



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:18 AM UTC

PDB ID : 6ERH / pdb_00006erh
Title : Complex of XLF and heterodimer Ku bound to DNA
Authors : Nemoz, C.; Legrand, P.; Ropars, V.; Charbonnier, J.B.
Deposited on : 2017-10-18
Resolution : 2.80 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

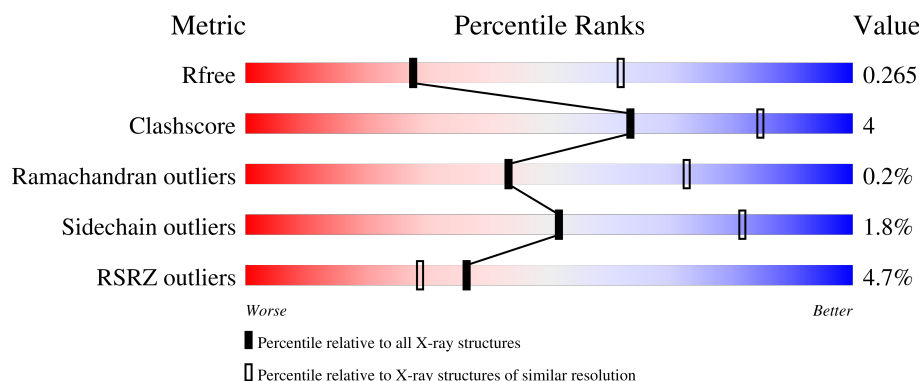
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	544	
1	C	544	
2	B	572	
2	D	572	
3	F	34	

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Mol	Chain	Length	Quality of chain
3	O	34	
4	K	21	
4	R	21	
5	M	19	
5	T	19	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18810 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 X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	0	0
			3955	2531	672	735	17			
1	C	493	Total	C	N	O	S	0	0	0
			3980	2547	677	738	18			

- Molecule 2 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	534	Total	C	N	O	S	0	0	0
			4301	2746	734	797	24			
2	D	535	Total	C	N	O	S	0	0	0
			4310	2752	736	798	24			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	MET	-	initiating methionine	UNP P13010
B	-15	HIS	-	expression tag	UNP P13010
B	-14	HIS	-	expression tag	UNP P13010
B	-13	HIS	-	expression tag	UNP P13010
B	-12	HIS	-	expression tag	UNP P13010
B	-11	HIS	-	expression tag	UNP P13010
B	-10	HIS	-	expression tag	UNP P13010
B	-9	HIS	-	expression tag	UNP P13010
B	-8	HIS	-	expression tag	UNP P13010
B	-7	HIS	-	expression tag	UNP P13010
B	-6	HIS	-	expression tag	UNP P13010
B	-5	GLU	-	expression tag	UNP P13010
B	-4	ASN	-	expression tag	UNP P13010
B	-3	LEU	-	expression tag	UNP P13010
B	-2	TYR	-	expression tag	UNP P13010
B	-1	PHE	-	expression tag	UNP P13010

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLN	-	expression tag	UNP P13010
B	1	GLY	-	expression tag	UNP P13010
D	-16	MET	-	initiating methionine	UNP P13010
D	-15	HIS	-	expression tag	UNP P13010
D	-14	HIS	-	expression tag	UNP P13010
D	-13	HIS	-	expression tag	UNP P13010
D	-12	HIS	-	expression tag	UNP P13010
D	-11	HIS	-	expression tag	UNP P13010
D	-10	HIS	-	expression tag	UNP P13010
D	-9	HIS	-	expression tag	UNP P13010
D	-8	HIS	-	expression tag	UNP P13010
D	-7	HIS	-	expression tag	UNP P13010
D	-6	HIS	-	expression tag	UNP P13010
D	-5	GLU	-	expression tag	UNP P13010
D	-4	ASN	-	expression tag	UNP P13010
D	-3	LEU	-	expression tag	UNP P13010
D	-2	TYR	-	expression tag	UNP P13010
D	-1	PHE	-	expression tag	UNP P13010
D	0	GLN	-	expression tag	UNP P13010
D	1	GLY	-	expression tag	UNP P13010

- Molecule 3 is a DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	32	Total	C	N	O	P	0	0	0
			646	309	123	183	31			
3	O	30	Total	C	N	O	P	0	0	0
			610	290	118	172	30			

