



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:43 AM UTC

PDB ID : 9FL8 / pdb_00009fl8
Title : Stapled peptide bound to NOT9-NOT1 complex
Authors : Pal, S.; Schmeing, S.; Gasper, R.; t Hart, P.
Deposited on : 2024-06-04
Resolution : 2.64 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

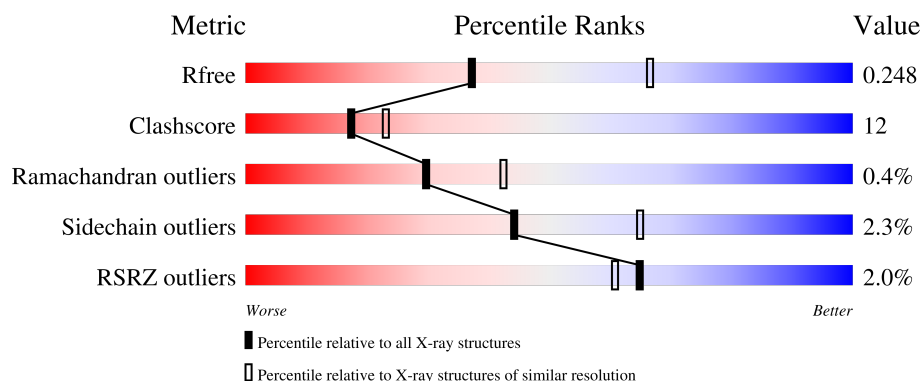
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	F	19	
1	G	19	
2	B	273	
2	C	273	
3	A	244	

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Mol	Chain	Length	Quality of chain
3	D	244	7% 57% 37% • 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8498 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 Protein bag of marbles.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	G	17	Total	C	N	O	0	0	0
			143	96	21	26			
1	F	18	Total	C	N	O	0	0	0
			146	98	21	27			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	16	ACE	-	acetylation	UNP P22745
G	19	MK8	HIS	engineered mutation	UNP P22745
G	23	MK8	GLN	engineered mutation	UNP P22745
G	24	NLE	MET	engineered mutation	UNP P22745
G	31	NLE	MET	engineered mutation	UNP P22745
G	34	NH2	-	amidation	UNP P22745
F	16	ACE	-	acetylation	UNP P22745
F	19	MK8	HIS	engineered mutation	UNP P22745
F	23	MK8	GLN	engineered mutation	UNP P22745
F	24	NLE	MET	engineered mutation	UNP P22745
F	31	NLE	MET	engineered mutation	UNP P22745
F	34	NH2	-	amidation	UNP P22745

- Molecule 2 is a protein called CCR4-NOT transcription complex subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	273	Total	C	N	O	S	0	2	0
			2194	1406	376	401	11			
2	C	273	Total	C	N	O	S	0	3	0
			2204	1413	381	399	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	13	GLY	-	expression tag	UNP Q92600
B	14	PRO	-	expression tag	UNP Q92600
B	15	HIS	-	expression tag	UNP Q92600
B	16	MET	-	expression tag	UNP Q92600
B	17	LEU	-	expression tag	UNP Q92600
B	18	GLU	-	expression tag	UNP Q92600
C	13	GLY	-	expression tag	UNP Q92600
C	14	PRO	-	expression tag	UNP Q92600
C	15	HIS	-	expression tag	UNP Q92600
C	16	MET	-	expression tag	UNP Q92600
C	17	LEU	-	expression tag	UNP Q92600
C	18	GLU	-	expression tag	UNP Q92600

