



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:00 PM UTC

PDB ID : 5W94 / pdb_00005w94
Title : Crystal structure of Scc4 in complex with Scc2n and Ctf19n
Authors : Hinshaw, S.M.; Harrison, S.C.
Deposited on : 2017-06-22
Resolution : 3.19 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:

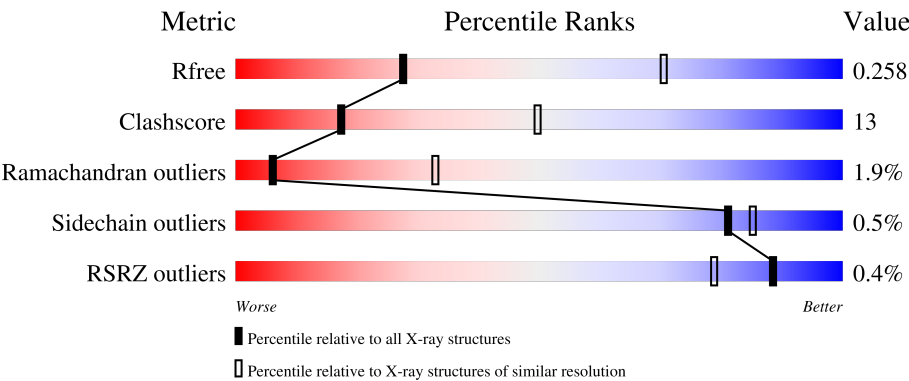
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	624	
1	C	624	
2	B	184	
2	D	184	
3	E	6	

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Mol	Chain	Length	Quality of chain
3	H	6	33%33%33%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11738 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 MAU2 chromatid cohesion factor homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	617	Total	C	N	O	S	0	0	0
			5008	3216	840	915	37			
1	C	605	Total	C	N	O	S	0	0	0
			4928	3168	826	897	37			

- Molecule 2 is a protein called Sister chromatid cohesion protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	114	Total	C	N	O	S	0	0	0
			874	553	150	170	1			
2	D	110	Total	C	N	O	S	0	0	0
			848	541	144	162	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	SER	-	expression tag	UNP Q04002
B	-1	ASN	-	expression tag	UNP Q04002
B	0	ALA	-	expression tag	UNP Q04002
D	-2	SER	-	expression tag	UNP Q04002
D	-1	ASN	-	expression tag	UNP Q04002
D	0	ALA	-	expression tag	UNP Q04002

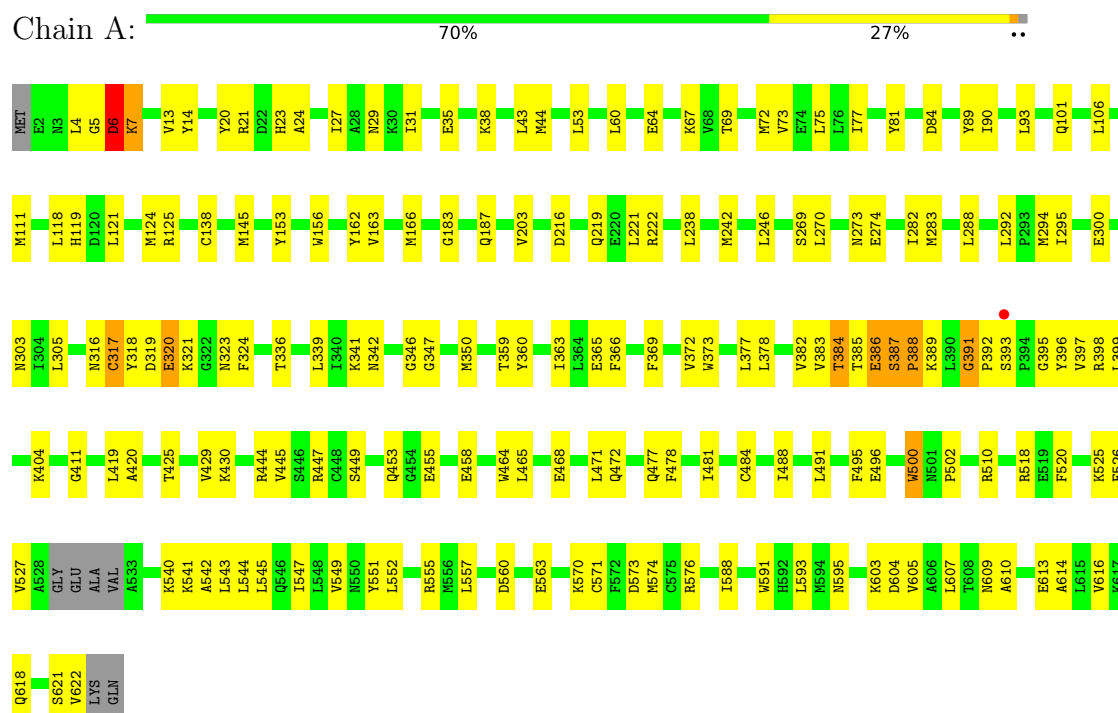
- Molecule 3 is a protein called Ctf19n.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	4	Total	C	N	O	P	0	0	0
			40	20	4	14	2			
3	H	4	Total	C	N	O	P	0	0	0
			40	20	4	14	2			

