



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:49 PM GMT

PDB ID : 4A0L
Title : Structure of DDB1-DDB2-CUL4B-RBX1 bound to a 12 bp abasic site containing DNA-duplex
Authors : Fischer, E.S.; Scrima, A.; Gut, H.; Thoma, N.H.
Deposited on : 2011-09-09
Resolution : 7.40 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

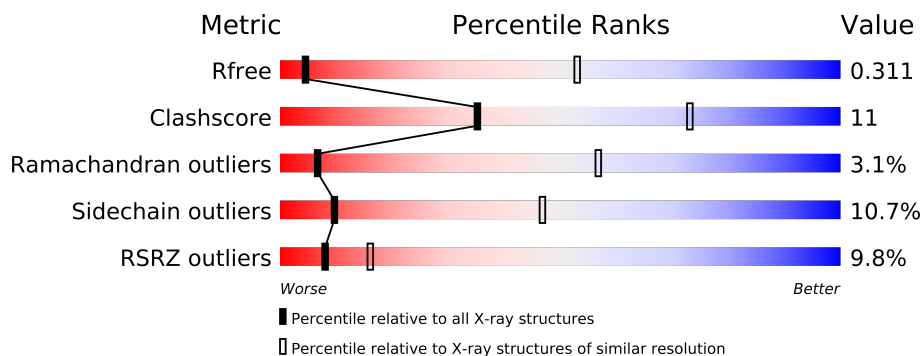
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 7.40 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}	66092	1098 (10.00-3.50)
Clashscore	79885	1039 (10.00-3.52)
Ramachandran outliers	78287	1291 (9.50-3.50)
Sidechain outliers	78261	1265 (9.50-3.50)
RSRZ outliers	66119	1097 (10.00-3.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1144	
1	C	1144	
2	B	382	
2	D	382	
3	E	726	
3	H	726	
4	F	98	
4	I	98	
5	R	12	
5	T	12	
6	S	12	
6	U	12	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 35553 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DNA DAMAGE-BINDING PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1105	Total	C	N	O	S	0	0	0
			8517	5403	1417	1652	45			
1	C	1105	Total	C	N	O	S	0	0	0
			8537	5409	1428	1655	45			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP Q16531
A	-2	GLY	-	EXPRESSION TAG	UNP Q16531
A	-1	GLY	-	EXPRESSION TAG	UNP Q16531
A	0	ARG	-	EXPRESSION TAG	UNP Q16531
C	-3	GLY	-	EXPRESSION TAG	UNP Q16531
C	-2	GLY	-	EXPRESSION TAG	UNP Q16531
C	-1	GLY	-	EXPRESSION TAG	UNP Q16531
C	0	ARG	-	EXPRESSION TAG	UNP Q16531

- Molecule 2 is a protein called DNA DAMAGE-BINDING PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	355	Total	C	N	O	S	0	0	0
			2819	1792	492	524	11			
2	D	355	Total	C	N	O	S	0	0	0
			2843	1806	499	527	11			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	76	MET	-	EXPRESSION TAG	UNP Q2YDS1
B	77	HIS	-	EXPRESSION TAG	UNP Q2YDS1
B	78	HIS	-	EXPRESSION TAG	UNP Q2YDS1
B	79	HIS	-	EXPRESSION TAG	UNP Q2YDS1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	80	HIS	-	EXPRESSION TAG	UNP Q2YDS1
B	81	HIS	-	EXPRESSION TAG	UNP Q2YDS1
B	82	HIS	-	EXPRESSION TAG	UNP Q2YDS1
B	83	ARG	-	EXPRESSION TAG	UNP Q2YDS1
B	84	ARG	-	EXPRESSION TAG	UNP Q2YDS1
B	85	LEU	-	EXPRESSION TAG	UNP Q2YDS1
B	86	VAL	-	EXPRESSION TAG	UNP Q2YDS1
B	87	PRO	-	EXPRESSION TAG	UNP Q2YDS1
B	88	ARG	-	EXPRESSION TAG	UNP Q2YDS1
B	89	GLY	-	EXPRESSION TAG	UNP Q2YDS1
B	90	SER	-	EXPRESSION TAG	UNP Q2YDS1
B	91	GLY	-	EXPRESSION TAG	UNP Q2YDS1
B	92	GLY	-	EXPRESSION TAG	UNP Q2YDS1
B	93	ARG	-	EXPRESSION TAG	UNP Q2YDS1
B	180	GLN	LEU	VARIANT	UNP Q2YDS1
B	214	ARG	TRP	VARIANT	UNP Q2YDS1
D	76	MET	-	EXPRESSION TAG	UNP Q2YDS1
D	77	HIS	-	EXPRESSION TAG	UNP Q2YDS1
D	78	HIS	-	EXPRESSION TAG	UNP Q2YDS1
D	79	HIS	-	EXPRESSION TAG	UNP Q2YDS1
D	80	HIS	-	EXPRESSION TAG	UNP Q2YDS1
D	81	HIS	-	EXPRESSION TAG	UNP Q2YDS1
D	82	HIS	-	EXPRESSION TAG	UNP Q2YDS1
D	83	ARG	-	EXPRESSION TAG	UNP Q2YDS1
D	84	ARG	-	EXPRESSION TAG	UNP Q2YDS1
D	85	LEU	-	EXPRESSION TAG	UNP Q2YDS1
D	86	VAL	-	EXPRESSION TAG	UNP Q2YDS1
D	87	PRO	-	EXPRESSION TAG	UNP Q2YDS1
D	88	ARG	-	EXPRESSION TAG	UNP Q2YDS1
D	89	GLY	-	EXPRESSION TAG	UNP Q2YDS1
D	90	SER	-	EXPRESSION TAG	UNP Q2YDS1
D	91	GLY	-	EXPRESSION TAG	UNP Q2YDS1
D	92	GLY	-	EXPRESSION TAG	UNP Q2YDS1
D	93	ARG	-	EXPRESSION TAG	UNP Q2YDS1
D	180	GLN	LEU	VARIANT	UNP Q2YDS1
D	214	ARG	TRP	VARIANT	UNP Q2YDS1

- Molecule 3 is a protein called CULLIN-4B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	709	Total	C	N	O	S	0	0	0
			5743	3659	979	1074	31			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	709	Total	C	N	O	S	0	0	0
			5773	3681	978	1082	32			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	189	GLY	-	EXPRESSION TAG	UNP Q13620
E	190	GLY	-	EXPRESSION TAG	UNP Q13620
E	191	GLY	-	EXPRESSION TAG	UNP Q13620
E	192	ARG	-	EXPRESSION TAG	UNP Q13620
H	189	GLY	-	EXPRESSION TAG	UNP Q13620
H	190	GLY	-	EXPRESSION TAG	UNP Q13620
H	191	GLY	-	EXPRESSION TAG	UNP Q13620
H	192	ARG	-	EXPRESSION TAG	UNP Q13620

- Molecule 4 is a protein called E3 UBIQUITIN-PROTEIN LIGASE RBX1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	21	Total	C	N	O	0	0	0
			175	118	31	26			
4	I	21	Total	C	N	O	0	0	0
			180	122	32	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	11	MET	-	EXPRESSION TAG	UNP P62878
I	11	MET	-	EXPRESSION TAG	UNP P62878

- Molecule 5 is a DNA chain called 12 BP THF CONTAINING DNA DUPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	R	12	Total	C	N	O	P	0	0	0
			234	111	41	70	12			
5	T	12	Total	C	N	O	P	0	0	0
			234	111	41	70	12			

- Molecule 6 is a DNA chain called 12 BP DNA DUPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	S	12	Total	C	N	O	P	0	0	0
			249	118	47	72	12			

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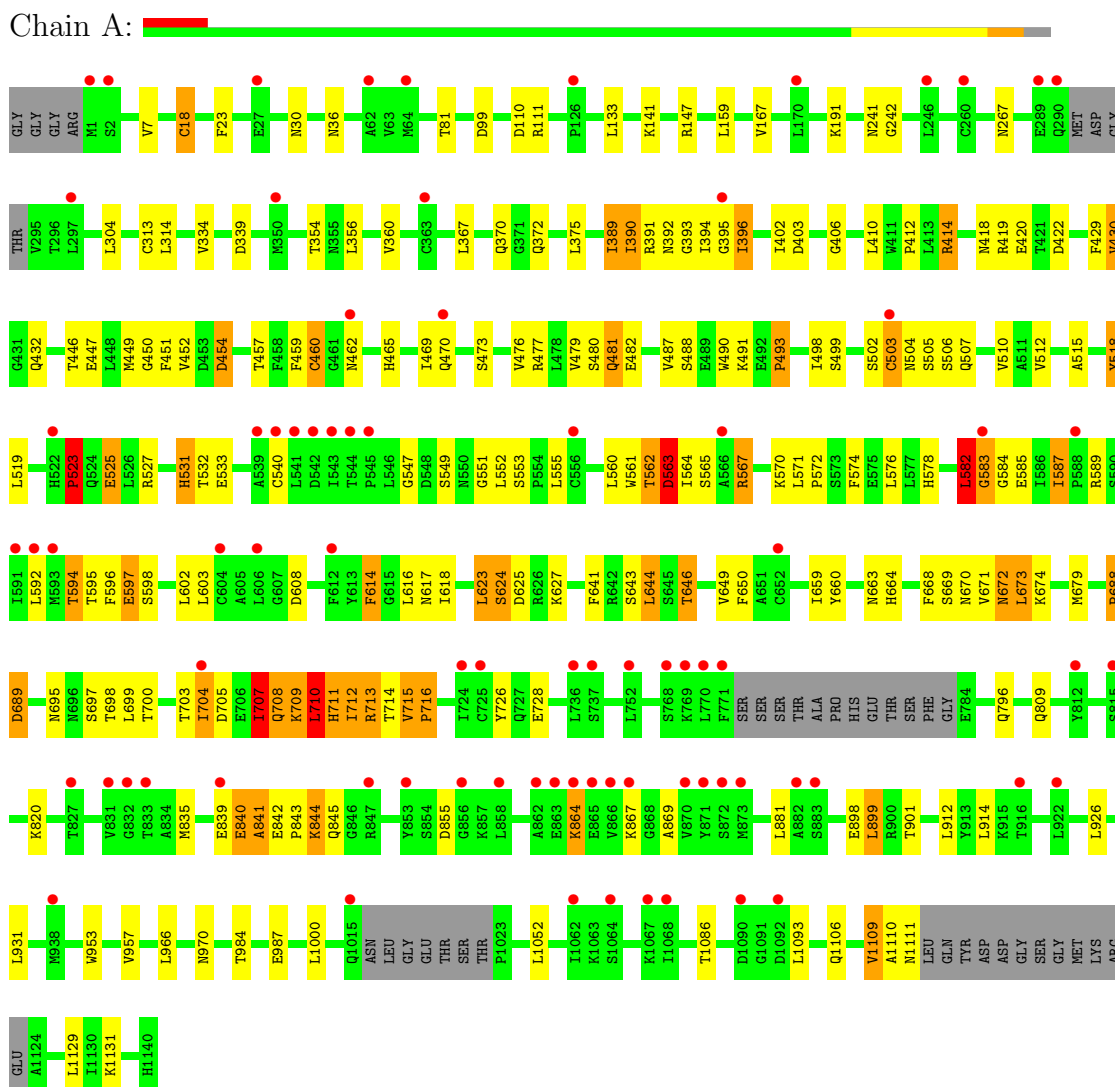
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	U	12	Total 249	C 118	N 47	O 72	P 12	0	0	0