- Molecule 4 is a DNA chain called DNA (21-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	21	Total	C	N	O	P	0	0	0
			431	208	71	132	20			
4	R	21	Total	C	N	O	P	0	0	0
			431	208	71	132	20			

- Molecule 5 is a protein called Non-homologous end-joining factor 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	M	7	Total	C	N	O	0	0	0
			56	37	11	8			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	T	6	Total	C	N	O	0	0	0
			47	31	9	7			

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		

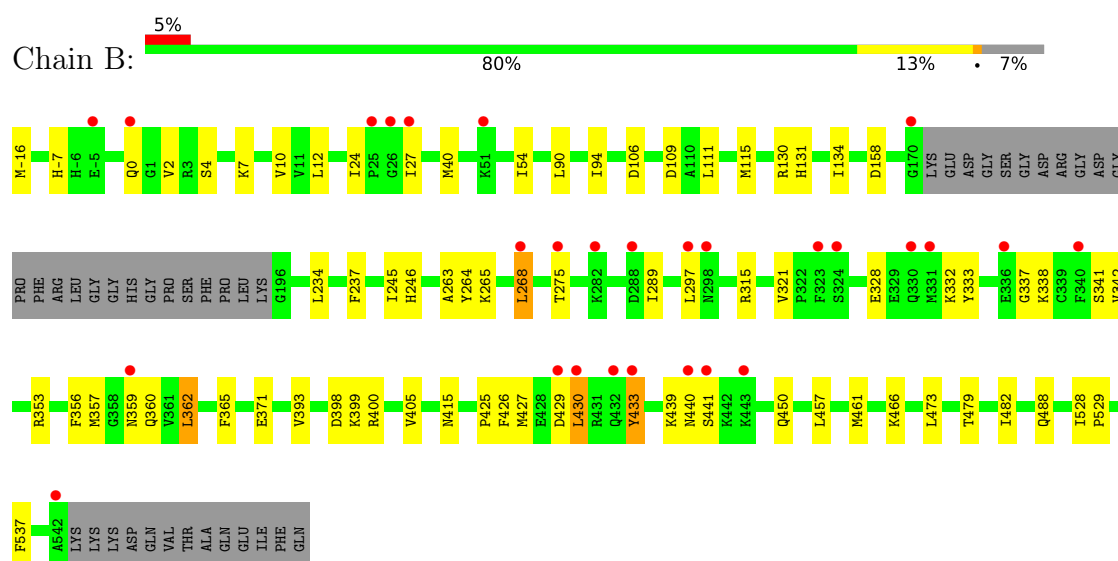
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	6	Total	O	0	0
			6	6		
7	B	5	Total	O	0	0
			5	5		
7	C	8	Total	O	0	0
			8	8		
7	D	8	Total	O	0	0
			8	8		
7	F	2	Total	O	0	0
			2	2		
7	O	2	Total	O	0	0
			2	2		

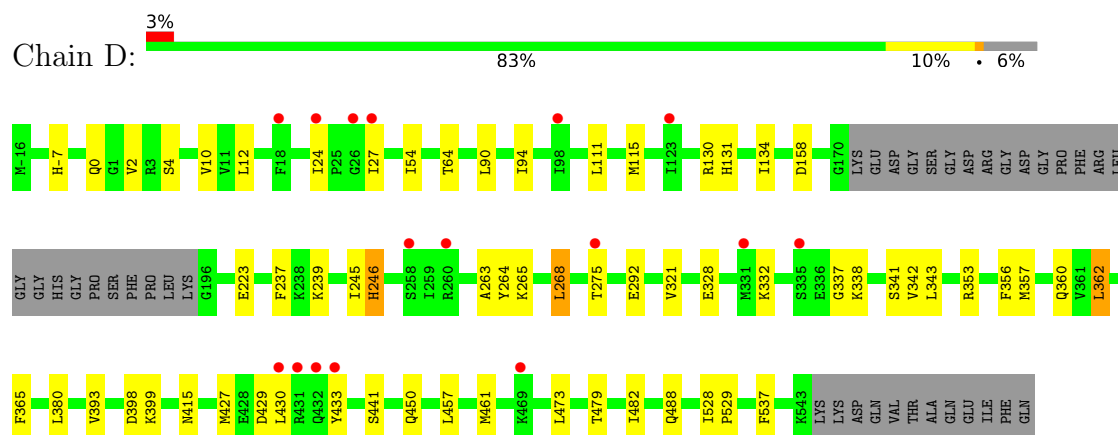
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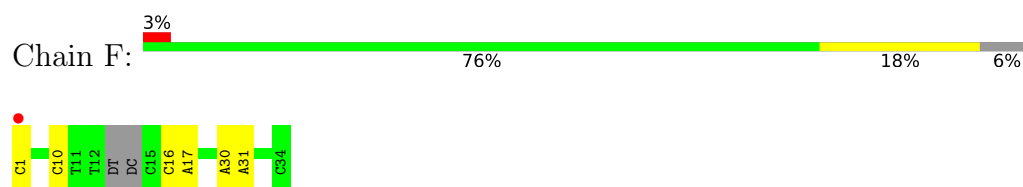
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	R	2	Total	O	0	0
			2	2		