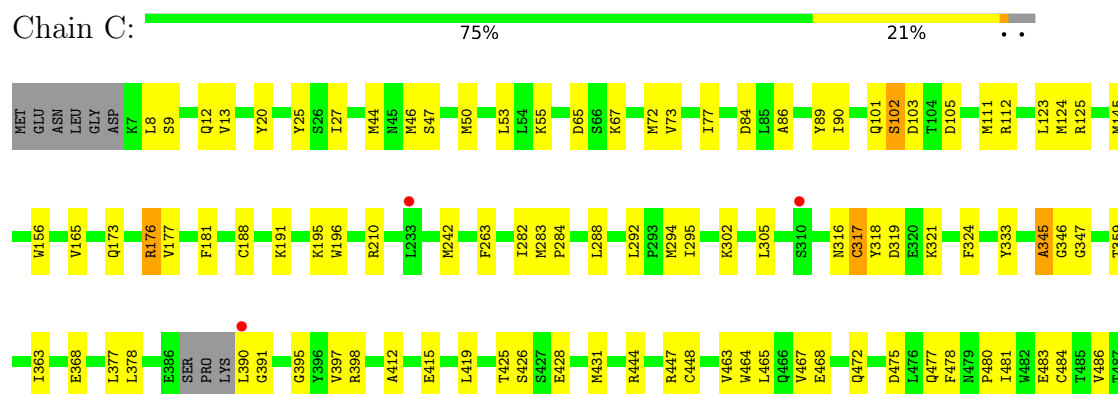
3 Residue-property plots

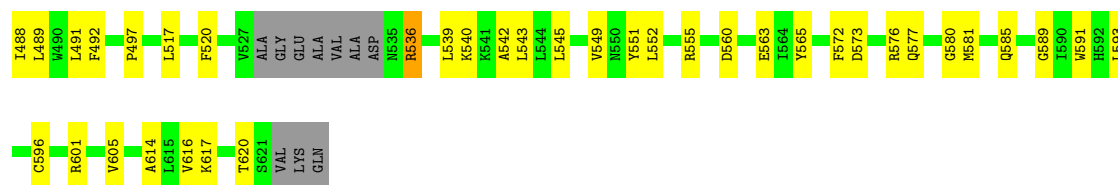
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: MAU2 chromatid cohesion factor homolog

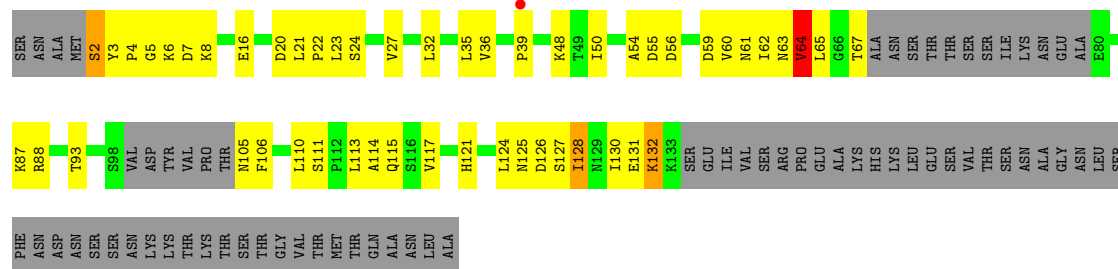
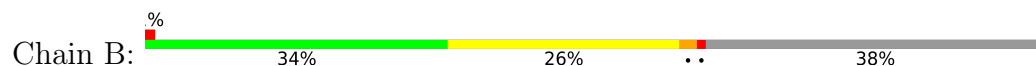


- Molecule 1: MAU2 chromatid cohesion factor homolog

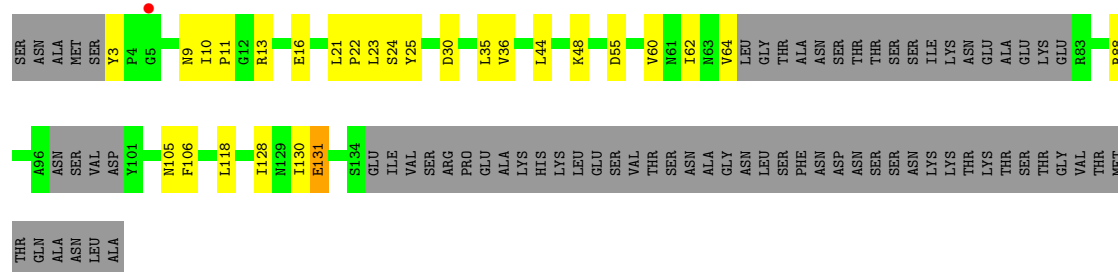




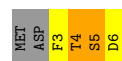
• Molecule 2: Sister chromatid cohesion protein 2



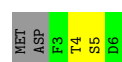
• Molecule 2: Sister chromatid cohesion protein 2



• Molecule 3: Ctf19n



• Molecule 3: Ctf19n



4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	172.97Å 172.97Å 145.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.94 – 3.19 39.94 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.1 (39.94-3.19) 99.0 (39.94-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 3.18Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.209 , 0.258 0.211 , 0.258	Depositor DCC
R_{free} test set	1998 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	112.6	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.037 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11738	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.54	0/5107	0.81	3/6888 (0.0%)
1	C	0.42	0/5025	0.72	1/6775 (0.0%)
2	B	0.65	0/887	1.00	2/1198 (0.2%)
2	D	0.44	0/863	0.76	0/1169
3	E	0.30	0/18	0.19	0/21
3	H	0.43	0/18	0.50	0/21
All	All	0.50	0/11918	0.78	6/16072 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	345	ALA	N-CA-C	-6.03	101.56	110.48
1	A	6	ASP	CA-C-N	5.74	132.50	121.54
1	A	6	ASP	C-N-CA	5.74	132.50	121.54
2	B	125	ASN	CA-C-N	5.28	131.23	122.62
2	B	125	ASN	C-N-CA	5.28	131.23	122.62
1	A	500	TRP	CA-CB-CG	5.08	123.24	113.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5008	0	5059	161	1
1	C	4928	0	4986	98	0
2	B	874	0	885	57	1
2	D	848	0	864	22	1
3	E	40	0	21	2	0
3	H	40	0	22	0	0
All	All	11738	0	11837	295	2

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 13.