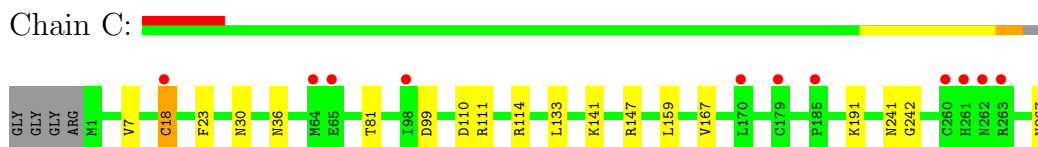
3 Residue-property plots

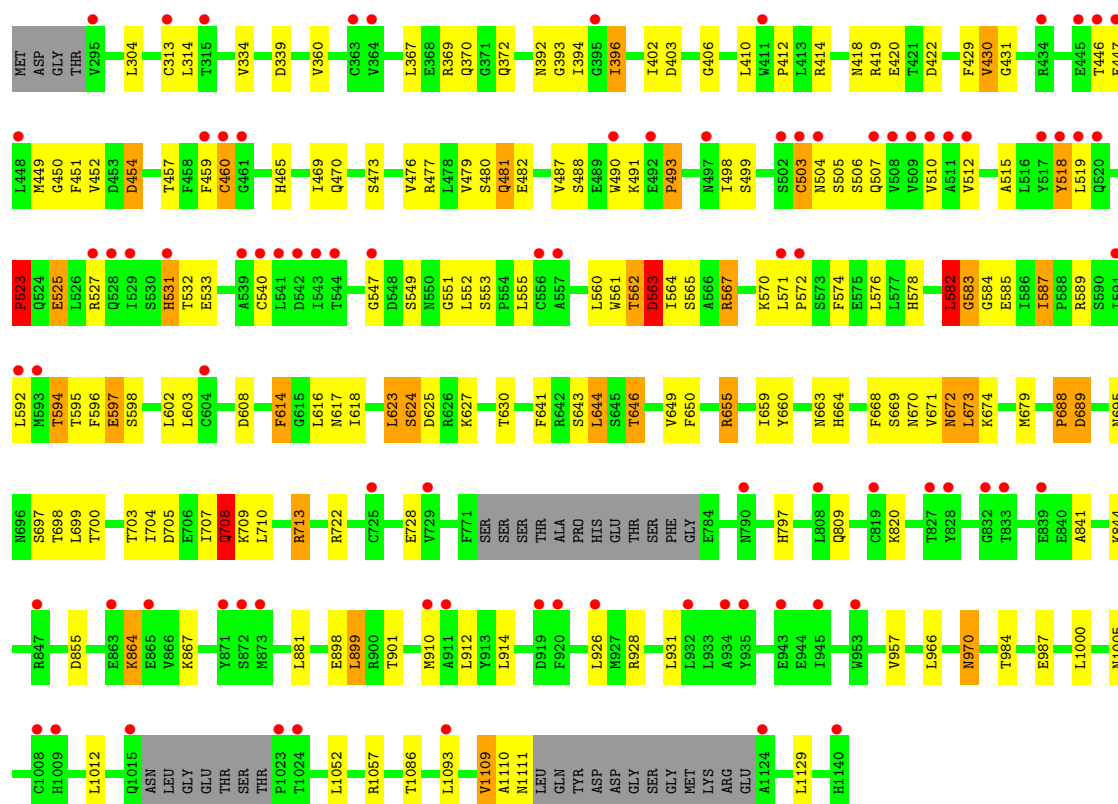
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: DNA DAMAGE-BINDING PROTEIN 1



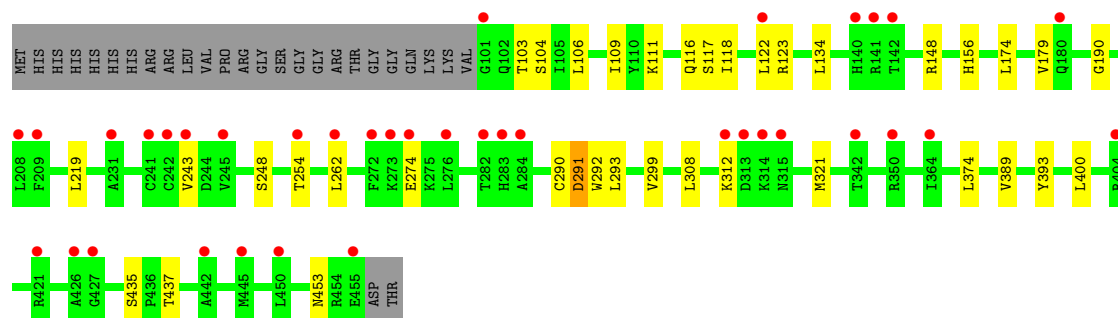
• Molecule 1: DNA DAMAGE-BINDING PROTEIN 1





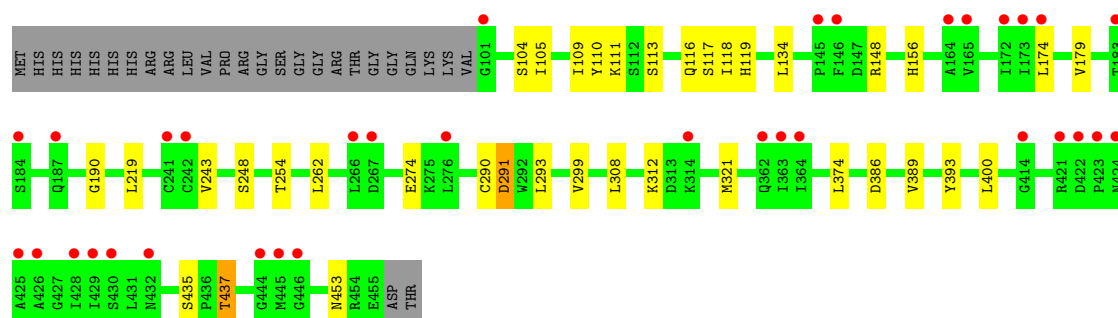
• Molecule 2: DNA DAMAGE-BINDING PROTEIN 2

Chain B:



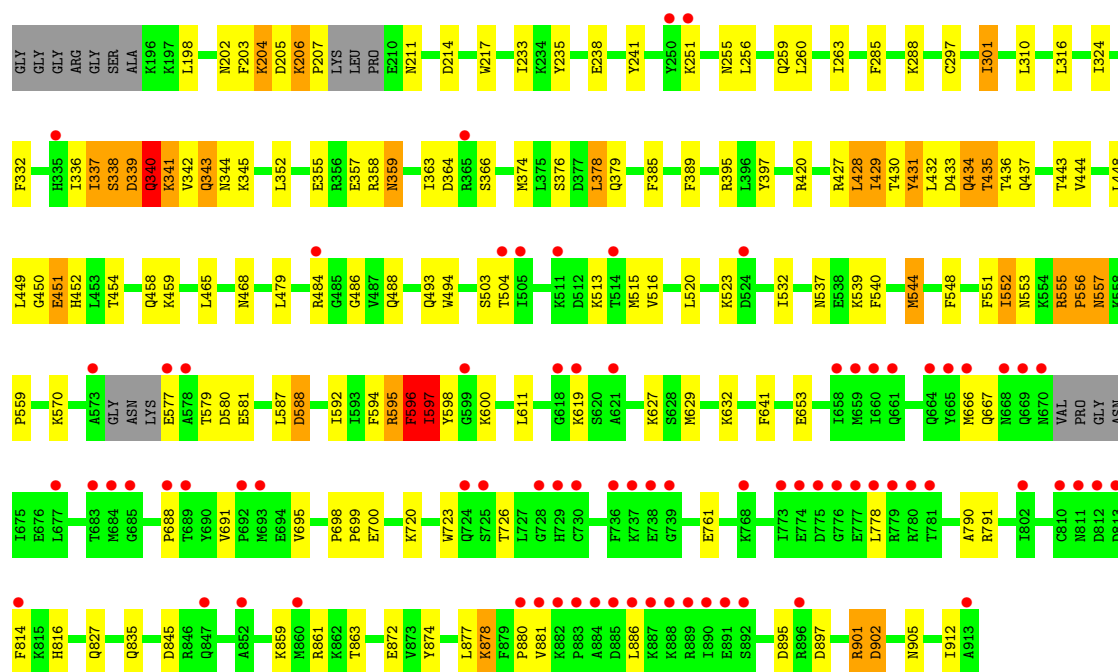
• Molecule 2: DNA DAMAGE-BINDING PROTEIN 2

Chain D:



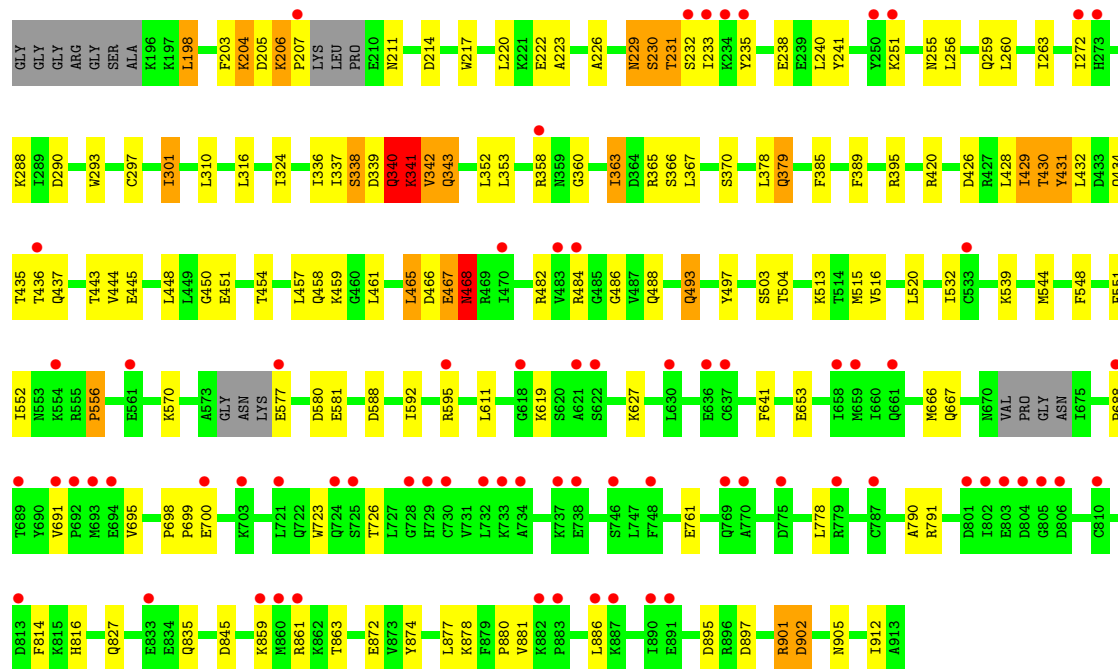
- Molecule 3: CULLIN-4B

Chain E:



