:249:ALA:C	2.57	0.47
2:D:45:ARG:C	2:D:47:GLY:H	2.21	0.47
1:A:274:ILE:HD13	1:B:274:ILE:HG13	1.97	0.47
2:C:14:LEU:HD23	3:C:2001:HOH:O	2.14	0.46
1:A:259:GLN:HA	1:A:262:GLN:HG2	1.97	0.46
1:A:290:THR:O	1:A:293:VAL:HB	2.16	0.46
1:A:328:GLN:HA	1:A:328:GLN:HE21	1.77	0.46
2:D:54:ALA:HB1	2:D:59:HIS:HB2	1.98	0.46
2:C:109:GLN:HA	2:C:114:LYS:O	2.16	0.45
2:D:42:ALA:O	2:D:49:THR:HA	2.16	0.45
2:C:25:GLY:HA2	2:C:62:ILE:HD13	1.98	0.45
2:D:117:PHE:HB2	3:D:2017:HOH:O	2.16	0.45
2:D:51:LEU:O	2:D:52:HIS:C	2.60	0.44
2:C:39:ASP:C	2:C:39:ASP:OD1	2.60	0.44
1:A:277:LEU:HD13	1:B:277:LEU:HB3	1.99	0.44
1:A:296:ALA:O	1:A:299:ASP:N	2.51	0.44
2:D:51:LEU:HB2	3:D:2008:HOH:O	2.17	0.44
1:A:308:GLU:OE2	1:B:309:ARG:NH1	2.51	0.44
1:A:317:GLU:O	1:A:318:LYS:C	2.61	0.44
2:D:51:LEU:HD12	2:D:51:LEU:HA	1.73	0.43
1:A:321:TYR:O	1:A:324:GLU:HB2	2.18	0.43
2:C:94:GLU:HA	2:C:97:GLU:HG3	2.01	0.43
1:A:324:GLU:HG2	3:A:2008:HOH:O	2.17	0.43
2:D:59:HIS:O	2:D:63:VAL:HG23	2.19	0.43
2:D:106:VAL:HG23	2:D:132:LEU:HD22	2.00	0.43
2:C:15:GLY:O	2:C:19:LEU:HG	2.18	0.43
2:C:61:GLU:CD	2:C:61:GLU:N	2.69	0.43
2:C:62:ILE:O	2:C:66:LEU:HG	2.19	0.43
2:D:45:ARG:C	2:D:47:GLY:N	2.77	0.43
1:A:277:LEU:HD23	1:A:277:LEU:HA	1.85	0.42
1:A:327:GLU:OE2	1:A:331:ARG:NH2	2.47	0.42
2:C:40:VAL:HG22	2:C:71:ALA:HB2	2.00	0.42
1:B:328:GLN:NE2	1:B:328:GLN:HA	2.34	0.42
2:D:110:ASP:OD1	2:D:110:ASP:C	2.63	0.42
1:A:255:ASP:O	1:A:259:GLN:HB2	2.20	0.42
2:D:61:GLU:CD	2:D:61:GLU:N	2.64	0.42
1:A:316:VAL:HG21	2:C:123:ASN:ND2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:40:VAL:HG22	2:C:40:VAL:O	2.19	0.41
2:C:88:ALA:O	2:C:89:LEU:C	2.63	0.41
1:B:323:GLN:HE22	2:D:92:HIS:HE1	1.67	0.41
1:B:263:ALA:O	1:B:267:LEU:N	2.49	0.41
1:A:326:LEU:HD23	1:A:326:LEU:HA	1.82	0.41
1:A:305:PHE:O	1:A:306:GLN:C	2.64	0.41
1:A:309:ARG:HD2	1:A:313:GLU:HG3	2.02	0.41
1:A:329:LEU:HD13	1:B:329:LEU:HB3	2.02	0.41
2:C:31:ARG:HE	2:C:65:VAL:HG21	1.86	0.41
2:D:18:LEU:HA	2:D:33:LEU:HD13	2.02	0.41
2:D:84:LEU:O	2:D:85:HIS:C	2.63	0.41
1:A:325:GLN:O	1:A:328:GLN:HB2	2.21	0.41
1:B:329:LEU:HD23	1:B:329:LEU:HA	1.62	0.40
2:D:49:THR:HB	2:D:50:PRO:CD	2.51	0.40
2:C:77:ASP:OD1	2:C:77:ASP:C	2.64	0.40
1:A:291:VAL:O	1:A:292:PRO:C	2.61	0.40
1:A:261:GLN:O	1:A:265:GLU:HG2	2.21	0.40
1:A:262:GLN:HG3	1:A:263:ALA:H	1.87	0.40
1:B:290:THR:O	1:B:294:LEU:HB2	2.21	0.40
1:B:319:LYS:O	1:B:320:GLU:C	2.64	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	96/110 (87%)	87 (91%)	9 (9%)	0	100	100
1	B	89/110 (81%)	84 (94%)	5 (6%)	0	100	100
2	C	123/136 (90%)	107 (87%)	15 (12%)	1 (1%)	16	44
2	D	126/136 (93%)	106 (84%)	17 (14%)	3 (2%)	4	18
All	All	434/492 (88%)	384 (88%)	46 (11%)	4 (1%)	14	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	93	LEU
2	D	110	ASP
2	D	46	LYS
2	D	77	ASP