All (295) 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)
2:B:65:LEU:HD11	2:B:121:HIS:CD2	1.49	1.45
2:B:65:LEU:CD1	2:B:121:HIS:HD2	1.42	1.30
2:B:65:LEU:CD1	2:B:121:HIS:CD2	2.22	1.18
1:A:6:ASP:O	1:A:7:LYS:HG3	1.53	1.08
2:B:61:ASN:ND2	2:B:63:ASN:OD1	1.99	0.93
1:A:6:ASP:OD1	2:B:63:ASN:OD1	1.87	0.92
1:A:318:TYR:OH	1:A:541:LYS:O	1.93	0.85
2:B:65:LEU:HD12	2:B:121:HIS:HD2	1.42	0.84
1:A:6:ASP:OD1	2:B:61:ASN:ND2	2.16	0.79
1:A:616:VAL:HG12	2:B:8:LYS:NZ	1.96	0.79
1:A:616:VAL:HG12	2:B:8:LYS:HZ3	1.47	0.79
1:A:111:MET:HE2	1:A:156:TRP:HB3	1.64	0.79
1:A:320:GLU:HG2	1:A:321:LYS:H	1.49	0.77
1:A:145:MET:HE1	1:A:156:TRP:HB2	1.67	0.76
1:A:525:LYS:O	1:A:527:VAL:N	2.15	0.76
1:A:491:LEU:HD12	1:A:552:LEU:HD21	1.67	0.75
1:C:483:GLU:OE2	1:C:536:ARG:NH1	2.21	0.74
1:C:8:LEU:HD12	2:D:62:ILE:HG21	1.67	0.74
1:C:555:ARG:HD3	1:C:591:TRP:NE1	2.02	0.73
1:A:465:LEU:HD23	1:A:468:GLU:HG3	1.72	0.72
1:C:283:MET:HE2	1:C:284:PRO:O	1.89	0.72
1:A:616:VAL:CG1	2:B:8:LYS:HD2	2.20	0.71
1:C:53:LEU:HD11	2:D:64:VAL:HG13	1.71	0.70
1:A:73:VAL:HG11	1:A:90:ILE:HD11	1.74	0.69
1:A:6:ASP:CG	2:B:63:ASN:OD1	2.35	0.69
2:B:88:ARG:HB3	2:B:131:GLU:HB2	1.73	0.69
1:A:84:ASP:OD1	1:A:125:ARG:NH2	2.26	0.69
1:A:145:MET:HE3	1:A:153:TYR:HD1	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:616:VAL:O	1:C:620:THR:OG1	2.12	0.67
2:B:128:ILE:HD11	2:B:130:ILE:HD11	1.76	0.67
1:C:560:ASP:HB3	1:C:563:GLU:HG3	1.77	0.67
1:C:173:GLN:OE1	1:C:176:ARG:NH1	2.26	0.67
1:C:27:ILE:HD13	2:D:106:PHE:HD2	1.60	0.67
1:C:283:MET:HG2	1:C:284:PRO:HD2	1.77	0.66
1:C:84:ASP:OD1	1:C:125:ARG:NH2	2.29	0.65
1:A:27:ILE:HG21	2:B:106:PHE:HB3	1.80	0.64
1:A:111:MET:HE2	1:A:156:TRP:CB	2.29	0.63
1:C:112:ARG:NE	2:D:44:LEU:O	2.30	0.63
1:C:27:ILE:HD13	2:D:106:PHE:CD2	2.34	0.62
1:A:269:SER:O	1:A:273:ASN:HB3	1.99	0.62
1:A:21:ARG:HG3	1:A:75:LEU:HD21	1.81	0.62
3:E:5:SEP:OG	3:E:6:ASP:N	2.33	0.61
1:A:6:ASP:O	1:A:7:LYS:CG	2.39	0.61
1:A:387:SER:O	1:A:389:LYS:N	2.34	0.61
1:A:398:ARG:HG3	1:A:419:LEU:HD13	1.83	0.61
2:B:130:ILE:HG22	2:B:131:GLU:H	1.65	0.61
1:A:373:TRP:CD1	2:B:27:VAL:HG22	2.36	0.60
1:C:67:LYS:HE3	2:D:48:LYS:O	2.01	0.60
1:A:203:VAL:HG11	1:A:221:LEU:HD22	1.83	0.60
1:A:145:MET:HE1	1:A:156:TRP:CB	2.31	0.60
1:A:464:TRP:NE1	1:A:468:GLU:OE2	2.33	0.60
2:B:65:LEU:HA	2:B:124:LEU:HD11	1.85	0.59
1:A:24:ALA:HB3	1:A:44:MET:HE2	1.86	0.58
1:C:492:PHE:HE1	1:C:552:LEU:HD13	1.68	0.58
2:B:65:LEU:HD12	2:B:121:HIS:CD2	2.22	0.58
1:C:491:LEU:HD12	1:C:552:LEU:HD21	1.86	0.58
1:A:20:TYR:OH	2:B:114:ALA:O	2.21	0.58
1:A:363:ILE:HG12	2:B:35:LEU:HD21	1.86	0.58
1:A:385:THR:HG22	1:A:386:GLU:H	1.69	0.58
1:C:419:LEU:HD12	1:C:425:THR:HG21	1.84	0.58
1:A:373:TRP:NE1	2:B:27:VAL:HG22	2.19	0.57
1:C:73:VAL:HG21	1:C:90:ILE:HD11	1.86	0.57
1:C:111:MET:HE2	1:C:156:TRP:HB3	1.86	0.57
1:A:4:LEU:HD11	1:A:7:LYS:N	2.20	0.57
1:C:20:TYR:HB2	1:C:47:SER:HB2	1.87	0.56
1:A:399:LEU:HD22	1:A:429:VAL:HG13	1.86	0.56
1:A:591:TRP:NE1	1:A:595:ASN:HD21	2.02	0.56
2:B:22:PRO:O	2:B:24:SER:N	2.38	0.56
2:B:62:ILE:O	2:B:62:ILE:HG13	2.02	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:TYR:CE1	1:C:44:MET:HE1	2.41	0.56
1:A:67:LYS:HE3	2:B:48:LYS:O	2.05	0.56
1:A:484:CYS:HB2	1:A:520:PHE:CE1	2.40	0.55
1:A:294:MET:HE1	1:A:360:TYR:CE1	2.41	0.55