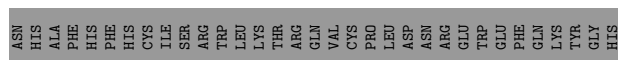
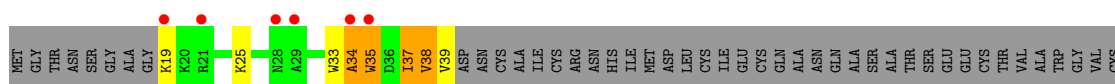
- Molecule 3: CULLIN-4B

Chain H:



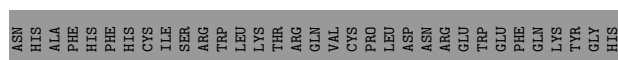
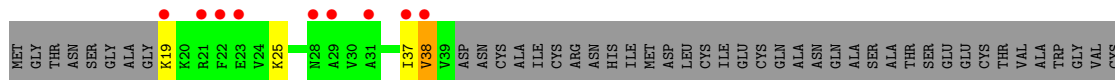
- Molecule 4: E3 UBIQUITIN-PROTEIN LIGASE RBX1

Chain F:



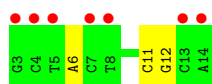
• Molecule 4: E3 UBIQUITIN-PROTEIN LIGASE RBX1

Chain I:



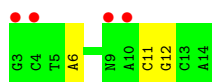
• Molecule 5: 12 BP THF CONTAINING DNA DUPLEX

Chain R:



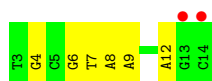
• Molecule 5: 12 BP THF CONTAINING DNA DUPLEX

Chain T:



• Molecule 6: 12 BP DNA DUPLEX

Chain S:



• Molecule 6: 12 BP DNA DUPLEX

Chain U:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	130.80Å 155.84Å 255.39Å 90.00° 94.17° 90.00°	Depositor
Resolution (Å)	29.86 – 7.40 29.86 – 7.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.86-7.40) 99.2 (29.86-7.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 7.23Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.318 , 0.320 0.313 , 0.311	Depositor DCC
R_{free} test set	1352 reflections (10.00%)	DCC
Wilson B-factor (Å ²)	444.7	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 160.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 13547 reflections	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	35553	wwPDB-VP
Average B, all atoms (Å ²)	253.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 3DR

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	0.43	2/8668 (0.0%)	0.66	7/11756 (0.1%)
1	C	0.43	2/8688 (0.0%)	0.66	8/11783 (0.1%)
2	B	0.38	0/2891	0.60	0/3928
2	D	0.38	0/2917	0.60	0/3962
3	E	0.40	3/5831 (0.1%)	0.55	1/7832 (0.0%)
3	H	0.38	0/5865	0.54	0/7878
4	F	0.35	0/179	0.39	0/241
4	I	0.42	0/186	0.43	0/251
5	R	0.92	1/248 (0.4%)	1.13	0/377
5	T	0.92	1/248 (0.4%)	1.12	0/377
6	S	0.89	0/279	1.36	1/429 (0.2%)
6	U	0.88	0/279	1.36	1/429 (0.2%)
All	All	0.43	9/36279 (0.0%)	0.64	18/49243 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	582	LEU	C-N	6.82	1.45	1.33
1	A	582	LEU	C-N	6.78	1.45	1.33
3	E	579	THR	C-N	-5.89	1.20	1.34
3	E	376	SER	C-N	5.80	1.47	1.34
5	R	11	DC	C1'-N1	5.47	1.56	1.49
5	T	11	DC	C1'-N1	5.41	1.56	1.49
3	E	537	ASN	C-N	-5.21	1.22	1.34
1	C	18	CYS	CB-SG	-5.18	1.73	1.81
1	A	18	CYS	CB-SG	-5.16	1.73	1.81