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	86/97 (89%)	67 (78%)	19 (22%)	1	3
1	B	81/97 (84%)	67 (83%)	14 (17%)	2	7
2	C	99/109 (91%)	81 (82%)	18 (18%)	2	6
2	D	101/109 (93%)	82 (81%)	19 (19%)	1	5
All	All	367/412 (89%)	297 (81%)	70 (19%)	1	5

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	VAL
1	A	244	ARG
1	A	248	MET
1	A	257	ARG
1	A	261	GLN
1	A	272	GLU
1	A	274	ILE
1	A	276	LYS
1	A	279	GLU
1	A	285	LYS
1	A	289	GLU
1	A	300	ILE
1	A	304	ASP
1	A	309	ARG
1	A	316	VAL
1	A	318	LYS

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Mol	Chain	Res	Type
1	A	328	GLN
1	A	330	GLN
1	A	335	LYS
1	B	250	SER
1	B	262	GLN
1	B	276	LYS
1	B	289	GLU
1	B	294	LEU
1	B	300	ILE
1	B	309	ARG
1	B	319	LYS
1	B	325	GLN
1	B	326	LEU
1	B	327	GLU
1	B	328	GLN
1	B	329	LEU
1	B	337	LYS
2	C	12	SER
2	C	27	ASP
2	C	28	ASP
2	C	36	ASN
2	C	45	ARG
2	C	46	LYS
2	C	53	LEU
2	C	60	LEU
2	C	61	GLU
2	C	68	LYS
2	C	86	LEU
2	C	101	LYS
2	C	106	VAL
2	C	109	GLN
2	C	115	THR
2	C	128	LEU
2	C	131	ILE
2	C	135	LEU
2	D	9	HIS
2	D	27	ASP
2	D	31	ARG
2	D	53	LEU
2	D	61	GLU
2	D	62	ILE
2	D	64	GLU

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Mol	Chain	Res	Type
2	D	81	SER
2	D	86	LEU
2	D	93	LEU
2	D	97	GLU
2	D	98	VAL
2	D	109	GLN
2	D	111	LYS
2	D	121	ILE
2	D	126	GLU
2	D	131	ILE
2	D	133	GLN
2	D	135	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	259	GLN
1	A	271	GLN
1	A	328	GLN
1	B	271	GLN
1	B	283	GLN
1	B	297	GLN
1	B	306	GLN
1	B	310	HIS
1	B	323	GLN
1	B	325	GLN
1	B	328	GLN
2	C	41	ASN
2	C	59	HIS
2	C	92	HIS
2	C	102	HIS
2	C	123	ASN
2	C	125	ASN
2	D	92	HIS
2	D	109	GLN
2	D	123	ASN
2	D	136	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](#)

There are no ligands in this entry.

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	98/110 (89%)	0.25	4 (4%)	41	33	38, 54, 70, 80	0
1	B	91/110 (82%)	0.28	3 (3%)	49	40	36, 54, 68, 76	0
2	C	125/136 (91%)	0.31	6 (4%)	35	28	35, 51, 63, 74	0
2	D	128/136 (94%)	-0.26	5 (3%)	43	35	39, 50, 62, 82	0
All	All	442/492 (89%)	0.13	18 (4%)	41	33	35, 52, 66, 82	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	11	GLY	3.3
2	C	136	ASN	3.1
1	B	286	ILE	2.9
2	C	134	LYS	2.9
1	A	336	LEU	2.8
2	D	136	ASN	2.8
1	A	240	GLY	2.6
1	A	241	LEU	2.6
1	A	250	SER	2.5
1	B	288	MET	2.4
2	C	37	GLY	2.4
2	C	132	LEU	2.4
2	C	32	ILE	2.4
2	C	131	ILE	2.2
2	D	9	HIS	2.2
2	D	10	HIS	2.2
2	D	134	LYS	2.1
1	B	247	HIS	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.