1:A:384:THR:HG23	1:A:385:THR:H	1.72	0.55
1:A:321:LYS:O	1:A:324:PHE:HB3	2.06	0.55
1:C:412:ALA:HA	1:C:415:GLU:HG2	1.88	0.55
1:A:616:VAL:HG11	2:B:8:LYS:HD2	1.89	0.55
1:C:210:ARG:HD2	1:C:475:ASP:OD2	2.07	0.54
2:D:22:PRO:O	2:D:24:SER:N	2.38	0.54
1:A:111:MET:HG3	1:A:156:TRP:CD2	2.41	0.54
1:A:455:GLU:O	1:A:458:GLU:HB3	2.07	0.54
1:A:525:LYS:C	1:A:527:VAL:H	2.11	0.54
1:A:77:ILE:HG23	1:A:124:MET:HG3	1.89	0.54
1:A:372:VAL:HG13	1:A:383:VAL:HG22	1.89	0.54
1:C:177:VAL:O	1:C:181:PHE:HB2	2.08	0.54
1:C:363:ILE:HG12	2:D:35:LEU:HD21	1.89	0.54
1:C:447:ARG:HB3	2:D:16:GLU:OE2	2.08	0.54
1:C:55:LYS:NZ	1:C:65:ASP:OD1	2.41	0.53
1:A:77:ILE:HD11	1:A:121:LEU:HG	1.89	0.53
2:D:128:ILE:HD11	2:D:130:ILE:HD11	1.91	0.53
1:C:210:ARG:NH1	1:C:475:ASP:OD2	2.36	0.53
1:A:81:TYR:CZ	2:B:87:LYS:HG2	2.43	0.53
1:A:518:ARG:NH1	1:A:557:LEU:HD22	2.24	0.53
1:A:573:ASP:O	1:A:576:ARG:HG2	2.08	0.53
1:A:4:LEU:HD13	1:A:5:GLY:N	2.24	0.53
1:A:111:MET:HG3	1:A:156:TRP:CE2	2.44	0.53
1:C:333:TYR:CE2	1:C:368:GLU:HG2	2.44	0.53
1:A:391:GLY:C	1:A:393:SER:H	2.16	0.52
1:C:188:CYS:HB3	1:C:195:LYS:HB2	1.90	0.52
1:A:73:VAL:HG21	1:A:90:ILE:HD11	1.91	0.52
1:A:53:LEU:HD23	2:B:62:ILE:HG22	1.90	0.52
1:C:497:PRO:HA	2:D:13:ARG:NH1	2.25	0.52
1:C:573:ASP:O	1:C:576:ARG:HG2	2.10	0.52
1:C:398:ARG:HG3	1:C:419:LEU:HD13	1.92	0.52
1:C:488:ILE:HD11	1:C:549:VAL:HG22	1.92	0.52
1:A:382:VAL:HG12	1:A:384:THR:H	1.75	0.51
1:A:542:ALA:HB3	1:A:545:LEU:HB3	1.92	0.51
1:A:616:VAL:CG1	2:B:8:LYS:NZ	2.72	0.51
1:A:472:GLN:O	1:A:477:GLN:NE2	2.44	0.51
1:C:492:PHE:CE1	1:C:552:LEU:HD13	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:PRO:O	1:A:389:LYS:HD3	2.10	0.51
1:C:242:MET:HE2	1:C:305:LEU:HD12	1.93	0.51
1:C:465:LEU:HD23	1:C:468:GLU:HG3	1.91	0.51
1:A:219:GLN:HG2	1:A:222:ARG:HH21	1.76	0.51
1:C:263:PHE:CE2	1:C:302:LYS:HD3	2.46	0.51
1:A:69:THR:HB	1:A:93:LEU:HD22	1.92	0.51
1:A:317:CYS:SG	1:A:378:LEU:HB2	2.51	0.51
1:A:481:ILE:HG23	1:A:545:LEU:HD22	1.93	0.51
2:B:65:LEU:HG	2:B:124:LEU:HG	1.93	0.50
1:C:565:TYR:CZ	1:C:601:ARG:HD3	2.47	0.50
1:A:359:THR:OG1	2:B:39:PRO:HD3	2.11	0.50
1:C:72:MET:HE1	1:C:89:TYR:CZ	2.47	0.50
1:A:366:PHE:CE1	1:A:392:PRO:HB2	2.47	0.50
1:A:540:LYS:O	1:A:542:ALA:N	2.42	0.50
1:C:282:ILE:HD11	1:C:288:LEU:HD12	1.92	0.50
1:A:72:MET:HE1	1:A:89:TYR:CZ	2.47	0.50
1:A:518:ARG:HG3	1:A:557:LEU:HD13	1.93	0.49
1:C:191:LYS:HG2	1:C:196:TRP:CZ2	2.47	0.49
1:A:14:TYR:CE1	2:B:50:ILE:HD11	2.47	0.49
1:A:555:ARG:HD3	1:A:591:TRP:NE1	2.28	0.49
1:A:551:TYR:CD1	1:A:588:ILE:HD13	2.47	0.49
1:C:77:ILE:HG23	1:C:124:MET:HG3	1.94	0.49
1:A:111:MET:HE2	1:A:156:TRP:CG	2.48	0.49
1:C:321:LYS:O	1:C:324:PHE:HB3	2.13	0.49
1:A:447:ARG:HB3	2:B:16:GLU:OE2	2.12	0.49
1:A:4:LEU:HD22	1:A:5:GLY:H	1.77	0.48
1:A:391:GLY:O	1:A:393:SER:N	2.46	0.48
1:C:543:LEU:HD22	1:C:577:GLN:HB2	1.94	0.48
1:A:73:VAL:HG21	1:A:90:ILE:CD1	2.43	0.48
1:A:119:HIS:HD2	1:A:163:VAL:HG22	1.78	0.48
1:C:86:ALA:O	1:C:90:ILE:HG12	2.12	0.48
1:C:614:ALA:HA	1:C:617:LYS:HE3	1.94	0.48
1:A:4:LEU:HD21	1:A:7:LYS:HB2	1.96	0.48
2:B:111:SER:O	2:B:115:GLN:HG3	2.13	0.48
1:C:165:VAL:HG11	1:C:181:PHE:CE2	2.48	0.48
1:A:5:GLY:O	1:A:6:ASP:HB2	2.14	0.48
1:A:593:LEU:HD11	1:A:605:VAL:HG13	1.95	0.48
1:A:119:HIS:CD2	1:A:163:VAL:HG22	2.49	0.48