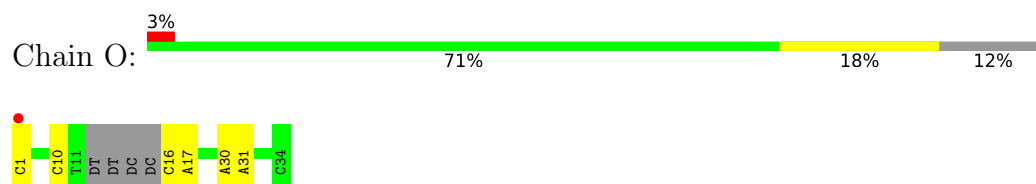
- Molecule 2: X-ray repair cross-complementing protein 5



- Molecule 3: DNA (34-MER)



- Molecule 3: DNA (34-MER)



- Molecule 4: DNA (21-MER)

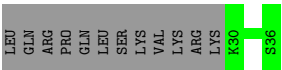




• Molecule 4: DNA (21-MER)



• Molecule 5: Non-homologous end-joining factor 1



• Molecule 5: Non-homologous end-joining factor 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.85Å 118.92Å 128.22Å 90.00° 93.11° 90.00°	Depositor
Resolution (Å)	49.38 – 2.80 49.38 – 2.80	Depositor EDS
% Data completeness (in resolution range)	50.4 (49.38-2.80) 50.4 (49.38-2.80)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.225 , 0.252 0.240 , 0.265	Depositor DCC
R_{free} test set	1918 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	62.9	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 64.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18810	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9723e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SO4

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	0.61	0/4030	1.18	5/5426 (0.1%)
1	C	0.64	2/4055 (0.0%)	1.21	6/5459 (0.1%)
2	B	0.61	0/4394	1.21	8/5929 (0.1%)
2	D	0.63	0/4403	1.25	2/5940 (0.0%)
3	F	0.42	0/724	0.55	0/1110
3	O	0.40	0/684	0.54	0/1048
4	K	0.39	0/481	0.63	0/743
4	R	0.37	0/481	0.63	0/743
5	M	0.63	0/57	1.14	0/74
5	T	0.57	0/48	1.21	0/62
All	All	0.60	2/19357 (0.0%)	1.15	21/26534 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	231	VAL	CA-C	5.72	1.59	1.52
1	C	446	MET	SD-CE	-5.47	1.65	1.79

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	ARG	CA-C-N	6.79	134.18	121.97
1	A	230	ARG	C-N-CA	6.79	134.18	121.97
1	C	323	GLY	CA-C-N	6.73	133.62	123.05
1	C	323	GLY	C-N-CA	6.73	133.62	123.05
1	A	195	ASP	CA-CB-CG	6.43	119.03	112.60
1	A	340	PHE	CA-CB-CG	6.33	120.13	113.80
1	C	340	PHE	CA-CB-CG	6.31	120.11	113.80
1	C	233	PHE	CA-CB-CG	5.66	119.46	113.80
2	B	297	LEU	CA-C-N	5.35	127.71	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	297	LEU	C-N-CA	5.35	127.71	120.38
1	A	263	LEU	N-CA-C	-5.28	105.70	111.82
2	D	321	VAL	N-CA-C	5.26	113.23	107.60
2	B	321	VAL	N-CA-C	5.25	113.21	107.60
1	C	263	LEU	N-CA-C	-5.21	105.77	111.82
2	D	415	ASN	CA-CB-CG	5.15	117.75	112.60
1	C	476	ASP	CA-CB-CG	5.13	117.73	112.60
2	B	440	ASN	CA-CB-CG	5.10	117.70	112.60
2	B	415	ASN	CA-CB-CG	5.08	117.68	112.60
2	B	466	LYS	CA-C-N	5.07	130.02	122.82
2	B	466	LYS	C-N-CA	5.07	130.02	122.82
2	B	405	VAL	N-CA-C	-5.06	101.09	108.17