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	624	SER	N-CA-C	7.04	130.01	111.00
1	C	624	SER	N-CA-C	7.02	129.95	111.00
1	A	688	PRO	N-CA-C	6.63	129.34	112.10
1	C	688	PRO	N-CA-C	6.56	129.16	112.10
1	A	689	ASP	N-CA-C	-6.55	93.32	111.00
1	C	689	ASP	N-CA-C	-6.45	93.59	111.00
6	U	4	DG	O4'-C1'-N9	6.19	112.33	108.00
6	S	4	DG	O4'-C1'-N9	6.07	112.25	108.00
1	C	688	PRO	CA-N-CD	-5.87	103.28	111.50
1	A	688	PRO	CA-N-CD	-5.85	103.31	111.50
1	C	624	SER	CB-CA-C	-5.84	99.00	110.10
1	A	624	SER	CB-CA-C	-5.81	99.07	110.10
1	C	710	LEU	N-CA-C	5.45	125.71	111.00
1	C	523	PRO	CA-N-CD	-5.28	104.11	111.50
1	A	422	ASP	CB-CG-OD2	5.24	123.02	118.30
3	E	376	SER	O-C-N	5.22	131.05	122.70
1	C	422	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	523	PRO	CA-N-CD	-5.19	104.23	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8517	0	0	135	0
1	C	8537	0	0	95	0
2	B	2819	0	0	22	0
2	D	2843	0	0	17	0
3	E	5743	0	0	72	0
3	H	5773	0	0	68	0
4	F	175	0	0	7	0
4	I	180	0	0	1	0
5	R	234	0	0	3	0
5	T	234	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	S	249	0	0	5	0
6	U	249	0	0	5	0
All	All	35553	0	0	378	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (378) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:E:555:ARG:CG	3:E:559:PRO:CD	2.22	1.17
1:A:354:THR:CG2	1:A:712:ILE:CG2	2.24	1.15
3:H:365:ARG:CB	3:H:430:THR:CG2	2.30	1.08
3:E:555:ARG:CB	3:E:559:PRO:CG	2.33	1.06
1:A:843:PRO:CB	2:B:104:SER:CB	2.36	1.04
3:E:552:ILE:CG2	3:E:597:ILE:CG1	2.35	1.03
3:E:555:ARG:CB	3:E:559:PRO:CD	2.36	1.02
1:A:354:THR:CG2	1:A:712:ILE:CD1	2.41	0.98
3:H:220:LEU:CD2	3:H:240:LEU:CD2	2.42	0.97
1:A:926:LEU:CD1	2:B:122:LEU:CD2	2.46	0.94
3:E:340:GLN:CG	3:E:341:LYS:N	2.30	0.92
3:E:494:TRP:CE3	3:E:540:PHE:CD2	2.57	0.92
1:A:111:ARG:CG	2:B:292:TRP:CZ2	2.53	0.90
1:A:704:ILE:N	1:A:704:ILE:CD1	2.30	0.90
3:H:226:ALA:CB	3:H:233:ILE:N	2.37	0.88
1:C:987:GLU:OE2	2:D:156:HIS:CE1	2.26	0.88
3:E:285:PHE:CE2	3:E:345:LYS:CD	2.58	0.87
1:A:375:LEU:O	1:A:389:ILE:CA	2.23	0.85
1:C:111:ARG:CZ	2:D:290:CYS:SG	2.64	0.85
1:C:841:ALA:O	2:D:104:SER:CA	2.25	0.85
1:C:499:SER:CB	3:H:238:GLU:CB	2.55	0.84
3:E:595:ARG:O	3:E:596:PHE:CG	2.30	0.84
1:A:111:ARG:NE	2:B:292:TRP:NE1	2.26	0.82
1:A:987:GLU:OE2	2:B:156:HIS:CE1	2.33	0.81
1:A:111:ARG:CB	2:B:292:TRP:CZ2	2.65	0.80
1:A:709:LYS:O	1:A:710:LEU:CD2	2.30	0.80
3:E:595:ARG:C	3:E:596:PHE:CG	2.55	0.79
1:A:708:GLN:O	1:A:709:LYS:CD	2.31	0.78
1:A:912:LEU:CD2	2:B:109:ILE:CG1	2.62	0.78
3:E:339:ASP:CG	3:E:340:GLN:N	2.37	0.78
3:E:449:LEU:CD1	3:E:479:LEU:CD2	2.62	0.77
1:A:708:GLN:O	1:A:709:LYS:CE	2.31	0.77
1:A:840:GLU:N	2:B:103:THR:CB	2.48	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:707:ILE:O	1:A:708:GLN:CB	2.33	0.76
3:E:429:ILE:O	3:E:429:ILE:CG1	2.35	0.75
3:E:595:ARG:O	3:E:596:PHE:CD2	2.40	0.74
1:A:375:LEU:O	1:A:389:ILE:CB	2.36	0.74
1:C:585:GLU:CG	3:H:301:ILE:CG2	2.66	0.74
3:H:363:ILE:C	3:H:363:ILE:CD1	2.53	0.74
1:A:987:GLU:CD	2:B:156:HIS:CE1	2.61	0.73
3:E:285:PHE:CZ	3:E:345:LYS:CD	2.71	0.73
1:C:585:GLU:OE2	3:H:301:ILE:CG2	2.38	0.72
3:E:588:ASP:CA	3:E:632:LYS:NZ	2.53	0.71
1:C:589:ARG:NH1	3:H:241:TYR:CE2	2.58	0.71
1:A:912:LEU:CD2	2:B:109:ILE:CG2	2.69	0.71
3:H:428:LEU:CA	3:H:432:LEU:CB	2.69	0.70
3:E:556:PRO:O	3:E:557:ASN:CG	2.30	0.70
3:E:428:LEU:CD2	3:E:432:LEU:CD2	2.69	0.70
1:A:715:VAL:O	1:A:715:VAL:CG1	2.40	0.70
1:C:561:TRP:O	1:C:587:ILE:CG2	2.40	0.70
3:E:597:ILE:O	3:E:600:LYS:CG	2.40	0.69
1:A:561:TRP:O	1:A:587:ILE:CG2	2.40	0.69
1:A:356:LEU:CD2	1:A:712:ILE:CG2	2.70	0.69
1:A:389:ILE:O	1:A:390:ILE:CB	2.40	0.69
1:C:708:GLN:NE2	1:C:708:GLN:CA	2.56	0.68
3:E:598:TYR:CD2	3:E:878:LYS:O	2.46	0.68
1:A:111:ARG:NH1	2:B:290:CYS:SG	2.67	0.67
1:A:840:GLU:CG	1:A:840:GLU:O	2.43	0.67
3:H:290:ASP:CG	3:H:367:LEU:CD1	2.64	0.67
1:C:454:ASP:OD1	1:C:454:ASP:N	2.28	0.66
1:A:714:THR:O	1:A:715:VAL:CB	2.44	0.66
3:E:397:TYR:CD2	3:E:444:VAL:CG1	2.78	0.66
1:A:710:LEU:O	1:A:711:HIS:C	2.34	0.66
1:C:630:THR:CB	1:C:797:HIS:CE1	2.78	0.66
3:E:720:LYS:CG	4:F:34:ALA:CB	2.74	0.66
3:E:553:ASN:CB	3:E:598:TYR:CB	2.73	0.66
1:C:582:LEU:O	1:C:583:GLY:O	2.14	0.65
1:C:695:ASN:OD1	1:C:697:SER:N	2.30	0.65
3:H:223:ALA:CB	3:H:240:LEU:CD1	2.75	0.65
1:A:582:LEU:O	1:A:583:GLY:O	2.14	0.65
1:A:695:ASN:OD1	1:A:697:SER:N	2.30	0.65
3:E:595:ARG:C	3:E:596:PHE:CD1	2.70	0.65
3:H:229:ASN:O	3:H:231:THR:N	2.30	0.65
1:A:454:ASP:N	1:A:454:ASP:OD1	2.28	0.65
3:E:203:PHE:O	3:E:204:LYS:C	2.35	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:711:HIS:O	1:A:713:ARG:N	2.30	0.65
1:A:562:THR:O	1:A:564:ILE:N	2.30	0.64
3:E:594:PHE:O	3:E:596:PHE:N	2.30	0.64
3:H:434:GLN:O	3:H:436:THR:N	2.30	0.64
3:E:434:GLN:O	3:E:436:THR:N	2.30	0.64
3:H:203:PHE:O	3:H:204:LYS:C	2.35	0.64
1:A:589:ARG:NH1	3:E:241:TYR:CE2	2.65	0.64
3:E:555:ARG:O	3:E:557:ASN:N	2.30	0.64
1:A:708:GLN:O	1:A:709:LYS:NZ	2.31	0.64
1:C:562:THR:O	1:C:564:ILE:N	2.30	0.64
3:E:450:GLY:O	3:E:452:HIS:N	2.30	0.64
1:A:715:VAL:N	1:A:716:PRO:CD	2.60	0.64
3:E:555:ARG:O	3:E:556:PRO:C	2.36	0.64
1:A:710:LEU:O	1:A:712:ILE:N	2.32	0.63
3:H:230:SER:O	3:H:232:SER:N	2.30	0.63
1:C:926:LEU:CD2	2:D:105:ILE:CD1	2.76	0.63
3:H:336:ILE:O	3:H:342:VAL:CB	2.45	0.63
3:E:359:ASN:OD1	3:E:359:ASN:N	2.32	0.63
3:H:229:ASN:N	3:H:229:ASN:OD1	2.30	0.63
4:F:38:VAL:O	4:F:39:VAL:CG2	2.47	0.62
1:C:928:ARG:NH1	2:D:437:THR:CG2	2.62	0.62
1:A:354:THR:CG2	1:A:712:ILE:CB	2.77	0.62
4:F:38:VAL:CG2	4:F:38:VAL:O	2.48	0.62
1:C:928:ARG:CZ	2:D:437:THR:CG2	2.78	0.61
1:C:111:ARG:NH2	2:D:290:CYS:SG	2.73	0.61
1:C:562:THR:O	1:C:564:ILE:CG1	2.49	0.61
5:R:12:DG:N2	6:S:6:DG:C2	2.69	0.61
5:T:12:DG:N2	6:U:6:DG:C2	2.69	0.61
1:A:562:THR:O	1:A:564:ILE:CG1	2.50	0.60
1:A:394:ILE:CG2	1:A:395:GLY:N	2.64	0.60
1:A:664:HIS:CB	1:A:1131:LYS:CE	2.80	0.60
3:H:206:LYS:CB	3:H:207:PRO:CD	2.79	0.60
3:E:587:LEU:CD2	3:E:629:MET:SD	2.90	0.60
3:H:290:ASP:OD1	3:H:367:LEU:CD1	2.50	0.60
3:H:339:ASP:O	3:H:340:GLN:CB	2.48	0.60
3:E:596:PHE:CD1	3:E:596:PHE:N	2.69	0.59
3:E:337:ILE:O	3:E:342:VAL:CB	2.50	0.59
1:C:910:MET:CE	2:D:105:ILE:CG2	2.81	0.59
3:E:374:MET:O	3:E:378:LEU:N	2.36	0.59
4:F:38:VAL:C	4:F:39:VAL:CG2	2.71	0.58
3:H:337:ILE:O	3:H:338:SER:C	2.41	0.58
1:A:841:ALA:N	2:B:103:THR:CB	2.65	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:336:ILE:O	3:H:342:VAL:CG1	2.51	0.58
3:H:340:GLN:O	3:H:341:LYS:C	2.41	0.58
3:E:374:MET:CG	3:E:378:LEU:CD2	2.83	0.57
1:A:669:SER:O	1:A:670:ASN:C	2.43	0.57
1:A:671:VAL:O	1:A:673:LEU:N	2.38	0.57
3:E:588:ASP:N	3:E:632:LYS:NZ	2.53	0.57
1:A:503:CYS:SG	1:A:504:ASN:N	2.78	0.57
1:C:503:CYS:SG	1:C:504:ASN:N	2.78	0.56
1:C:429:PHE:O	1:C:430:VAL:O	2.22	0.56
3:E:339:ASP:OD1	3:E:340:GLN:N	2.38	0.56
3:E:597:ILE:O	3:E:600:LYS:CE	2.53	0.56
1:C:393:GLY:O	1:C:709:LYS:N	2.38	0.56
1:C:669:SER:O	1:C:670:ASN:C	2.43	0.56
1:A:111:ARG:CZ	2:B:290:CYS:SG	2.94	0.56
1:C:518:TYR:CD1	1:C:519:LEU:N	2.74	0.56
1:C:392:ASN:CB	1:C:1012:LEU:O	2.54	0.56
3:H:353:LEU:CD2	3:H:363:ILE:CB	2.84	0.56
3:H:434:GLN:C	3:H:436:THR:N	2.59	0.56
1:A:518:TYR:C	1:A:518:TYR:CD1	2.80	0.56
1:A:429:PHE:O	1:A:430:VAL:O	2.22	0.56
1:A:703:THR:OG1	1:A:704:ILE:N	2.39	0.55
1:C:671:VAL:O	1:C:673:LEU:N	2.38	0.55
3:H:363:ILE:O	3:H:363:ILE:CD1	2.54	0.55
1:A:532:THR:CG2	1:A:533:GLU:N	2.69	0.55
1:A:525:GLU:OE2	1:A:527:ARG:NH2	2.39	0.55
1:C:532:THR:CG2	1:C:533:GLU:N	2.69	0.55
1:A:518:TYR:CD1	1:A:519:LEU:N	2.75	0.55
1:A:663:ASN:O	1:A:1131:LYS:CE	2.55	0.55
1:C:525:GLU:OE2	1:C:527:ARG:NH2	2.39	0.55
3:H:226:ALA:O	3:H:232:SER:N	2.40	0.55
3:H:428:LEU:O	3:H:432:LEU:CB	2.55	0.55
3:E:357:GLU:O	3:E:427:ARG:NH2	2.41	0.54
1:C:614:PHE:CD1	1:C:614:PHE:N	2.75	0.54
1:A:525:GLU:OE2	1:A:527:ARG:NE	2.41	0.54
1:C:525:GLU:OE2	1:C:527:ARG:NE	2.41	0.54
3:E:430:THR:O	3:E:431:TYR:CB	2.54	0.54
1:C:111:ARG:NH2	2:D:290:CYS:CA	2.71	0.54
1:C:518:TYR:C	1:C:518:TYR:CD1	2.79	0.54
1:A:614:PHE:CD1	1:A:614:PHE:N	2.75	0.54
1:C:570:LYS:O	1:C:574:PHE:N	2.41	0.54
1:A:649:VAL:CG1	1:A:650:PHE:N	2.71	0.54
3:H:378:LEU:O	3:H:379:GLN:CB	2.56	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:229:ASN:C	3:H:231:THR:N	2.61	0.54
1:A:111:ARG:CZ	2:B:292:TRP:NE1	2.71	0.53
3:H:231:THR:O	3:H:232:SER:C	2.45	0.53
4:F:37:ILE:CG1	4:F:38:VAL:N	2.71	0.53
1:A:714:THR:CG2	1:A:716:PRO:CD	2.86	0.53
1:A:695:ASN:OD1	1:A:698:THR:N	2.42	0.53
1:C:695:ASN:OD1	1:C:698:THR:N	2.42	0.53
1:A:841:ALA:C	2:B:103:THR:O	2.46	0.53
3:H:340:GLN:CG	3:H:341:LYS:N	2.71	0.53
1:C:465:HIS:ND1	1:C:523:PRO:CD	2.72	0.53
1:A:1109:VAL:O	1:A:1111:ASN:N	2.42	0.53
3:H:222:GLU:O	3:H:233:ILE:CB	2.57	0.53
3:H:445:GLU:O	3:H:450:GLY:N	2.41	0.53
3:E:552:ILE:CD1	3:E:597:ILE:CD1	2.86	0.53
1:A:465:HIS:ND1	1:A:523:PRO:CD	2.72	0.53
1:A:570:LYS:O	1:A:574:PHE:N	2.42	0.53
1:C:649:VAL:CG1	1:C:650:PHE:N	2.71	0.53
3:H:365:ARG:O	3:H:431:TYR:CB	2.57	0.52
3:H:272:ILE:CD1	3:H:340:GLN:NE2	2.73	0.52
3:E:338:SER:O	3:E:343:GLN:CB	2.57	0.52
1:A:594:THR:CG2	1:A:595:THR:N	2.73	0.52