1:A:295:ILE:HD11	2:B:36:VAL:HA	1.96	0.47
1:C:73:VAL:HG21	1:C:90:ILE:CD1	2.44	0.47
1:A:162:TYR:CE2	1:A:166:MET:HE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:PHE:CE1	1:A:510:ARG:HG2	2.50	0.47
1:A:242:MET:HE2	1:A:305:LEU:HD12	1.97	0.47
1:A:4:LEU:HD11	1:A:7:LYS:C	2.39	0.47
1:A:384:THR:CG2	1:A:404:LYS:HE3	2.45	0.47
1:C:173:GLN:OE1	1:C:176:ARG:HD3	2.15	0.47
1:A:447:ARG:HB3	2:B:16:GLU:CD	2.40	0.47
1:C:428:GLU:O	1:C:431:MET:N	2.47	0.47
1:C:316:ASN:HB3	1:C:319:ASP:OD1	2.15	0.47
2:D:88:ARG:HG2	2:D:131:GLU:HG2	1.96	0.47
1:A:488:ILE:HD11	1:A:549:VAL:HG22	1.96	0.46
1:C:391:GLY:CA	1:C:397:VAL:HG23	2.44	0.46
1:C:543:LEU:HD23	1:C:581:MET:HE2	1.97	0.46
1:C:589:GLY:O	1:C:593:LEU:N	2.45	0.46
1:A:24:ALA:CB	1:A:44:MET:HE2	2.46	0.46
1:A:477:GLN:HG3	1:A:478:PHE:CE1	2.50	0.46
2:B:54:ALA:C	2:B:56:ASP:H	2.23	0.46
1:A:320:GLU:O	1:A:323:ASN:HB2	2.16	0.46
1:A:346:GLY:HA3	1:A:347:GLY:HA2	1.77	0.46
1:A:111:MET:HE1	1:A:145:MET:SD	2.56	0.46
1:A:318:TYR:CE2	1:A:543:LEU:HB2	2.50	0.46
1:C:25:TYR:O	1:C:345:ALA:HB1	2.16	0.46
1:C:572:PHE:CE1	1:C:585:GLN:HG2	2.51	0.46
1:A:270:LEU:O	1:A:274:GLU:HB2	2.16	0.46
3:E:3:PHE:HD1	3:E:4:TPO:N	2.14	0.46
1:C:9:SER:N	1:C:12:GLN:OE1	2.46	0.45
1:A:500:TRP:CD1	2:B:16:GLU:OE2	2.69	0.45
1:C:601:ARG:O	1:C:605:VAL:HG23	2.15	0.45
1:A:616:VAL:CG1	2:B:8:LYS:CD	2.93	0.45
1:C:377:LEU:HD23	1:C:377:LEU:HA	1.79	0.45
1:A:27:ILE:O	1:A:31:ILE:HD12	2.17	0.45
1:C:426:SER:HB3	2:D:30:ASP:CG	2.42	0.45
1:C:444:ARG:O	1:C:448:CYS:HB2	2.16	0.45
1:A:316:ASN:O	1:A:318:TYR:N	2.50	0.45
1:A:560:ASP:HB3	1:A:563:GLU:HG3	1.99	0.45
1:A:616:VAL:HG13	2:B:8:LYS:HD2	1.95	0.45
1:A:29:ASN:HA	2:B:93:THR:HB	1.99	0.45
1:A:300:GLU:HG3	1:A:339:LEU:HD13	1.99	0.45
1:C:555:ARG:HG2	1:C:591:TRP:CZ2	2.52	0.45
1:A:216:ASP:OD1	1:A:216:ASP:N	2.50	0.44
1:C:13:VAL:HG13	1:C:50:MET:HE3	1.99	0.44
1:C:294:MET:HE3	1:C:359:THR:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LEU:CD1	1:A:6:ASP:H	2.31	0.44
1:C:464:TRP:CH2	1:C:486:VAL:HG13	2.53	0.44
1:C:472:GLN:O	1:C:477:GLN:NE2	2.50	0.44
1:A:282:ILE:HD11	1:A:288:LEU:HD12	2.00	0.44
1:A:607:LEU:O	1:A:610:ALA:N	2.50	0.44
1:A:465:LEU:HD23	1:A:465:LEU:HA	1.78	0.44
1:C:596:CYS:HB3	1:C:605:VAL:HG22	2.00	0.44
2:B:32:LEU:HA	2:B:32:LEU:HD23	1.78	0.44
1:C:292:LEU:HA	1:C:292:LEU:HD23	1.77	0.44
1:A:377:LEU:HD23	1:A:377:LEU:HA	1.83	0.44
2:D:88:ARG:HB3	2:D:131:GLU:HA	2.00	0.44
1:C:101:GLN:O	1:C:103:ASP:N	2.51	0.44
1:A:4:LEU:HD13	1:A:6:ASP:H	1.83	0.44
1:A:53:LEU:HA	1:A:53:LEU:HD12	1.66	0.44
1:A:419:LEU:HD12	1:A:425:THR:HG21	1.98	0.44
1:C:390:LEU:HB3	1:C:391:GLY:H	1.65	0.44
1:A:373:TRP:HE1	2:B:27:VAL:HG22	1.82	0.43
1:A:81:TYR:CE1	2:B:87:LYS:HG2	2.53	0.43
1:A:106:LEU:HD23	1:A:106:LEU:HA	1.78	0.43
2:B:64:VAL:HB	2:B:65:LEU:H	1.39	0.43
1:A:283:MET:HE2	1:A:283:MET:HB3	1.73	0.43
1:A:341:LYS:HG2	1:A:342:ASN:OD1	2.18	0.43
1:A:90:ILE:HG23	1:A:90:ILE:HD12	1.74	0.43
2:B:21:LEU:HD12	2:B:21:LEU:HA	1.63	0.43
1:C:477:GLN:HG3	1:C:478:PHE:CE1	2.54	0.43
2:B:132:LYS:HB3	2:B:132:LYS:HE2	1.65	0.43
2:D:10:ILE:HG23	2:D:11:PRO:HD2	2.00	0.43
2:B:105:ASN:C	2:B:106:PHE:CD1	2.96	0.43
1:A:246:LEU:HD12	1:A:246:LEU:HA	1.76	0.43
1:A:318:TYR:O	1:A:318:TYR:CD1	2.72	0.43
1:A:477:GLN:HG3	1:A:478:PHE:CD1	2.53	0.43