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	3955	0	4034	37	0
1	C	3980	0	4064	32	0
2	B	4301	0	4308	42	0
2	D	4310	0	4321	36	0
3	F	646	0	360	5	0
3	O	610	0	336	4	0
4	K	431	0	243	9	0
4	R	431	0	243	6	0
5	M	56	0	60	0	0
5	T	47	0	48	2	0
6	A	5	0	0	0	0
6	C	5	0	0	0	0
7	A	6	0	0	0	0
7	B	5	0	0	0	0
7	C	8	0	0	0	0
7	D	8	0	0	0	0
7	F	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	O	2	0	0	0	0
7	R	2	0	0	0	0
All	All	18810	0	18017	146	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 4.

All (146) 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:446:MET:HE1	2:D:264:TYR:HB2	1.40	1.03
2:D:263:ALA:HB1	2:D:362:LEU:HD22	1.41	0.97
2:B:263:ALA:HB1	2:B:362:LEU:HD22	1.50	0.92
1:A:446:MET:HE1	2:B:264:TYR:HB2	1.56	0.87
2:D:263:ALA:HB1	2:D:362:LEU:CD2	2.15	0.77
2:B:400:ARG:HH12	4:K:13:DT:H4'	1.51	0.75
1:A:143:LEU:H	1:A:176:HIS:HE1	1.37	0.73
1:C:143:LEU:H	1:C:176:HIS:HE1	1.36	0.72
3:O:1:DC:H5	4:R:21:DG:H22	1.40	0.68
1:A:350:PHE:HB3	1:A:394:VAL:CG1	2.26	0.65
1:A:350:PHE:HB3	1:A:394:VAL:HG11	1.78	0.65
2:D:24:ILE:HD12	2:D:27:ILE:HD11	1.79	0.64
1:C:350:PHE:HB3	1:C:394:VAL:CG1	2.28	0.64
2:B:338:LYS:HG2	2:B:398:ASP:HA	1.80	0.64
2:D:338:LYS:HG2	2:D:398:ASP:HA	1.79	0.64
2:B:263:ALA:HB1	2:B:362:LEU:CD2	2.25	0.64
1:C:350:PHE:HB3	1:C:394:VAL:HG11	1.79	0.64
2:B:24:ILE:HD12	2:B:27:ILE:HD11	1.80	0.63
2:B:111:LEU:HD13	2:B:134:ILE:HD11	1.81	0.63
1:C:40:PHE:HE2	1:C:83:LEU:HD23	1.65	0.62
1:A:40:PHE:HE2	1:A:83:LEU:HD23	1.63	0.61
2:B:328:GLU:O	2:B:332:LYS:HB2	2.00	0.61
2:B:0:GLN:HA	2:B:4:SER:HB3	1.81	0.61
2:D:265:LYS:HD3	2:D:268:LEU:HD11	1.82	0.61
2:B:265:LYS:HD3	2:B:268:LEU:HD11	1.81	0.61
2:D:111:LEU:HD13	2:D:134:ILE:HD11	1.81	0.60
3:F:10:DC:H42	3:F:17:DA:H61	1.50	0.60
2:D:328:GLU:O	2:D:332:LYS:HB2	2.02	0.60
3:F:1:DC:H5	4:K:21:DG:H22	1.49	0.59
2:D:0:GLN:HA	2:D:4:SER:HB3	1.82	0.59
1:A:253:LYS:HG2	2:B:433:TYR:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:THR:HG23	1:C:318:ARG:HH12	1.69	0.58
2:B:400:ARG:NH1	4:K:13:DT:H4'	2.17	0.57
1:C:48:MET:HA	1:C:59:PRO:HG2	1.86	0.57
2:D:237:PHE:H	2:D:488:GLN:HE22	1.52	0.57
3:O:10:DC:H42	3:O:17:DA:H61	1.52	0.57
1:A:48:MET:HA	1:A:59:PRO:HG2	1.86	0.57
1:A:278:GLN:HE22	4:K:5:DT:H3'	1.69	0.56
2:B:90:LEU:O	2:B:94:ILE:HG12	2.04	0.56
2:D:342:VAL:HA	2:D:393:VAL:HG12	1.87	0.56
2:D:90:LEU:O	2:D:94:ILE:HG12	2.06	0.56
2:B:2:VAL:HG21	2:B:245:ILE:HD13	1.88	0.56
2:B:237:PHE:H	2:B:488:GLN:HE22	1.52	0.56
2:B:342:VAL:HA	2:B:393:VAL:HG12	1.87	0.56