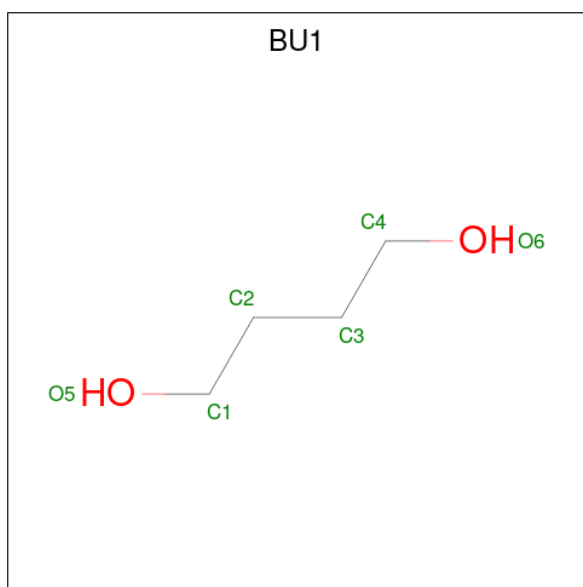
- Molecule 3 is a protein called CCR4-NOT transcription complex subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	235	Total	C	N	O	S	0	3	0
			1882	1170	345	347	20			
3	D	233	Total	C	N	O	S	0	0	0
			1847	1151	337	341	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1345	GLY	-	expression tag	UNP A5YKK6
A	1346	PRO	-	expression tag	UNP A5YKK6
A	1347	HIS	-	expression tag	UNP A5YKK6
A	1348	MET	-	expression tag	UNP A5YKK6
A	1349	LEU	-	expression tag	UNP A5YKK6
A	1350	GLU	-	expression tag	UNP A5YKK6
D	1345	GLY	-	expression tag	UNP A5YKK6
D	1346	PRO	-	expression tag	UNP A5YKK6
D	1347	HIS	-	expression tag	UNP A5YKK6
D	1348	MET	-	expression tag	UNP A5YKK6
D	1349	LEU	-	expression tag	UNP A5YKK6
D	1350	GLU	-	expression tag	UNP A5YKK6

- Molecule 4 is 1,4-BUTANEDIOL (CCD ID: BU1) (formula: C₄H₁₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			6	4	2		
4	B	1	Total	C	O	0	0
			6	4	2		
4	B	1	Total	C	O	0	0
			6	4	2		
4	A	1	Total	C	O	0	0
			6	4	2		
4	A	1	Total	C	O	0	0
			6	4	2		
4	C	1	Total	C	O	0	0
			6	4	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	3	Total	O	0	0
			3	3		
5	B	4	Total	O	0	0
			4	4		
5	A	24	Total	O	0	0
			24	24		
5	C	14	Total	O	0	0
			14	14		
5	D	1	Total	O	0	0
			1	1		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

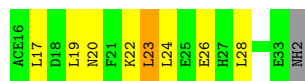
- Molecule 1: Protein bag of marbles

Chain G: 



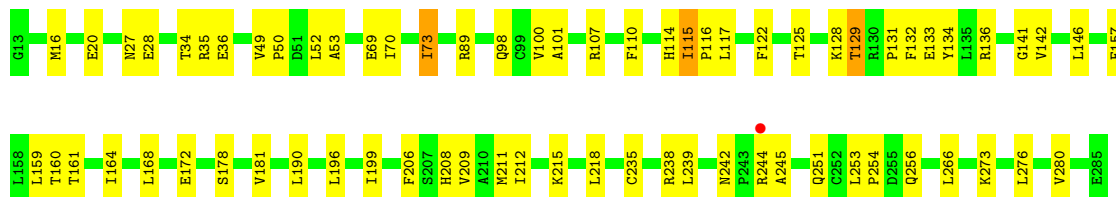
- Molecule 1: Protein bag of marbles

Chain F: 



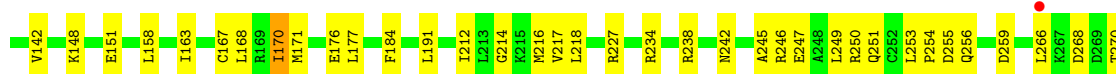
- Molecule 2: CCR4-NOT transcription complex subunit 9

Chain B: 



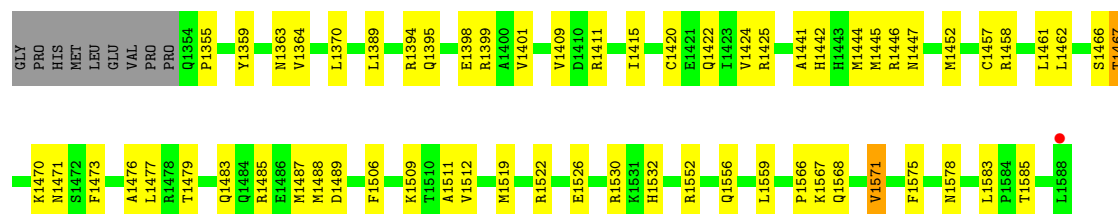
- Molecule 2: CCR4-NOT transcription complex subunit 9

Chain C: 