2:B:20:ASP:OD1	2:B:20:ASP:N	2.48	0.43
1:C:391:GLY:HA2	1:C:397:VAL:HG23	2.01	0.43
1:A:145:MET:HE2	1:A:153:TYR:O	2.19	0.42
2:B:124:LEU:C	2:B:126:ASP:H	2.27	0.42
1:C:295:ILE:HD11	2:D:36:VAL:HG13	2.01	0.42
1:C:395:GLY:HA2	1:C:398:ARG:HE	1.84	0.42
1:A:238:LEU:HD23	1:A:238:LEU:HA	1.75	0.42
2:B:59:ASP:OD1	2:B:59:ASP:N	2.52	0.42
1:C:123:LEU:HD23	1:C:123:LEU:HA	1.85	0.42
1:A:365:GLU:C	1:A:392:PRO:HG3	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:ASN:C	2:B:106:PHE:HD1	2.26	0.42
1:C:463:VAL:O	1:C:467:VAL:HG23	2.19	0.42
1:C:491:LEU:CD1	1:C:517:LEU:HD22	2.49	0.42
1:A:445:VAL:HG13	1:A:453:GLN:HE21	1.84	0.42
1:A:574:MET:O	1:A:576:ARG:N	2.52	0.42
1:C:481:ILE:HD11	1:C:540:LYS:HB2	2.01	0.42
1:A:23:HIS:HD2	1:A:43:LEU:HD11	1.85	0.42
1:A:124:MET:HE1	2:B:87:LYS:NZ	2.35	0.42
1:A:145:MET:HE2	1:A:145:MET:HB3	1.77	0.42
1:A:303:ASN:OD1	1:A:336:THR:OG1	2.32	0.42
1:C:484:CYS:HA	1:C:520:PHE:CE2	2.55	0.42
1:A:544:LEU:HA	1:A:544:LEU:HD12	1.80	0.42
1:A:570:LYS:O	1:A:571:CYS:C	2.62	0.42
1:C:317:CYS:SG	1:C:378:LEU:HB2	2.60	0.42
1:A:292:LEU:HD23	1:A:292:LEU:HA	1.93	0.42
1:A:614:ALA:O	1:A:618:GLN:HG3	2.20	0.42
1:C:543:LEU:CD2	1:C:581:MET:HE2	2.50	0.42
1:A:547:ILE:HD11	1:A:574:MET:HB2	2.00	0.42
2:B:3:TYR:HB2	2:B:4:PRO:HD2	2.01	0.42
1:C:145:MET:HB3	1:C:145:MET:HE2	1.81	0.42
1:C:346:GLY:HA3	1:C:347:GLY:HA2	1.67	0.42
1:A:350:MET:HE2	1:A:350:MET:HB3	1.96	0.41
1:A:13:VAL:HG21	2:B:60:VAL:HB	2.02	0.41
1:C:580:GLY:O	2:D:21:LEU:HD13	2.20	0.41
1:A:183:GLY:O	1:A:187:GLN:NE2	2.28	0.41
1:A:369:PHE:CZ	1:A:396:TYR:CD2	3.08	0.41
1:A:609:ASN:O	1:A:613:GLU:HG3	2.20	0.41
1:C:8:LEU:O	2:D:60:VAL:N	2.47	0.41
1:A:60:LEU:HD22	1:A:64:GLU:HB3	2.01	0.41
1:A:496:GLU:HG3	1:A:502:PRO:HG3	2.03	0.41
2:B:5:GLY:O	2:B:6:LYS:C	2.63	0.41
1:A:395:GLY:C	1:A:397:VAL:N	2.77	0.41
1:A:449:SER:O	1:A:453:GLN:HB2	2.19	0.41
2:B:113:LEU:O	2:B:117:VAL:HG23	2.20	0.41
1:C:398:ARG:H	1:C:398:ARG:HG2	1.73	0.41
1:A:4:LEU:HD13	1:A:4:LEU:C	2.45	0.41
1:A:111:MET:CE	1:A:156:TRP:HB3	2.44	0.41
1:C:545:LEU:HB2	2:D:25:TYR:CE2	2.55	0.41
1:A:391:GLY:C	1:A:393:SER:N	2.79	0.41
1:A:420:ALA:HA	1:A:430:LYS:HG2	2.03	0.41
2:B:110:LEU:HA	2:B:110:LEU:HD23	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:GLN:HG3	1:C:102:SER:N	2.35	0.41
1:C:145:MET:HE1	1:C:156:TRP:CB	2.51	0.41
1:C:395:GLY:HA2	1:C:398:ARG:HG2	2.03	0.41
1:C:545:LEU:HB2	2:D:25:TYR:CD2	2.56	0.41
1:C:318:TYR:CE2	1:C:543:LEU:HB2	2.56	0.41
2:D:44:LEU:HD12	2:D:44:LEU:HA	1.60	0.41
1:A:411:GLY:HA3	1:A:444:ARG:NH2	2.36	0.40
1:C:46:MET:HG3	2:D:118:LEU:HD13	2.03	0.40
1:C:73:VAL:HG13	1:C:86:ALA:HB1	2.04	0.40
1:A:35:GLU:O	1:A:38:LYS:N	2.54	0.40
1:A:118:LEU:HD13	1:A:138:CYS:HA	2.03	0.40
1:A:145:MET:HE3	1:A:153:TYR:CD1	2.47	0.40
1:A:383:VAL:O	1:A:385:THR:N	2.54	0.40
1:A:471:LEU:O	1:A:477:GLN:HB3	2.21	0.40
1:C:480:PRO:HB2	1:C:539:LEU:HD23	2.03	0.40
1:C:542:ALA:HB3	1:C:545:LEU:HB3	2.03	0.40
1:A:242:MET:HB3	1:A:242:MET:HE3	1.83	0.40
1:A:386:GLU:HB2	1:A:387:SER:H	1.48	0.40
1:A:551:TYR:O	1:A:552:LEU:C	2.65	0.40
1:A:603:LYS:HE3	1:A:604:ASP:N	2.36	0.40
1:C:489:LEU:HD23	1:C:489:LEU:HA	1.85	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:SER:OG	2:D:3:TYR:N[4_445]	1.31	0.89
1:A:101:GLN:OE1	1:A:603:LYS:NZ[3_545]	2.06	0.14