2:B:479:THR:HA	2:B:482:ILE:HD12	1.88	0.55
2:D:2:VAL:HG21	2:D:245:ILE:HD13	1.88	0.55
1:A:316:THR:HG23	1:A:318:ARG:HH12	1.71	0.55
2:B:111:LEU:HG	2:B:115:MET:HE2	1.89	0.55
1:C:433:GLN:HE22	2:D:353:ARG:HG3	1.70	0.55
2:D:479:THR:HA	2:D:482:ILE:HD12	1.88	0.54
2:B:337:GLY:HA2	2:B:399:LYS:HA	1.89	0.54
2:D:111:LEU:HG	2:D:115:MET:HE2	1.89	0.53
2:D:427:MET:O	2:D:430:LEU:HD23	2.08	0.53
1:A:352:PRO:HG3	2:B:473:LEU:HD21	1.90	0.53
2:B:457:LEU:HD11	2:B:461:MET:HE3	1.91	0.52
2:D:337:GLY:HA2	2:D:399:LYS:HA	1.91	0.52
2:B:275:THR:HG21	4:K:9:DT:H5'	1.92	0.51
2:B:426:PHE:O	2:B:429:ASP:OD1	2.27	0.51
2:D:265:LYS:HB3	2:D:268:LEU:HD11	1.93	0.51
1:A:340:PHE:HB2	1:A:408:PRO:HD3	1.92	0.50
3:F:16:DC:H4'	3:F:17:DA:OP1	2.12	0.50
1:C:340:PHE:HB2	1:C:408:PRO:HD3	1.92	0.50
2:D:457:LEU:HD11	2:D:461:MET:HE3	1.93	0.50
2:B:528:ILE:HB	2:B:529:PRO:HD3	1.94	0.50
2:B:265:LYS:HB3	2:B:268:LEU:HD11	1.93	0.50
2:D:-7:HIS:O	2:D:2:VAL:HG22	2.12	0.49
2:B:-7:HIS:O	2:B:2:VAL:HG22	2.12	0.49
2:B:425:PRO:HB2	2:B:429:ASP:OD1	2.12	0.49
1:A:433:GLN:HE22	2:B:353:ARG:HG3	1.77	0.49
1:C:217:TYR:HA	1:C:220:ILE:HB	1.94	0.49
2:B:353:ARG:HA	2:B:356:PHE:CD1	2.48	0.48
1:A:446:MET:CE	2:B:365:PHE:HE2	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:400:ARG:HH12	4:K:13:DT:C4'	2.24	0.48
2:D:528:ILE:HB	2:D:529:PRO:HD3	1.95	0.48
1:C:278:GLN:HE22	4:R:5:DT:H3'	1.79	0.47
1:A:452:ILE:HD13	2:B:371:GLU:HG3	1.95	0.47
1:C:147:LEU:HB3	1:C:193:LEU:HD11	1.96	0.47
2:D:353:ARG:HA	2:D:356:PHE:CD1	2.49	0.47
1:A:482:VAL:HG22	2:B:333:TYR:HD2	1.80	0.47
1:A:217:TYR:HA	1:A:220:ILE:HB	1.97	0.47
1:C:143:LEU:H	1:C:176:HIS:CE1	2.26	0.46
1:C:193:LEU:HD13	1:C:200:LEU:HD21	1.96	0.46
1:A:147:LEU:HB3	1:A:193:LEU:HD11	1.96	0.46
1:C:95:ASN:ND2	1:C:102:ILE:HB	2.30	0.46
1:A:165:ARG:HG3	1:A:199:PHE:HB2	1.98	0.46
4:R:6:DT:H2''	4:R:7:DA:C8	2.50	0.46
1:A:193:LEU:HD13	1:A:200:LEU:HD21	1.98	0.46
1:A:311:LEU:HD13	2:B:289:ILE:HD12	1.98	0.46
1:C:38:LEU:HD22	1:C:250:GLU:HG2	1.97	0.46
1:C:165:ARG:HG3	1:C:199:PHE:HB2	1.98	0.46
4:K:6:DT:H2''	4:K:7:DA:C8	2.50	0.46
1:A:163:HIS:HB2	1:A:252:ARG:NH1	2.30	0.46
1:A:38:LEU:HD22	1:A:250:GLU:HG2	1.97	0.46
1:C:462:MET:HG2	2:D:380:LEU:HA	1.97	0.46
1:A:461:LYS:HG3	1:A:528:LEU:HD12	1.98	0.45
1:C:303:PHE:HE2	2:D:292:GLU:HB2	1.80	0.45
2:D:275:THR:HG21	4:R:9:DT:H5'	1.98	0.45
1:C:440:ALA:O	2:D:239:LYS:HE3	2.16	0.45
1:A:72:ILE:HG12	1:A:116:ILE:HD13	1.98	0.45
1:A:95:ASN:ND2	1:A:102:ILE:HB	2.31	0.45