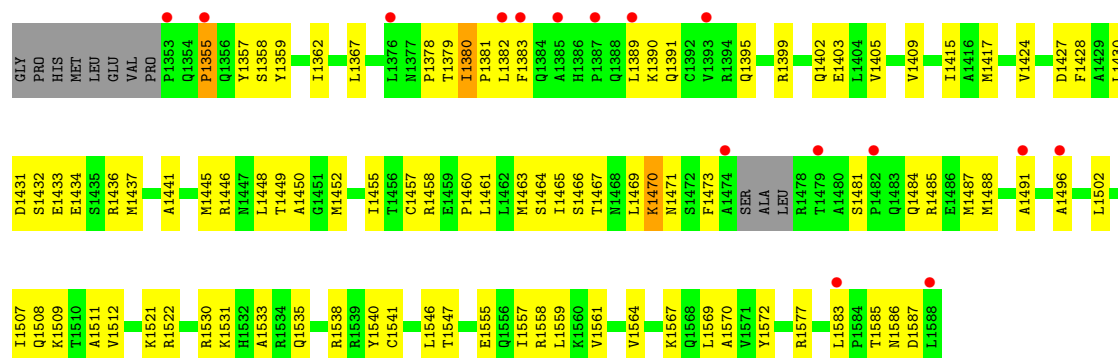
- Molecule 3: CCR4-NOT transcription complex subunit 1

Chain A:  71% 25% . .



- Molecule 3: CCR4-NOT transcription complex subunit 1

Chain D:  7% 57% 37% . 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	106.56Å 106.56Å 262.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.14 – 2.64 46.14 – 2.65	Depositor EDS
% Data completeness (in resolution range)	50.7 (46.14-2.64) 50.7 (46.14-2.65)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487)	Depositor
R, R_{free}	0.203 , 0.249 0.203 , 0.248	Depositor DCC
R_{free} test set	1304 reflections (2.53%)	wwPDB-VP
Wilson B-factor (Å ²)	60.8	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8498	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: ACE, MK8, NLE, BU1

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	F	0.18	0/108	0.35	0/140
1	G	0.11	0/107	0.20	0/138
2	B	0.13	0/2244	0.28	0/3048
2	C	0.16	0/2254	0.34	0/3060
3	A	0.16	0/1915	0.36	0/2586
3	D	0.17	0/1880	0.37	0/2538
All	All	0.15	0/8508	0.33	0/11510

There are no bond length outliers.

There are no bond angle outliers.

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	F	146	0	148	9	0
1	G	143	0	143	4	0
2	B	2194	0	2265	49	0
2	C	2204	0	2284	55	0
3	A	1882	0	1887	47	0
3	D	1847	0	1853	60	1
4	A	12	0	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	12	0	20	1	0
4	C	6	0	10	1	0
4	F	6	0	10	1	0
5	A	24	0	0	6	0
5	B	4	0	0	0	0
5	C	14	0	0	0	0
5	D	1	0	0	0	0
5	G	3	0	0	1	0
All	All	8498	0	8640	213	1

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 12.