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	613/624 (98%)	566 (92%)	36 (6%)	11 (2%)	6	34
1	C	599/624 (96%)	561 (94%)	33 (6%)	5 (1%)	16	50
2	B	108/184 (59%)	89 (82%)	13 (12%)	6 (6%)	1	11
2	D	104/184 (56%)	90 (86%)	9 (9%)	5 (5%)	2	14
All	All	1424/1616 (88%)	1306 (92%)	91 (6%)	27 (2%)	6	33

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	7	LYS
1	A	317	CYS
1	A	384	THR
1	A	386	GLU
1	A	387	SER
1	A	526	PHE
2	B	55	ASP
2	B	64	VAL
2	B	127	SER
2	B	128	ILE
2	B	132	LYS
2	D	9	ASN
2	D	55	ASP
1	A	319	ASP
1	C	102	SER
2	D	23	LEU
2	D	105	ASN
1	A	320	GLU
2	B	23	LEU
1	C	317	CYS
2	D	131	GLU
1	C	105	ASP
1	C	536	ARG
1	C	551	TYR
1	A	388	PRO
1	A	391	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	558/564 (99%)	556 (100%)	2 (0%)	84	86
1	C	550/564 (98%)	549 (100%)	1 (0%)	87	89
2	B	99/161 (62%)	95 (96%)	4 (4%)	28	61
2	D	97/161 (60%)	97 (100%)	0	100	100
3	E	2/4 (50%)	2 (100%)	0	100	100
3	H	2/4 (50%)	2 (100%)	0	100	100
All	All	1308/1458 (90%)	1301 (100%)	7 (0%)	81	85