1:C:507:THR:O	2:D:343:LEU:HD21	2.16	0.45
1:C:461:LYS:HG3	1:C:528:LEU:HD12	1.99	0.44
2:D:10:VAL:HG22	2:D:131:HIS:HB2	1.99	0.44
2:B:10:VAL:HG22	2:B:131:HIS:HB2	1.99	0.44
4:R:11:DT:H2''	4:R:12:DA:C8	2.53	0.44
2:B:450:GLN:HB3	2:B:537:PHE:CZ	2.53	0.44
1:A:286:ILE:HD13	2:B:315:ARG:HG3	2.00	0.43
1:C:95:ASN:ND2	1:C:99:PHE:HB2	2.32	0.43
4:R:16:DG:H2''	4:R:17:DG:C8	2.53	0.43
4:K:11:DT:H2''	4:K:12:DA:C8	2.53	0.43
1:A:262:LYS:HG2	1:A:268:VAL:HG22	2.01	0.43
4:K:16:DG:H2''	4:K:17:DG:C8	2.54	0.43
1:A:95:ASN:ND2	1:A:99:PHE:HB2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:427:MET:O	2:B:430:LEU:HG	2.19	0.43
1:A:85:VAL:HG21	1:A:119:LEU:HD21	2.00	0.43
1:C:72:ILE:HG12	1:C:116:ILE:HD13	2.01	0.43
1:C:262:LYS:HG2	1:C:268:VAL:HG22	2.01	0.43
3:F:16:DC:H2''	3:F:17:DA:C5	2.54	0.43
1:C:85:VAL:HG21	1:C:119:LEU:HD21	2.00	0.42
2:B:130:ARG:HH21	2:B:158:ASP:HB3	1.83	0.42
2:D:130:ARG:HH21	2:D:158:ASP:HB3	1.85	0.42
1:C:446:MET:CE	2:D:365:PHE:HE2	2.32	0.42
2:D:131:HIS:CD2	5:T:33:GLY:HA2	2.55	0.42
3:O:16:DC:H5''	3:O:17:DA:OP1	2.19	0.42
2:D:450:GLN:HB3	2:D:537:PHE:CZ	2.54	0.42
1:A:70:VAL:O	1:A:74:LYS:HG2	2.20	0.42
1:A:400:TYR:CE2	1:A:402:PRO:HG3	2.55	0.42
2:B:40:MET:HB3	2:B:234:LEU:HB3	2.02	0.42
2:B:12:LEU:HD11	2:B:54:ILE:HD11	2.02	0.41
2:B:106:ASP:HB3	2:B:109:ASP:HB2	2.02	0.41
1:A:530:TYR:HA	1:A:531:PRO:HD3	1.96	0.41
3:F:30:DA:H2''	3:F:31:DA:C8	2.56	0.41
1:A:275:ASN:C	1:A:277:VAL:H	2.29	0.41
1:A:289:TYR:CE2	1:A:291:GLU:HB2	2.56	0.41
1:A:390:LEU:HG	1:A:415:PRO:HB2	2.03	0.41
1:C:70:VAL:O	1:C:74:LYS:HG2	2.20	0.41
2:D:12:LEU:HD11	2:D:54:ILE:HD11	2.03	0.41
1:C:275:ASN:C	1:C:277:VAL:H	2.29	0.41
1:A:75:ILE:HD12	1:A:116:ILE:HD11	2.03	0.40
1:C:289:TYR:CE2	1:C:291:GLU:HB2	2.57	0.40
1:C:402:PRO:HD2	1:C:406:ILE:HG21	2.04	0.40
1:A:233:PHE:CD2	1:A:245:LYS:HG2	2.56	0.40
1:C:420:LEU:HD23	1:C:426:GLN:HA	2.03	0.40
3:O:30:DA:H2''	3:O:31:DA:C8	2.56	0.40
2:D:223:GLU:HG3	5:T:32:ARG:HH21	1.86	0.40
2:D:246:HIS:HB2	2:D:264:TYR:CE1	2.56	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	482/544 (89%)	467 (97%)	14 (3%)	1 (0%)	43	72
1	C	485/544 (89%)	470 (97%)	14 (3%)	1 (0%)	43	72
2	B	530/572 (93%)	512 (97%)	17 (3%)	1 (0%)	43	72
2	D	531/572 (93%)	512 (96%)	17 (3%)	2 (0%)	30	60
5	M	5/19 (26%)	5 (100%)	0	0	100	100
5	T	4/19 (21%)	4 (100%)	0	0	100	100
All	All	2037/2270 (90%)	1970 (97%)	62 (3%)	5 (0%)	43	72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	441	SER
2	B	433	TYR
2	D	433	TYR
1	C	250	GLU
1	A	250	GLU