All (213) 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)
3:A:1485:ARG:NH1	5:A:1701:HOH:O	2.04	0.89
3:D:1417:MET:HE1	3:D:1522:ARG:HG3	1.66	0.78
3:D:1466:SER:HA	3:D:1469:LEU:HD12	1.66	0.76
2:B:196:LEU:HD22	2:B:238:ARG:HE	1.51	0.74
3:A:1457[A]:CYS:SG	3:A:1458:ARG:N	2.62	0.73
2:C:253:LEU:HD12	2:C:254:PRO:HD2	1.71	0.72
3:A:1395:GLN:HE22	3:A:1399:ARG:HD2	1.54	0.71
2:B:253:LEU:HD12	2:B:254:PRO:HD2	1.72	0.71
2:C:83:THR:HG23	2:C:86:GLN:H	1.55	0.70
2:C:14:PRO:HG2	2:C:16:MET:HG2	1.73	0.69
2:B:36:GLU:HB2	2:B:89:ARG:HH21	1.58	0.69
3:D:1381:PRO:HD2	3:D:1491:ALA:HB2	1.74	0.68
3:A:1467:THR:O	3:A:1471:ASN:ND2	2.26	0.68
2:C:176:GLU:OE2	2:C:227:ARG:NH1	2.27	0.68
2:C:270:THR:HA	2:C:273:LYS:HE3	1.74	0.68
3:D:1463:MET:O	3:D:1467:THR:OG1	2.12	0.68
2:C:168:LEU:HB3	2:C:212:ILE:HG13	1.75	0.68
2:B:128:LYS:H	2:B:136:ARG:HH22	1.43	0.67
3:D:1380:ILE:HG12	3:D:1383:PHE:HB2	1.75	0.67
3:D:1415:ILE:HG21	3:D:1452:MET:HE2	1.75	0.67
3:D:1585:THR:OG1	3:D:1586:ASN:N	2.27	0.67
2:C:24:GLN:HE22	2:C:28:GLU:HG3	1.60	0.66
1:G:20:ASN:ND2	5:G:101:HOH:O	2.27	0.66
2:C:68:GLN:O	2:C:72:ASN:ND2	2.30	0.64
3:A:1415:ILE:HG21	3:A:1452:MET:HE2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1469:LEU:O	3:D:1471:ASN:N	2.30	0.64
3:D:1446:ARG:HG3	3:D:1512:VAL:HG11	1.79	0.64
3:A:1425:ARG:NH1	5:A:1703:HOH:O	2.29	0.64
3:D:1577:ARG:HD2	3:D:1587:ASP:HA	1.80	0.63
3:D:1457:CYS:SG	3:D:1458:ARG:N	2.70	0.63
2:C:16:MET:O	2:C:20:GLU:HG2	1.99	0.63
2:C:247:GLU:HA	2:C:250:ARG:HH11	1.64	0.63
2:B:244:ARG:O	2:B:244:ARG:NH1	2.33	0.62
3:A:1424:VAL:HG11	3:A:1441:ALA:HB2	1.79	0.62
2:C:247:GLU:HA	2:C:250:ARG:HD2	1.80	0.62
3:A:1422:GLN:NE2	5:A:1703:HOH:O	2.33	0.62
3:A:1394:ARG:NH1	3:A:1398:GLU:OE1	2.32	0.62
3:A:1552:ARG:NH1	5:A:1704:HOH:O	2.32	0.62
3:A:1473:PHE:HB3	3:A:1488:MET:HG2	1.82	0.61
2:C:24:GLN:O	2:C:27:ASN:N	2.32	0.61
2:B:159:LEU:HD23	2:B:164:ILE:HD11	1.82	0.61
2:B:101:ALA:HB1	2:B:146:LEU:HD11	1.82	0.61
3:A:1447:ASN:ND2	3:A:1578:ASN:O	2.34	0.60
2:C:71:VAL:HG21	3:D:1448:LEU:HD22	1.83	0.60
2:B:242:ASN:HB3	2:B:245:ALA:HB3	1.83	0.60
2:C:250:ARG:HG2	2:C:251:GLN:HG2	1.83	0.60
2:B:251:GLN:N	2:B:251:GLN:OE1	2.35	0.60
1:F:20:ASN:HA	1:F:23:MK8:HDA	1.83	0.60
2:B:53:ALA:HB1	2:B:100:VAL:HA	1.83	0.60
2:C:177:LEU:H	4:C:301:BU1:H42	1.67	0.59
2:C:255:ASP:O	2:C:259:ASP:HB2	2.02	0.59
2:B:168:LEU:HG	2:B:212:ILE:HG13	1.83	0.59
2:B:129:THR:HG22	2:B:131:PRO:HD2	1.85	0.58
2:B:69:GLU:OE2	2:B:89:ARG:NH1	2.36	0.58
2:B:117:LEU:HD13	3:A:1415:ILE:HG23	1.86	0.58
3:D:1367:LEU:HD12	3:D:1367:LEU:H	1.67	0.58
3:D:1481:SER:HB2	3:D:1484:GLN:HG3	1.85	0.57
2:C:266:LEU:O	2:C:273:LYS:HE2	2.04	0.57
3:D:1399:ARG:O	3:D:1403:GLU:HG2	2.05	0.57
3:A:1522:ARG:NH1	5:A:1709:HOH:O	2.38	0.56
3:D:1437:MET:HE1	3:D:1530:ARG:CZ	2.35	0.56