1:C:970:ASN:OD1	2:D:119:HIS:ND1	2.42	0.52
1:C:1109:VAL:O	1:C:1111:ASN:N	2.42	0.52
1:C:597:GLU:OE1	1:C:664:HIS:N	2.43	0.52
1:C:594:THR:CG2	1:C:595:THR:N	2.73	0.52
3:E:594:PHE:C	3:E:596:PHE:N	2.63	0.52
1:A:597:GLU:OE1	1:A:664:HIS:N	2.43	0.52
1:A:912:LEU:CD2	2:B:109:ILE:CD1	2.88	0.51
1:C:562:THR:C	1:C:564:ILE:N	2.64	0.51
4:F:38:VAL:O	4:F:39:VAL:CB	2.57	0.51
1:C:402:ILE:CD1	3:H:198:LEU:CB	2.87	0.51
1:C:578:HIS:CE1	1:C:623:LEU:CD1	2.93	0.51
1:A:394:ILE:O	1:A:672:ASN:N	2.43	0.51
1:A:578:HIS:CE1	1:A:623:LEU:CD1	2.93	0.51
3:E:340:GLN:O	3:E:344:ASN:OD1	2.28	0.51
1:A:459:PHE:CD2	1:A:460:CYS:N	2.79	0.51
3:H:465:LEU:CB	3:H:497:TYR:CZ	2.93	0.51
1:C:459:PHE:CD2	1:C:460:CYS:N	2.79	0.51
1:A:23:PHE:N	1:A:30:ASN:ND2	2.59	0.51
1:C:369:ARG:CB	1:C:668:PHE:CB	2.89	0.51
1:A:711:HIS:O	1:A:711:HIS:CD2	2.64	0.51
1:C:23:PHE:N	1:C:30:ASN:ND2	2.59	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:490:TRP:CG	1:C:491:LYS:N	2.79	0.50
1:A:391:ARG:O	1:A:393:GLY:N	2.44	0.50
3:E:450:GLY:C	3:E:452:HIS:N	2.64	0.50
3:H:444:VAL:O	3:H:448:LEU:N	2.44	0.50
1:A:571:LEU:O	1:A:572:PRO:C	2.50	0.50
1:A:490:TRP:CG	1:A:491:LYS:N	2.79	0.49
3:E:587:LEU:CB	3:E:632:LYS:CD	2.90	0.49
1:A:668:PHE:N	1:A:668:PHE:CD1	2.80	0.49
1:C:490:TRP:CD2	1:C:491:LYS:N	2.81	0.49
1:A:490:TRP:CD2	1:A:491:LYS:N	2.81	0.49
1:A:394:ILE:CG2	1:A:705:ASP:CB	2.91	0.49
1:C:707:ILE:O	1:C:708:GLN:O	2.30	0.49
3:E:494:TRP:CZ3	3:E:540:PHE:CD2	3.00	0.49
3:H:365:ARG:CB	3:H:430:THR:O	2.60	0.49
1:A:664:HIS:O	1:A:1131:LYS:NZ	2.46	0.49
1:C:507:GLN:NE2	1:C:552:LEU:CA	2.76	0.49
1:C:571:LEU:O	1:C:572:PRO:C	2.50	0.49
3:H:230:SER:C	3:H:232:SER:N	2.67	0.49
1:A:562:THR:C	1:A:564:ILE:N	2.64	0.49
1:C:707:ILE:O	1:C:707:ILE:CG2	2.60	0.49
3:E:397:TYR:CE2	3:E:444:VAL:CG1	2.96	0.49
3:H:340:GLN:NE2	3:H:342:VAL:CG2	2.76	0.49
3:E:332:PHE:CE1	3:E:336:ILE:CG2	2.96	0.49
1:A:840:GLU:O	1:A:841:ALA:O	2.30	0.48
3:H:465:LEU:CB	3:H:497:TYR:CE2	2.96	0.48
1:C:512:VAL:N	1:C:515:ALA:O	2.46	0.48
1:A:507:GLN:NE2	1:A:552:LEU:CA	2.76	0.48
1:C:655:ARG:NH1	1:C:713:ARG:NE	2.60	0.48
1:C:1005:ASN:ND2	2:D:113:SER:O	2.46	0.48
3:E:340:GLN:CG	3:E:341:LYS:CG	2.91	0.48
1:A:450:GLY:O	1:A:477:ARG:NH2	2.45	0.48
1:A:835:MET:CG	1:A:845:GLN:O	2.61	0.48
1:A:446:THR:CG2	1:A:447:GLU:N	2.75	0.48
1:C:722:ARG:NH2	2:D:110:TYR:CD2	2.82	0.48
1:C:446:THR:CG2	1:C:447:GLU:N	2.75	0.48
3:H:353:LEU:CD2	3:H:363:ILE:CG1	2.92	0.48
1:A:512:VAL:N	1:A:515:ALA:O	2.46	0.48
1:C:450:GLY:O	1:C:477:ARG:NH2	2.46	0.48
1:A:679:MET:C	1:A:679:MET:SD	2.92	0.48
1:A:711:HIS:O	1:A:711:HIS:CG	2.66	0.48
1:C:578:HIS:CD2	1:C:623:LEU:CD1	2.97	0.48
1:A:459:PHE:CG	1:A:460:CYS:N	2.82	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:114:ARG:NH2	2:D:386:ASP:OD2	2.47	0.48
3:E:203:PHE:O	3:E:205:ASP:N	2.47	0.48
1:A:479:VAL:CG1	1:A:480:SER:N	2.77	0.48
3:H:358:ARG:O	3:H:420:ARG:NH1	2.47	0.47
1:C:679:MET:SD	1:C:679:MET:C	2.92	0.47
1:A:578:HIS:CD2	1:A:623:LEU:CD1	2.97	0.47
3:E:355:GLU:O	3:E:359:ASN:OD1	2.32	0.47
1:C:459:PHE:CG	1:C:460:CYS:N	2.82	0.47
3:E:206:LYS:CB	3:E:207:PRO:CD	2.92	0.47
1:C:479:VAL:CG1	1:C:480:SER:N	2.77	0.47
1:C:18:CYS:CB	1:C:313:CYS:SG	3.03	0.47
3:H:426:ASP:O	3:H:429:ILE:CG2	2.63	0.47
1:A:843:PRO:N	2:B:104:SER:CB	2.78	0.47
1:A:531:HIS:ND1	1:A:532:THR:N	2.63	0.47
1:A:840:GLU:O	1:A:841:ALA:C	2.54	0.46
1:C:531:HIS:ND1	1:C:532:THR:N	2.63	0.46
1:C:643:SER:OG	1:C:644:LEU:N	2.46	0.46
3:H:430:THR:O	3:H:431:TYR:CB	2.61	0.46
3:H:205:ASP:O	3:H:205:ASP:CG	2.53	0.46
1:A:18:CYS:CB	1:A:313:CYS:SG	3.03	0.46
1:C:396:ILE:N	1:C:396:ILE:CD1	2.78	0.46
1:A:664:HIS:O	1:A:1131:LYS:CE	2.64	0.46
1:A:585:GLU:OE2	3:E:301:ILE:CG2	2.63	0.46
1:A:869:ALA:CB	2:B:106:LEU:CB	2.93	0.46
1:A:709:LYS:C	1:A:710:LEU:CG	2.84	0.46
4:F:33:TRP:O	4:F:34:ALA:O	2.34	0.46
3:H:226:ALA:CB	3:H:233:ILE:CB	2.94	0.46
1:A:664:HIS:C	1:A:1131:LYS:CE	2.84	0.46
1:A:396:ILE:N	1:A:396:ILE:CD1	2.78	0.46
3:H:698:PRO:O	3:H:700:GLU:N	2.48	0.46
3:E:698:PRO:O	3:E:700:GLU:N	2.48	0.46
1:C:910:MET:SD	2:D:105:ILE:CD1	3.04	0.46
3:E:434:GLN:C	3:E:436:THR:N	2.68	0.45
1:A:715:VAL:O	1:A:716:PRO:C	2.55	0.45
3:H:229:ASN:O	3:H:230:SER:OG	2.34	0.45
1:C:402:ILE:N	1:C:699:LEU:O	2.49	0.45
1:A:643:SER:OG	1:A:644:LEU:N	2.47	0.45
1:A:842:GLU:O	1:A:844:LYS:CD	2.65	0.45
1:A:589:ARG:CZ	3:E:241:TYR:CE2	3.00	0.45
3:H:901:ARG:O	3:H:902:ASP:CB	2.65	0.45
6:S:7:DT:C7	6:S:8:DA:C6	2.99	0.45
6:U:7:DT:C7	6:U:8:DA:C6	3.00	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:402:ILE:N	1:A:699:LEU:O	2.49	0.45
1:C:864:LYS:NZ	1:C:899:LEU:O	2.50	0.45
1:A:841:ALA:CA	2:B:103:THR:O	2.65	0.45
3:H:861:ARG:NH1	3:H:872:GLU:OE2	2.50	0.45
1:A:864:LYS:NZ	1:A:899:LEU:O	2.50	0.45
3:E:339:ASP:O	3:E:340:GLN:CB	2.66	0.44
1:C:912:LEU:CD2	2:D:109:ILE:CD1	2.95	0.44
3:E:385:PHE:O	3:E:389:PHE:N	2.51	0.44
1:A:659:ILE:CG2	1:A:660:TYR:N	2.79	0.44
3:H:385:PHE:O	3:H:389:PHE:N	2.51	0.44
3:E:901:ARG:O	3:E:902:ASP:CB	2.65	0.44
4:I:37:ILE:O	4:I:38:VAL:C	2.56	0.44
2:B:248:SER:OG	2:B:291:ASP:OD1	2.36	0.44
3:H:336:ILE:O	3:H:342:VAL:CG2	2.65	0.44
3:H:457:LEU:CB	3:H:493:GLN:NE2	2.81	0.44
3:E:444:VAL:O	3:E:448:LEU:N	2.50	0.44
1:C:659:ILE:CG2	1:C:660:TYR:N	2.80	0.44
1:A:953:TRP:CZ2	2:B:123:ARG:NH1	2.86	0.44
1:A:564:ILE:O	1:A:564:ILE:CG2	2.66	0.44
3:E:556:PRO:C	3:E:557:ASN:CG	2.77	0.44
1:A:562:THR:O	1:A:563:ASP:C	2.56	0.44
2:D:248:SER:OG	2:D:291:ASP:OD1	2.36	0.44
5:T:12:DG:C2	6:U:6:DG:C2	3.06	0.43
1:A:582:LEU:CD1	1:A:583:GLY:N	2.81	0.43
1:C:582:LEU:CD1	1:C:583:GLY:N	2.81	0.43
3:E:861:ARG:NH1	3:E:872:GLU:OE2	2.51	0.43
5:R:12:DG:C2	6:S:6:DG:C2	3.06	0.43
3:H:466:ASP:OD1	3:H:497:TYR:OH	2.37	0.43
3:E:202:ASN:O	3:E:204:LYS:N	2.52	0.43
1:C:465:HIS:CE1	1:C:523:PRO:CD	3.02	0.43
3:H:466:ASP:O	3:H:468:ASN:N	2.51	0.43
1:A:451:PHE:CD1	1:A:470:GLN:CB	3.02	0.43
1:C:705:ASP:OD1	1:C:707:ILE:CG1	2.66	0.43
5:R:6:DA:C2	6:S:12:DA:C2	3.07	0.43
1:A:465:HIS:CE1	1:A:523:PRO:CD	3.02	0.42
3:H:467:GLU:O	3:H:468:ASN:CB	2.66	0.42
1:A:562:THR:CG2	1:A:563:ASP:N	2.82	0.42
1:A:432:GLN:NE2	3:E:207:PRO:CG	2.82	0.42
5:T:6:DA:C2	6:U:12:DA:C2	3.07	0.42
1:A:505:SER:OG	1:A:506:SER:N	2.52	0.42
1:C:641:PHE:CD1	1:C:641:PHE:C	2.93	0.42
1:A:709:LYS:C	1:A:710:LEU:CD2	2.88	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:643:SER:N	1:A:646:THR:O	2.53	0.42
1:C:451:PHE:CD1	1:C:470:GLN:CB	3.02	0.42
3:E:523:LYS:CE	3:E:544:MET:CE	2.98	0.42
3:E:363:ILE:O	3:E:364:ASP:C	2.58	0.42
3:H:340:GLN:CG	3:H:341:LYS:CG	2.98	0.42
3:E:552:ILE:CG2	3:E:597:ILE:CD1	2.97	0.42
1:C:562:THR:O	1:C:563:ASP:C	2.56	0.42
3:H:445:GLU:OE2	3:H:482:ARG:NE	2.53	0.42
1:C:643:SER:N	1:C:646:THR:O	2.53	0.42
1:C:505:SER:OG	1:C:506:SER:N	2.52	0.42
3:H:340:GLN:O	3:H:343:GLN:N	2.52	0.42
3:H:466:ASP:O	3:H:467:GLU:C	2.55	0.42
1:A:502:SER:O	1:A:503:CYS:CB	2.68	0.41
3:H:434:GLN:O	3:H:437:GLN:N	2.53	0.41
1:A:708:GLN:C	1:A:709:LYS:CD	2.88	0.41
1:C:111:ARG:NE	2:D:290:CYS:SG	2.93	0.41
1:C:562:THR:CG2	1:C:563:ASP:N	2.82	0.41
1:A:499:SER:CB	3:E:238:GLU:CB	2.98	0.41
1:A:641:PHE:CD1	1:A:641:PHE:C	2.93	0.41
1:A:712:ILE:O	1:A:713:ARG:O	2.38	0.41
1:A:111:ARG:NH2	2:B:292:TRP:CD1	2.89	0.41
1:A:708:GLN:C	1:A:709:LYS:CE	2.88	0.41
1:C:564:ILE:CG2	1:C:564:ILE:O	2.66	0.41
1:C:430:VAL:CG1	1:C:431:GLY:N	2.83	0.41
1:C:110:ASP:OD1	1:C:141:LYS:NZ	2.54	0.41
1:C:565:SER:OG	1:C:567:ARG:NH1	2.54	0.41
1:A:705:ASP:OD1	1:A:705:ASP:C	2.59	0.41
3:E:596:PHE:O	3:E:597:ILE:CG1	2.68	0.41
1:A:643:SER:O	1:A:644:LEU:C	2.59	0.41
1:C:643:SER:O	1:C:644:LEU:C	2.59	0.41
3:H:461:LEU:CD2	3:H:493:GLN:CB	2.99	0.41
1:A:110:ASP:OD1	1:A:141:LYS:NZ	2.54	0.41
1:A:498:ILE:CD1	1:A:498:ILE:N	2.84	0.41
1:C:457:THR:CG2	1:C:459:PHE:O	2.69	0.41
6:S:8:DA:C2	6:S:9:DA:N6	2.88	0.41
1:A:705:ASP:O	1:A:707:ILE:N	2.55	0.40
1:C:507:GLN:NE2	1:C:553:SER:N	2.69	0.40
6:U:8:DA:C2	6:U:9:DA:N6	2.88	0.40
1:A:726:TYR:OH	1:A:796:GLN:NE2	2.54	0.40
1:C:498:ILE:N	1:C:498:ILE:CD1	2.84	0.40
1:C:394:ILE:O	1:C:672:ASN:N	2.54	0.40
1:C:392:ASN:ND2	1:C:1012:LEU:O	2.54	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:450:GLY:O	3:H:451:GLU:CB	2.69	0.40
1:A:414:ARG:CB	1:A:462:ASN:ND2	2.85	0.40
1:A:565:SER:OG	1:A:567:ARG:NH1	2.54	0.40
3:H:293:TRP:CH2	3:H:370:SER:CB	3.05	0.40
1:C:1057:ARG:NH1	1:C:1109:VAL:O	2.55	0.40
1:A:457:THR:CG2	1:A:459:PHE:O	2.69	0.40
1:A:507:GLN:NE2	1:A:553:SER:N	2.70	0.40
1:C:585:GLU:CD	3:H:301:ILE:CG2	2.89	0.40
3:E:358:ARG:O	3:E:420:ARG:NH2	2.55	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	1095/1144 (96%)	948 (87%)	105 (10%)	42 (4%)	5	51
1	C	1095/1144 (96%)	967 (88%)	97 (9%)	31 (3%)	8	59
2	B	353/382 (92%)	333 (94%)	16 (4%)	4 (1%)	21	78
2	D	353/382 (92%)	333 (94%)	16 (4%)	4 (1%)	21	78
3	E	701/726 (97%)	603 (86%)	73 (10%)	25 (4%)	5	52
3	H	701/726 (97%)	604 (86%)	72 (10%)	25 (4%)	5	52
4	F	19/98 (19%)	14 (74%)	2 (10%)	3 (16%)	0	8
4	I	19/98 (19%)	16 (84%)	2 (10%)	1 (5%)	3	41
All	All	4336/4700 (92%)	3818 (88%)	383 (9%)	135 (3%)	7	57