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	621	SER
1	A	622	VAL
2	B	2	SER
2	B	7	ASP
2	B	64	VAL
2	B	67	THR
1	C	176	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	266	ASN
1	A	309	GLN
1	A	375	GLN
1	A	595	ASN
2	B	97	ASN
2	B	121	HIS
2	B	125	ASN
1	C	15	HIS
1	C	52	GLN
1	C	143	GLN
1	C	208	ASN
1	C	266	ASN
1	C	375	GLN

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Mol	Chain	Res	Type
1	C	609	ASN
1	C	618	GLN
2	D	37	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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
3	SEP	E	5	3	8,9,10	1.83	3 (37%)	7,12,14	1.88	1 (14%)
3	TPO	H	4	3	8,10,11	1.98	3 (37%)	10,14,16	1.76	1 (10%)
3	SEP	H	5	3	8,9,10	1.77	3 (37%)	7,12,14	1.77	1 (14%)
3	TPO	E	4	3	8,10,11	2.17	3 (37%)	10,14,16	1.98	1 (10%)

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
3	SEP	E	5	3	-	4/6/8/10	-
3	TPO	H	4	3	-	1/9/11/13	-
3	SEP	H	5	3	-	5/6/8/10	-
3	TPO	E	4	3	-	3/9/11/13	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4	TPO	P-O1P	3.89	1.62	1.50
3	E	5	SEP	P-O1P	3.83	1.62	1.50
3	H	4	TPO	P-O1P	3.83	1.62	1.50
3	H	5	SEP	P-O1P	3.71	1.62	1.50
3	E	4	TPO	CB-CA	3.18	1.60	1.53
3	H	4	TPO	P-OG1	2.24	1.63	1.59
3	H	4	TPO	P-O2P	2.19	1.62	1.54
3	E	5	SEP	P-O2P	2.09	1.62	1.54
3	E	5	SEP	P-O3P	2.08	1.62	1.54
3	E	4	TPO	P-O3P	2.05	1.62	1.54
3	H	5	SEP	P-O3P	2.04	1.62	1.54
3	H	5	SEP	P-O2P	2.03	1.62	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	4	TPO	P-OG1-CB	-5.85	107.44	123.33
3	H	4	TPO	P-OG1-CB	-4.81	110.26	123.33
3	E	5	SEP	OG-CB-CA	4.41	112.43	108.14
3	H	5	SEP	OG-CB-CA	4.03	112.07	108.14

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	4	TPO	N-CA-CB-CG2
3	E	4	TPO	N-CA-CB-OG1
3	E	4	TPO	C-CA-CB-CG2
3	E	5	SEP	C-CA-CB-OG
3	H	5	SEP	CB-OG-P-O3P
3	H	5	SEP	CB-OG-P-O1P
3	E	5	SEP	CB-OG-P-O2P
3	H	5	SEP	CB-OG-P-O2P
3	E	5	SEP	CA-CB-OG-P
3	E	5	SEP	N-CA-CB-OG
3	H	5	SEP	N-CA-CB-OG
3	H	4	TPO	CB-OG1-P-O1P
3	H	5	SEP	C-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5	SEP	1	0
3	E	4	TPO	1	0

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	617/624 (98%)	-0.47	1 (0%) 91 85	67, 101, 151, 191	0
1	C	605/624 (96%)	-0.35	3 (0%) 87 76	90, 125, 161, 182	0
2	B	114/184 (61%)	-0.20	1 (0%) 81 64	80, 107, 148, 165	0
2	D	110/184 (59%)	-0.09	1 (0%) 81 64	95, 142, 171, 180	0
3	E	2/6 (33%)	0.59	0 100 100	182, 182, 182, 183	0
3	H	2/6 (33%)	0.50	0 100 100	170, 170, 170, 177	0
All	All	1450/1628 (89%)	-0.37	6 (0%) 88 79	67, 116, 161, 191	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	390	LEU	2.6
1	C	310	SER	2.4
2	B	39	PRO	2.3
2	D	5	GLY	2.2
1	C	233	LEU	2.2
1	A	393	SER	2.1

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TPO	E	4	11/12	0.49	0.12	194,208,242,254	0
3	TPO	H	4	11/12	0.53	0.10	183,196,215,229	0
3	SEP	H	5	10/11	0.66	0.07	176,197,209,213	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SEP	E	5	10/11	0.73	0.07	189,200,212,225	0

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.