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	444/492 (90%)	438 (99%)	6 (1%)	59	85
1	C	447/492 (91%)	440 (98%)	7 (2%)	55	83
2	B	483/513 (94%)	471 (98%)	12 (2%)	42	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	484/513 (94%)	475 (98%)	9 (2%)	50	81
5	M	6/18 (33%)	6 (100%)	0	100	100
5	T	5/18 (28%)	5 (100%)	0	100	100
All	All	1869/2046 (91%)	1835 (98%)	34 (2%)	51	82

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	MET
1	A	222	SER
1	A	231	VAL
1	A	243	LEU
1	A	277	VAL
1	A	409	TYR
2	B	-16	MET
2	B	7	LYS
2	B	246	HIS
2	B	268	LEU
2	B	341	SER
2	B	357	MET
2	B	359	ASN
2	B	360	GLN
2	B	362	LEU
2	B	430	LEU
2	B	439	LYS
2	B	441	SER
1	C	167	MET
1	C	220	ILE
1	C	222	SER
1	C	243	LEU
1	C	277	VAL
1	C	363	ARG
1	C	409	TYR
2	D	64	THR
2	D	246	HIS
2	D	268	LEU
2	D	341	SER
2	D	357	MET
2	D	360	GLN
2	D	362	LEU
2	D	429	ASP

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Mol	Chain	Res	Type
2	D	473	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	176	HIS
1	A	275	ASN
1	A	320	GLN
1	A	360	HIS
1	A	433	GLN
2	B	-12	HIS
2	B	-9	HIS
2	B	-8	HIS
2	B	6	ASN
2	B	22	ASN
2	B	73	GLN
2	B	99	GLN
2	B	120	HIS
2	B	131	HIS
2	B	152	HIS
2	B	243	HIS
2	B	298	ASN
2	B	415	ASN
2	B	488	GLN
2	B	511	HIS
1	C	95	ASN
1	C	176	HIS
1	C	275	ASN
1	C	360	HIS
1	C	433	GLN
1	C	515	ASN
2	D	-12	HIS
2	D	-9	HIS
2	D	-8	HIS
2	D	-4	ASN
2	D	0	GLN
2	D	6	ASN
2	D	22	ASN
2	D	99	GLN
2	D	131	HIS
2	D	243	HIS

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Mol	Chain	Res	Type
2	D	298	ASN
2	D	488	GLN
2	D	511	HIS

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](#)

2 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	$\# Z > 2$
6	SO4	A	601	-	4,4,4	0.25	0	6,6,6	0.09	0
6	SO4	C	601	-	4,4,4	0.25	0	6,6,6	0.19	0