All (135) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	LEU
1	A	390	ILE
1	A	430	VAL

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Mol	Chain	Res	Type
1	A	583	GLY
1	A	598	SER
1	A	672	ASN
1	A	707	ILE
1	A	708	GLN
1	A	711	HIS
1	A	712	ILE
1	A	713	ARG
1	A	715	VAL
1	A	841	ALA
1	C	367	LEU
1	C	430	VAL
1	C	583	GLY
1	C	598	SER
1	C	672	ASN
1	C	674	LYS
1	C	708	GLN
3	E	204	LYS
3	E	431	TYR
3	E	515	MET
3	E	556	PRO
3	E	595	ARG
3	E	597	ILE
3	E	902	ASP
4	F	34	ALA
4	F	38	VAL
3	H	204	LYS
3	H	431	TYR
3	H	515	MET
3	H	902	ASP
4	I	38	VAL
1	A	389	ILE
1	A	392	ASN
1	A	549	SER
1	A	562	THR
1	A	563	ASP
1	A	584	GLY
1	A	674	LYS
1	A	855	ASP
1	A	1110	ALA
2	B	117	SER
1	C	547	GLY

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Mol	Chain	Res	Type
1	C	549	SER
1	C	562	THR
1	C	563	ASP
1	C	584	GLY
1	C	855	ASP
1	C	1110	ALA
2	D	117	SER
3	E	337	ILE
3	E	435	THR
3	E	596	PHE
3	E	761	GLU
3	E	880	PRO
3	E	912	ILE
3	H	206	LYS
3	H	230	SER
3	H	231	THR
3	H	338	SER
3	H	435	THR
3	H	761	GLU
3	H	880	PRO
3	H	912	ILE
1	A	372	GLN
1	A	418	ASN
1	A	449	MET
1	A	481	GLN
1	A	547	GLY
1	A	624	SER
1	A	644	LEU
1	A	710	LEU
1	A	1109	VAL
1	C	418	ASN
1	C	449	MET
1	C	481	GLN
1	C	624	SER
1	C	644	LEU
1	C	1109	VAL
3	E	557	ASN
3	H	340	GLN
3	H	341	LYS
3	H	468	ASN
1	A	36	ASN
1	A	488	SER

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Mol	Chain	Res	Type
2	B	190	GLY
1	C	36	ASN
1	C	372	GLN
1	C	488	SER
1	C	503	CYS
2	D	190	GLY
3	E	338	SER
3	E	340	GLN
3	E	451	GLU
3	E	699	PRO
3	H	699	PRO
1	A	503	CYS
1	A	592	LEU
1	C	242	GLY
1	C	592	LEU
2	D	291	ASP
3	E	790	ALA
3	H	360	GLY
3	H	467	GLU
3	H	556	PRO
3	H	790	ALA
1	A	242	GLY
1	A	460	CYS
2	B	291	ASP
1	C	460	CYS
4	F	35	TRP
1	A	493	PRO
1	A	551	GLY
2	B	118	ILE
1	C	493	PRO
1	C	551	GLY
2	D	118	ILE
3	E	301	ILE
3	E	688	PRO
3	E	881	VAL
3	H	301	ILE
3	H	688	PRO
3	H	881	VAL
1	A	406	GLY
1	C	406	GLY
3	E	516	VAL
3	H	516	VAL

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Mol	Chain	Res	Type
1	A	523	PRO
1	A	716	PRO
1	C	523	PRO
3	E	206	LYS
3	E	486	GLY
3	H	486	GLY

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	938/1000 (94%)	847 (90%)	91 (10%)	12	51
1	C	944/1000 (94%)	854 (90%)	90 (10%)	12	52
2	B	306/335 (91%)	283 (92%)	23 (8%)	19	65
2	D	313/335 (93%)	290 (93%)	23 (7%)	20	66
3	E	625/660 (95%)	535 (86%)	90 (14%)	5	31
3	H	631/660 (96%)	548 (87%)	83 (13%)	6	35
4	F	17/83 (20%)	13 (76%)	4 (24%)	1	9
4	I	16/83 (19%)	14 (88%)	2 (12%)	7	38
All	All	3790/4156 (91%)	3384 (89%)	406 (11%)	10	47

All (406) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	81	THR
1	A	99	ASP
1	A	133	LEU
1	A	147	ARG
1	A	159	LEU
1	A	167	VAL
1	A	191	LYS
1	A	241	ASN
1	A	267	ASN
1	A	304	LEU

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Mol	Chain	Res	Type
1	A	314	LEU
1	A	334	VAL
1	A	339	ASP
1	A	360	VAL
1	A	370	GLN
1	A	396	ILE
1	A	403	ASP
1	A	410	LEU
1	A	412	PRO
1	A	414	ARG
1	A	419	ARG
1	A	420	GLU
1	A	452	VAL
1	A	454	ASP
1	A	469	ILE
1	A	473	SER
1	A	476	VAL
1	A	481	GLN
1	A	482	GLU
1	A	487	VAL
1	A	493	PRO
1	A	510	VAL
1	A	518	TYR
1	A	523	PRO
1	A	525	GLU
1	A	531	HIS
1	A	540	CYS
1	A	555	LEU
1	A	560	LEU
1	A	563	ASP
1	A	567	ARG
1	A	576	LEU
1	A	582	LEU
1	A	587	ILE
1	A	594	THR
1	A	596	PHE
1	A	597	GLU
1	A	602	LEU
1	A	603	LEU
1	A	608	ASP
1	A	614	PHE
1	A	616	LEU

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Mol	Chain	Res	Type
1	A	617	ASN
1	A	618	ILE
1	A	623	LEU
1	A	625	ASP
1	A	627	LYS
1	A	646	THR
1	A	673	LEU
1	A	688	PRO
1	A	689	ASP
1	A	700	THR
1	A	704	ILE
1	A	707	ILE
1	A	709	LYS
1	A	710	LEU
1	A	728	GLU
1	A	809	GLN
1	A	820	LYS
1	A	839	GLU
1	A	840	GLU
1	A	844	LYS
1	A	864	LYS
1	A	867	LYS
1	A	881	LEU
1	A	898	GLU
1	A	899	LEU
1	A	901	THR
1	A	914	LEU
1	A	931	LEU
1	A	957	VAL
1	A	966	LEU
1	A	970	ASN
1	A	984	THR
1	A	1000	LEU
1	A	1052	LEU
1	A	1086	THR
1	A	1093	LEU
1	A	1106	GLN
1	A	1129	LEU
2	B	111	LYS
2	B	116	GLN
2	B	134	LEU
2	B	148	ARG

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Mol	Chain	Res	Type
2	B	174	LEU
2	B	179	VAL
2	B	219	LEU
2	B	243	VAL
2	B	254	THR
2	B	262	LEU
2	B	274	GLU
2	B	293	LEU
2	B	299	VAL
2	B	308	LEU
2	B	312	LYS
2	B	321	MET
2	B	374	LEU
2	B	389	VAL
2	B	393	TYR
2	B	400	LEU
2	B	435	SER
2	B	437	THR
2	B	453	ASN
1	C	7	VAL
1	C	81	THR
1	C	99	ASP
1	C	133	LEU
1	C	147	ARG
1	C	159	LEU
1	C	167	VAL
1	C	191	LYS
1	C	241	ASN
1	C	267	ASN
1	C	304	LEU
1	C	314	LEU
1	C	334	VAL
1	C	339	ASP
1	C	360	VAL
1	C	370	GLN
1	C	396	ILE
1	C	403	ASP
1	C	410	LEU
1	C	412	PRO
1	C	414	ARG
1	C	419	ARG
1	C	420	GLU

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Mol	Chain	Res	Type
1	C	452	VAL
1	C	454	ASP
1	C	469	ILE
1	C	473	SER
1	C	476	VAL
1	C	481	GLN
1	C	482	GLU
1	C	487	VAL
1	C	493	PRO
1	C	510	VAL
1	C	518	TYR
1	C	523	PRO
1	C	525	GLU
1	C	531	HIS
1	C	540	CYS
1	C	555	LEU
1	C	560	LEU
1	C	563	ASP
1	C	567	ARG
1	C	576	LEU
1	C	582	LEU
1	C	587	ILE
1	C	594	THR
1	C	596	PHE
1	C	597	GLU
1	C	602	LEU
1	C	603	LEU
1	C	608	ASP
1	C	614	PHE
1	C	616	LEU
1	C	617	ASN
1	C	618	ILE
1	C	623	LEU
1	C	625	ASP
1	C	627	LYS
1	C	646	THR
1	C	655	ARG
1	C	663	ASN
1	C	673	LEU
1	C	688	PRO
1	C	689	ASP
1	C	700	THR

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Mol	Chain	Res	Type
1	C	703	THR
1	C	704	ILE
1	C	708	GLN
1	C	713	ARG
1	C	728	GLU
1	C	809	GLN
1	C	820	LYS
1	C	844	LYS
1	C	864	LYS
1	C	867	LYS
1	C	881	LEU
1	C	898	GLU
1	C	899	LEU
1	C	901	THR
1	C	914	LEU
1	C	931	LEU
1	C	957	VAL
1	C	966	LEU
1	C	970	ASN
1	C	984	THR
1	C	1000	LEU
1	C	1052	LEU
1	C	1086	THR
1	C	1093	LEU
1	C	1129	LEU
2	D	111	LYS
2	D	116	GLN
2	D	134	LEU
2	D	148	ARG
2	D	174	LEU
2	D	179	VAL
2	D	219	LEU
2	D	243	VAL
2	D	254	THR
2	D	262	LEU
2	D	274	GLU
2	D	293	LEU
2	D	299	VAL
2	D	308	LEU
2	D	312	LYS
2	D	321	MET
2	D	374	LEU

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Mol	Chain	Res	Type
2	D	389	VAL
2	D	393	TYR
2	D	400	LEU
2	D	435	SER
2	D	437	THR
2	D	453	ASN
3	E	198	LEU
3	E	211	ASN
3	E	214	ASP
3	E	217	TRP
3	E	233	ILE
3	E	235	TYR
3	E	251	LYS
3	E	255	ASN
3	E	256	LEU
3	E	259	GLN
3	E	260	LEU
3	E	263	ILE
3	E	288	LYS
3	E	297	CYS
3	E	310	LEU
3	E	316	LEU
3	E	324	ILE
3	E	339	ASP
3	E	340	GLN
3	E	341	LYS
3	E	343	GLN
3	E	352	LEU
3	E	359	ASN
3	E	366	SER
3	E	378	LEU
3	E	379	GLN
3	E	395	ARG
3	E	428	LEU
3	E	429	ILE
3	E	433	ASP
3	E	434	GLN
3	E	435	THR
3	E	437	GLN
3	E	443	THR
3	E	451	GLU
3	E	454	THR

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Mol	Chain	Res	Type
3	E	458	GLN
3	E	459	LYS
3	E	465	LEU
3	E	468	ASN
3	E	484	ARG
3	E	488	GLN
3	E	493	GLN
3	E	503	SER
3	E	504	THR
3	E	513	LYS
3	E	520	LEU
3	E	532	ILE
3	E	539	LYS
3	E	544	MET
3	E	548	PHE
3	E	551	PHE
3	E	552	ILE
3	E	555	ARG
3	E	570	LYS
3	E	577	GLU
3	E	580	ASP
3	E	581	GLU
3	E	588	ASP
3	E	592	ILE
3	E	596	PHE
3	E	597	ILE
3	E	611	LEU
3	E	619	LYS
3	E	627	LYS
3	E	641	PHE
3	E	653	GLU
3	E	666	MET
3	E	667	GLN
3	E	691	VAL
3	E	695	VAL
3	E	723	TRP
3	E	726	THR
3	E	778	LEU
3	E	791	ARG
3	E	814	PHE
3	E	816	HIS
3	E	827	GLN

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Mol	Chain	Res	Type
3	E	835	GLN
3	E	845	ASP
3	E	859	LYS
3	E	863	THR
3	E	874	TYR
3	E	877	LEU
3	E	878	LYS
3	E	886	LEU
3	E	895	ASP
3	E	897	ASP
3	E	901	ARG
3	E	905	ASN
4	F	19	LYS
4	F	25	LYS
4	F	35	TRP
4	F	37	ILE
3	H	198	LEU
3	H	211	ASN
3	H	214	ASP
3	H	217	TRP
3	H	229	ASN
3	H	235	TYR
3	H	251	LYS
3	H	255	ASN
3	H	256	LEU
3	H	259	GLN
3	H	260	LEU
3	H	263	ILE
3	H	288	LYS
3	H	297	CYS
3	H	310	LEU
3	H	316	LEU
3	H	324	ILE
3	H	340	GLN
3	H	341	LYS
3	H	342	VAL
3	H	343	GLN
3	H	352	LEU
3	H	363	ILE
3	H	366	SER
3	H	379	GLN
3	H	395	ARG

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Mol	Chain	Res	Type
3	H	429	ILE
3	H	430	THR
3	H	443	THR
3	H	454	THR
3	H	458	GLN
3	H	459	LYS
3	H	465	LEU
3	H	468	ASN
3	H	484	ARG
3	H	488	GLN
3	H	493	GLN
3	H	503	SER
3	H	504	THR
3	H	513	LYS
3	H	520	LEU
3	H	532	ILE
3	H	539	LYS
3	H	544	MET
3	H	548	PHE
3	H	551	PHE
3	H	552	ILE
3	H	556	PRO
3	H	570	LYS
3	H	577	GLU
3	H	580	ASP
3	H	581	GLU
3	H	588	ASP
3	H	592	ILE
3	H	595	ARG
3	H	611	LEU
3	H	619	LYS
3	H	627	LYS
3	H	641	PHE
3	H	653	GLU
3	H	666	MET
3	H	667	GLN
3	H	691	VAL
3	H	695	VAL
3	H	723	TRP
3	H	726	THR
3	H	778	LEU
3	H	791	ARG

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Mol	Chain	Res	Type
3	H	814	PHE
3	H	816	HIS
3	H	827	GLN
3	H	835	GLN
3	H	845	ASP
3	H	859	LYS
3	H	863	THR
3	H	874	TYR
3	H	877	LEU
3	H	878	LYS
3	H	886	LEU
3	H	895	ASP
3	H	897	ASP
3	H	901	ARG
3	H	905	ASN
4	I	19	LYS
4	I	25	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
5	3DR	R	9	5	9,11,12	1.54	1 (11%)	11,14,17	0.85	0
5	3DR	T	9	5	9,11,12	1.51	1 (11%)	11,14,17	0.85	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	3DR	R	9	5	-	0/4/15/16	0/1/1/1
5	3DR	T	9	5	-	0/4/15/16	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	9	3DR	P-OP1	4.51	1.51	1.46
5	T	9	3DR	P-OP1	4.42	1.51	1.46

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates 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, 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	1105/1144 (96%)	0.76	80 (7%) 15 22	98, 183, 251, 326	0
1	C	1105/1144 (96%)	0.79	99 (8%) 10 18	130, 197, 349, 378	0
2	B	355/382 (92%)	0.98	37 (10%) 7 15	275, 328, 394, 423	0
2	D	355/382 (92%)	0.81	34 (9%) 8 16	193, 275, 343, 370	0
3	E	709/726 (97%)	0.87	78 (11%) 6 14	131, 321, 394, 414	0
3	H	709/726 (97%)	0.87	72 (10%) 7 15	226, 289, 381, 399	0
4	F	21/98 (21%)	1.20	6 (28%) 1 4	368, 383, 396, 398	0
4	I	21/98 (21%)	1.78	9 (42%) 1 3	340, 358, 380, 389	0
5	R	12/12 (100%)	2.52	7 (58%) 0 3	301, 328, 376, 403	0
5	T	12/12 (100%)	1.71	4 (33%) 1 4	257, 350, 356, 358	0
6	S	12/12 (100%)	1.49	2 (16%) 2 8	317, 326, 386, 386	0
6	U	12/12 (100%)	1.67	6 (50%) 0 3	286, 320, 350, 363	0
All	All	4428/4748 (93%)	0.84	434 (9%) 8 16	98, 240, 379, 423	0

All (434) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	770	LEU	12.6
3	E	775	ASP	11.3
1	A	771	PHE	10.3
1	A	865	GLU	8.4
3	E	810	CYS	8.1
1	A	769	LYS	7.6
3	E	774	GLU	6.9
3	H	860	MET	6.6
5	R	3	DG	6.5
3	E	779	ARG	6.4
1	C	503	CYS	6.4

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Mol	Chain	Res	Type	RSRZ
1	C	934	ALA	5.5
2	B	242	CYS	5.3
1	A	540	CYS	5.3
1	A	832	GLY	5.3
3	E	684	MET	5.2
3	E	778	LEU	5.0
3	E	621	ALA	4.9
3	E	889	ARG	4.9
3	E	776	GLY	4.9
1	C	542	ASP	4.8
1	C	460	CYS	4.8
3	E	669	GLN	4.8
3	H	803	GLU	4.8
1	C	517	TYR	4.8
5	T	3	DG	4.7
6	U	14	DC	4.7
1	C	540	CYS	4.7
2	B	180	GLN	4.7
2	D	173	ILE	4.7
2	B	426	ALA	4.6
2	B	241	CYS	4.4
3	H	621	ALA	4.4
3	E	777	GLU	4.4
2	B	142	THR	4.4
3	E	661	GLN	4.4
2	D	174	LEU	4.3
2	D	242	CYS	4.3
2	B	141	ARG	4.2
1	A	503	CYS	4.2
3	E	811	ASN	4.2
3	E	737	LYS	4.2
1	A	768	SER	4.2
2	B	342	THR	4.2
3	E	665	TYR	4.2
1	A	863	GLU	4.2
2	D	429	ILE	4.1
3	E	813	ASP	4.1
3	E	693	MET	4.1
1	A	289	GLU	4.1
3	H	738	GLU	4.0
2	B	284	ALA	4.0
3	E	882	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
3	H	250	TYR	4.0
2	D	101	GLY	3.9
3	E	618	GLY	3.9
2	B	313	ASP	3.9
3	H	692	PRO	3.9
1	C	18	CYS	3.9
2	B	140	HIS	3.9
5	R	4	DC	3.9
3	H	728	GLY	3.9
3	E	685	GLY	3.9
1	C	289	GLU	3.9
2	B	312	LYS	3.9
5	R	14	DA	3.8
3	E	883	PRO	3.8
2	D	422	ASP	3.7
3	E	773	ILE	3.7
1	C	1015	GLN	3.7
2	D	430	SER	3.7
3	H	733	LYS	3.7
1	C	492	GLU	3.7
3	E	885	ASP	3.7
2	B	350	ARG	3.7
1	A	544	THR	3.7
1	A	871	TYR	3.7
2	B	445	MET	3.7
3	H	693	MET	3.7
3	E	890	ILE	3.7
3	H	802	ILE	3.6
1	C	290	GLN	3.6
3	H	694	GLU	3.6
2	B	314	LYS	3.6
3	E	577	GLU	3.6
3	E	736	PHE	3.5
6	S	14	DC	3.5
3	H	658	ILE	3.5
3	E	812	ASP	3.5
1	A	873	MET	3.5
3	E	666	MET	3.5
3	H	729	HIS	3.5
3	E	887	LYS	3.5
1	C	556	CYS	3.4
3	H	805	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	544	THR	3.4
3	H	730	CYS	3.4
1	C	832	GLY	3.4
2	D	363	ILE	3.4
1	C	64	MET	3.4
3	H	618	GLY	3.4
1	A	542	ASP	3.4
3	E	251	LYS	3.4
1	C	510	VAL	3.4
6	U	11	DT	3.3
1	A	725	CYS	3.3
3	H	577	GLU	3.3
3	H	861	ARG	3.3
3	E	504	THR	3.3
2	B	276	LEU	3.3
3	E	891	GLU	3.3
3	E	913	ALA	3.3
2	D	145	PRO	3.3
3	H	804	ASP	3.3
3	H	810	CYS	3.3
1	C	518	TYR	3.3
1	A	872	SER	3.3
1	C	262	ASN	3.3
3	E	860	MET	3.2
1	A	853	TYR	3.2
3	E	659	MET	3.2
5	T	10	DA	3.2
1	A	27	GLU	3.2
1	C	943	GLU	3.2
1	A	604	CYS	3.2
1	C	725	CYS	3.2
3	E	881	VAL	3.2
3	E	683	THR	3.1
1	C	593	MET	3.1
3	H	886	LEU	3.1
1	C	572	PRO	3.1
2	D	432	ASN	3.1
1	C	543	ILE	3.1
6	S	13	DG	3.1
1	C	591	ILE	3.1
4	I	29	ALA	3.1
3	E	689	THR	3.0