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	490/544 (90%)	0.67	32 (6%)	25	18	36, 92, 166, 194	0
1	C	493/544 (90%)	0.41	23 (4%)	36	29	26, 72, 153, 178	0
2	B	534/572 (93%)	0.50	28 (5%)	33	25	30, 78, 151, 190	0
2	D	535/572 (93%)	0.37	16 (2%)	52	42	25, 73, 130, 187	0
3	F	32/34 (94%)	0.67	1 (3%)	51	41	52, 126, 175, 190	0
3	O	30/34 (88%)	0.46	1 (3%)	49	39	50, 108, 160, 181	0
4	K	21/21 (100%)	0.25	0	100	100	71, 90, 147, 164	0
4	R	21/21 (100%)	0.42	1 (4%)	35	28	65, 91, 140, 155	0
5	M	7/19 (36%)	0.66	0	100	100	41, 45, 75, 83	0
5	T	6/19 (31%)	0.38	0	100	100	39, 44, 67, 73	0
All	All	2169/2380 (91%)	0.49	102 (4%)	36	29	25, 80, 155, 194	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	534	TYR	4.2
1	A	534	TYR	4.1
2	B	359	ASN	4.1
1	C	157	VAL	4.0
2	D	430	LEU	3.8
1	A	51	SER	3.5
2	B	430	LEU	3.5
1	C	209	GLY	3.1
2	B	27	ILE	3.1
2	B	323	PHE	3.1
2	D	18	PHE	3.0
2	B	298	ASN	3.0
2	B	51	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	498	MET	2.9
1	A	501	GLU	2.8
1	A	280	ALA	2.8
1	A	503	ALA	2.8
1	A	117	LEU	2.8
1	A	500	PRO	2.8
1	C	506	LEU	2.8
2	D	432	GLN	2.8
1	C	134	MET	2.8
1	C	275	ASN	2.8
1	A	510	LYS	2.8
1	C	135	MET	2.7
2	D	431	ARG	2.7
2	B	26	GLY	2.7
1	A	137	HIS	2.7
1	C	510	LYS	2.6
3	O	1	DC	2.6
1	A	506	LEU	2.6
1	C	52	GLN	2.6
1	C	137	HIS	2.6
2	B	432	GLN	2.6
1	A	135	MET	2.6
1	A	225	GLU	2.6
2	D	275	THR	2.5
1	C	247	ARG	2.5
3	F	1	DC	2.5
2	D	469	LYS	2.5
2	B	25	PRO	2.5
2	B	331	MET	2.5
1	C	158	GLN	2.5
1	C	475	SER	2.5
1	C	507	THR	2.5
2	B	275	THR	2.5
1	C	341	ASP	2.5
2	D	335	SER	2.5
1	C	231	VAL	2.5
1	A	226	ASP	2.4
1	A	521	LEU	2.4
2	B	297	LEU	2.4
2	B	288	ASP	2.4
1	A	504	VAL	2.4
1	A	224	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	330	GLN	2.4
2	D	98	ILE	2.4
2	B	440	ASN	2.4
2	B	170	GLY	2.4
1	A	502	GLN	2.4
2	D	433	TYR	2.4
2	B	282	LYS	2.3
2	B	429	ASP	2.3
1	A	507	THR	2.3
2	D	27	ILE	2.3
1	A	530	TYR	2.3
1	C	302	THR	2.2
1	C	313	PRO	2.2
2	B	441	SER	2.2
1	A	164	LYS	2.2
1	A	279	LYS	2.2
1	C	225	GLU	2.2
1	A	275	ASN	2.2
2	D	123	ILE	2.2
1	A	163	HIS	2.2
1	C	34	GLY	2.2
1	A	493	LEU	2.2
2	D	26	GLY	2.2
1	A	324	SER	2.2
1	A	231	VAL	2.1
1	C	498	MET	2.1
2	B	324	SER	2.1
2	B	340	PHE	2.1
2	B	433	TYR	2.1
1	A	457	GLU	2.1
1	A	174	ASN	2.1
1	A	195	ASP	2.1
1	A	216	PHE	2.1
1	C	230	ARG	2.1
2	B	542	ALA	2.1
2	B	-5	GLU	2.1
2	B	443	LYS	2.0
2	B	268	LEU	2.0
2	D	24	ILE	2.0
4	R	21	DG	2.0
2	D	331	MET	2.0
2	B	0	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	258	SER	2.0
2	D	260	ARG	2.0
1	C	425	ILE	2.0
2	B	336	GLU	2.0
1	A	459	VAL	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
6	SO4	A	601	5/5	0.85	0.10	96,96,96,97	0
6	SO4	C	601	5/5	0.86	0.12	94,94,95,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.