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Mol	Chain	Res	Type	RSRZ
3	E	664	GLN	3.0
3	H	890	ILE	3.0
2	B	209	PHE	3.0
1	A	592	LEU	3.0
2	B	315	ASN	3.0
2	B	364	ILE	3.0
2	D	362	GLN	3.0
1	A	833	THR	3.0
1	C	847	ARG	3.0
2	B	450	LEU	3.0
3	H	732	LEU	3.0
2	D	445	MET	3.0
1	C	490	TRP	3.0
3	H	659	MET	2.9
1	C	512	VAL	2.9
1	A	260	CYS	2.9
1	A	847	ARG	2.9
1	C	511	ALA	2.9
1	C	541	LEU	2.9
1	C	547	GLY	2.9
4	F	29	ALA	2.9
1	A	883	SER	2.9
3	E	573	ALA	2.9
3	E	524	ASP	2.9
3	E	814	PHE	2.9
1	C	604	CYS	2.8
3	H	882	LYS	2.8
1	C	263	ARG	2.8
1	C	519	LEU	2.8
1	C	592	LEU	2.8
2	D	424	ASN	2.8
1	C	910	MET	2.8
3	E	658	ILE	2.8
1	A	856	GLY	2.8
1	A	1062	ILE	2.8
2	B	427	GLY	2.8
1	C	363	CYS	2.8
1	A	591	ILE	2.8
4	I	31	ALA	2.8
1	A	815	SER	2.8
3	H	233	ILE	2.8
2	B	274	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
3	H	251	LYS	2.7
2	D	266	LEU	2.7
1	C	434	ARG	2.7
1	A	297	LEU	2.7
3	E	578	ALA	2.7
1	C	819	CYS	2.7
3	E	728	GLY	2.7
1	A	1	MET	2.7
2	D	183	THR	2.7
1	C	520	GLN	2.7
3	E	781	THR	2.7
3	H	234	LYS	2.7
2	B	231	ALA	2.7
1	C	935	TYR	2.7
3	H	207	PRO	2.7
3	H	859	LYS	2.7
3	H	725	SER	2.7
1	A	606	LEU	2.7
1	C	571	LEU	2.7
1	C	260	CYS	2.7
2	B	455	GLU	2.7
1	A	916	THR	2.7
2	D	164	ALA	2.7
4	I	23	GLU	2.7
4	I	38	VAL	2.7
1	A	593	MET	2.7
1	A	363	CYS	2.7
3	H	561	GLU	2.7
2	B	283	HIS	2.7
3	E	886	LEU	2.6
3	H	235	TYR	2.6
3	H	883	PRO	2.6
2	D	446	GLY	2.6
1	C	839	GLU	2.6
1	C	445	GLU	2.6
1	C	919	ASP	2.6
3	H	232	SER	2.6
1	C	504	ASN	2.6
1	C	1009	HIS	2.6
3	H	887	LYS	2.6
3	H	779	ARG	2.6
1	C	863	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1068	ILE	2.6
2	B	254	THR	2.6
4	I	37	ILE	2.6
5	R	13	DC	2.6
3	H	700	GLU	2.6
1	C	447	GLU	2.6
1	A	350	MET	2.6
1	C	827	THR	2.6
2	D	364	ILE	2.6
1	A	539	ALA	2.6
1	A	170	LEU	2.6
1	C	871	TYR	2.6
5	T	9	3DR	2.6
1	A	588	PRO	2.5
1	A	839	GLU	2.5
6	U	3	DT	2.5
1	A	652	CYS	2.5
3	E	738	GLU	2.5
1	C	461	GLY	2.5
3	H	748	PHE	2.5
4	I	28	ASN	2.5
3	E	884	ALA	2.5
3	E	660	ILE	2.5
1	A	541	LEU	2.5
3	H	787	CYS	2.5
1	A	290	GLN	2.5
4	F	21	ARG	2.5
1	A	870	VAL	2.5
2	B	404	ARG	2.5
3	H	721	LEU	2.5
1	C	411	TRP	2.5
3	E	729	HIS	2.5
3	H	630	LEU	2.5
2	B	421	ARG	2.5
1	C	313	CYS	2.5
2	B	272	PHE	2.5
1	C	790	ASN	2.4
2	B	208	LEU	2.4
1	A	470	GLN	2.4
1	A	938	MET	2.4
3	H	661	GLN	2.4
3	E	484	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	865	GLU	2.4
1	C	920	PHE	2.4
1	C	729	VAL	2.4
2	B	101	GLY	2.4
3	E	888	LYS	2.4
3	E	730	CYS	2.4
1	C	1023	PRO	2.4
1	C	945	ILE	2.4
4	I	19	LYS	2.4
3	H	637	CYS	2.4
3	E	852	ALA	2.4
1	C	364	VAL	2.4
2	D	423	PRO	2.4
1	C	873	MET	2.4
3	E	250	TYR	2.4
1	A	246	LEU	2.4
6	U	4	DG	2.4
1	C	509	VAL	2.4
1	C	539	ALA	2.4
3	H	595	ARG	2.4
3	H	689	THR	2.4
1	C	911	ALA	2.4
1	A	831	VAL	2.3
1	C	932	LEU	2.3
3	E	692	PRO	2.3
3	E	619	LYS	2.3
1	C	98	ILE	2.3
1	A	866	VAL	2.3
3	H	801	ASP	2.3
1	A	862	ALA	2.3
1	C	179	CYS	2.3
3	H	769	GLN	2.3
1	A	724	ILE	2.3
1	C	1124	ALA	2.3
3	H	358	ARG	2.3
3	H	533	CYS	2.3
3	E	668	ASN	2.3
3	H	470	ILE	2.3
3	H	724	GLN	2.3
3	E	677	LEU	2.3
3	E	802	ILE	2.3
2	D	426	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
3	E	780	ARG	2.3
3	H	554	LYS	2.3
1	C	315	THR	2.3
1	C	288	GLU	2.3
3	E	725	SER	2.3
2	D	276	LEU	2.3
1	A	1015	GLN	2.3
3	H	688	PRO	2.3
1	C	508	VAL	2.3
1	A	882	ALA	2.3
1	A	737	SER	2.3
1	C	446	THR	2.3
2	D	425	ALA	2.3
1	A	543	ILE	2.3
3	H	436	THR	2.3
2	B	273	LYS	2.3
3	H	691	VAL	2.3
1	A	864	LYS	2.2
1	C	531	HIS	2.2
2	D	414	GLY	2.2
3	E	670	ASN	2.2
1	C	185	PRO	2.2
3	H	806	ASP	2.2
2	D	314	LYS	2.2
3	H	775	ASP	2.2
1	C	1008	CYS	2.2
3	E	739	GLY	2.2
1	C	448	LEU	2.2
1	A	545	PRO	2.2
1	C	497	ASN	2.2
1	C	953	TRP	2.2
2	D	444	GLY	2.2
3	E	688	PRO	2.2
3	H	737	LYS	2.2
3	E	847	GLN	2.2
2	B	262	LEU	2.2
2	D	421	ARG	2.2
1	C	529	ILE	2.2
1	A	752	LEU	2.2
4	F	19	LYS	2.2
5	R	8	DT	2.2
5	T	4	DC	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	126	PRO	2.2
3	H	813	ASP	2.2
2	B	282	THR	2.2
3	E	505	ILE	2.2
1	A	2	SER	2.2
3	H	770	ALA	2.2
1	C	261	HIS	2.2
3	H	833	GLU	2.2
1	A	922	LEU	2.2
1	A	1067	LYS	2.2
1	C	65	GLU	2.2
3	E	880	PRO	2.2
1	C	459	PHE	2.2
3	H	273	HIS	2.2
2	B	122	LEU	2.2
3	E	896	ARG	2.2
1	C	170	LEU	2.2
1	C	295	VAL	2.2
1	A	704	ILE	2.2
3	H	891	GLU	2.2
1	A	858	LEU	2.2
1	C	502	SER	2.1
1	C	808	LEU	2.1
2	B	243	VAL	2.1
2	D	241	CYS	2.1
1	A	395	GLY	2.1
1	C	926	LEU	2.1
2	D	184	SER	2.1
3	H	484	ARG	2.1
3	H	636	GLU	2.1
1	C	872	SER	2.1
1	C	828	TYR	2.1
1	A	867	LYS	2.1
1	C	1024	THR	2.1
2	D	172	ILE	2.1
1	C	1140	HIS	2.1
2	D	165	VAL	2.1
1	A	1064	SER	2.1
1	A	462	ASN	2.1
3	E	514	THR	2.1
1	C	528	GLN	2.1
3	H	734	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
4	F	35	TRP	2.1
1	A	736	LEU	2.1
3	H	272	ILE	2.1
1	C	507	GLN	2.1
4	F	34	ALA	2.1
1	A	827	THR	2.1
5	R	7	DC	2.1
6	U	12	DA	2.1
5	R	5	DT	2.1
2	D	146	PHE	2.1
1	A	1092	ASP	2.1
3	E	365	ARG	2.1
3	E	892	SER	2.1
4	I	22	PHE	2.1
1	A	62	ALA	2.1
1	C	1093	LEU	2.1
3	E	511	LYS	2.1
1	C	527	ARG	2.1
6	U	13	DG	2.1
2	B	442	ALA	2.1
1	A	583	GLY	2.1
1	A	1090	ASP	2.1
2	B	245	VAL	2.1
3	E	724	GLN	2.1
3	H	483	VAL	2.1
3	H	746	SER	2.1
3	H	622	SER	2.0
1	C	833	THR	2.0
3	E	335	HIS	2.0
1	A	64	MET	2.0
1	A	566	ALA	2.0
3	H	703	LYS	2.0
1	A	522	HIS	2.0
1	C	557	ALA	2.0
3	E	599	GLY	2.0
3	E	768	LYS	2.0
2	D	267	ASP	2.0
2	D	428	ILE	2.0
1	A	612	PHE	2.0
1	A	556	CYS	2.0
1	C	395	GLY	2.0
1	A	812	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
4	F	28	ASN	2.0
4	I	21	ARG	2.0
2	D	187	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	3DR	T	9	11/12	0.59	1.93	347,358,362,362	0
5	3DR	R	9	11/12	0.40	0.36	318,324,336,339	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.