2:C:114:HIS:HB3	2:C:117:LEU:HD13	1.87	0.56
3:A:1447:ASN:HB3	3:A:1575:PHE:HD1	1.70	0.55
2:B:190:LEU:HD21	2:B:199:ILE:HD12	1.89	0.55
3:A:1566:PRO:O	3:A:1567:LYS:HB2	2.06	0.55
2:C:148:LYS:HD2	2:C:184:PHE:HZ	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:PHE:O	2:B:161:THR:HG23	2.06	0.55
3:D:1470:LYS:HD3	3:D:1473:PHE:HB2	1.87	0.55
3:D:1431:ASP:OD2	3:D:1436:ARG:NH2	2.40	0.54
2:C:123:LEU:O	2:C:170:ILE:HD11	2.07	0.54
2:C:253:LEU:HD22	2:C:283:LEU:HD12	1.90	0.54
3:D:1541:CYS:HB3	3:D:1546:LEU:HD22	1.89	0.54
1:F:17:LEU:HD11	2:B:134:TYR:CD2	2.43	0.54
2:B:35:ARG:HH11	2:B:69:GLU:HG2	1.73	0.54
3:A:1370:LEU:HD11	3:A:1401:VAL:HG11	1.90	0.54
2:B:28:GLU:O	2:B:34:THR:OG1	2.26	0.53
3:D:1355:PRO:HB2	3:D:1583:LEU:HD22	1.91	0.53
2:C:42:LEU:HB3	2:C:96:LEU:HD21	1.91	0.53
2:C:212:ILE:O	2:C:216:MET:HG3	2.08	0.53
2:C:98:GLN:HB2	2:C:142:VAL:HG22	1.91	0.53
3:D:1378:PRO:O	3:D:1380:ILE:HG13	2.09	0.52
2:B:208:HIS:O	2:B:212:ILE:HG12	2.10	0.52
2:C:117:LEU:HD12	2:C:117:LEU:H	1.74	0.52
3:A:1363:ASN:ND2	5:A:1711:HOH:O	2.42	0.51
3:A:1526:GLU:HB3	3:A:1530:ARG:HH12	1.74	0.51
2:B:73:ILE:HD11	2:B:122:PHE:CE1	2.46	0.51
3:D:1432:SER:OG	3:D:1540:TYR:O	2.25	0.51
2:B:211:MET:HE2	2:B:215:LYS:HE2	1.92	0.50
3:A:1477:LEU:O	3:A:1479:THR:N	2.38	0.50
3:A:1446[B]:ARG:HG2	3:A:1512:VAL:HG13	1.93	0.50
2:C:51:ASP:O	2:C:55:MET:HG3	2.11	0.50
2:C:158:LEU:HB3	2:C:163:ILE:HG21	1.93	0.50
3:A:1571:VAL:HG12	3:A:1575:PHE:HE2	1.77	0.50
3:A:1457[A]:CYS:SG	3:A:1458:ARG:HG2	2.51	0.50
3:A:1457[B]:CYS:SG	3:A:1461:LEU:HD22	2.52	0.50
1:F:23:MK8:HB1A	1:F:26:GLU:HB2	1.93	0.49
2:B:218:LEU:HG	2:B:256:GLN:NE2	2.27	0.49
2:C:242:ASN:HB3	2:C:245:ALA:HB3	1.93	0.49
3:D:1383:PHE:CE2	3:D:1390:LYS:HA	2.47	0.49
2:B:16:MET:HE3	2:B:20:GLU:HG3	1.95	0.49
2:C:55:MET:HB3	3:D:1557:ILE:HD12	1.94	0.49
3:D:1390:LYS:HG3	3:D:1391:GLN:HG2	1.95	0.49
3:D:1445:MET:SD	3:D:1449:THR:OG1	2.70	0.49
3:A:1411:ARG:O	3:A:1415:ILE:HG13	2.13	0.49
2:C:32:PRO:HD3	3:D:1570:ALA:HB1	1.94	0.49
3:D:1533:ALA:HB1	3:D:1538:ARG:HG2	1.93	0.49
2:B:172[A]:GLU:HG3	2:B:212:ILE:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:THR:OG1	3:D:1521:LYS:HD3	2.13	0.48
3:D:1367:LEU:HD21	3:D:1402:GLN:HG3	1.96	0.48
3:D:1431:ASP:OD2	3:D:1564:VAL:HG23	2.13	0.48
3:D:1382:LEU:HG	3:D:1488:MET:HG2	1.94	0.48
2:B:133:GLU:OE2	2:B:136:ARG:NH1	2.46	0.48
3:A:1359:TYR:CZ	3:A:1509:LYS:HG3	2.48	0.48
3:D:1382:LEU:HD11	3:D:1389:LEU:HD22	1.96	0.47
1:F:19:MK8:HB1A	1:F:22:LYS:HB2	1.95	0.47
3:A:1389:LEU:HD11	3:A:1477:LEU:HG	1.95	0.47
3:A:1420:CYS:HB3	3:A:1519:MET:HE1	1.97	0.47
3:D:1450:ALA:O	3:D:1508:GLN:NE2	2.41	0.47
3:A:1409:VAL:HG22	3:A:1511:ALA:HB2	1.95	0.47
3:A:1532:HIS:CD2	3:A:1532:HIS:C	2.93	0.47
1:G:28:LEU:O	1:G:32:VAL:HG13	2.15	0.47
2:B:98:GLN:HB2	2:B:142:VAL:HG22	1.97	0.47
2:C:158:LEU:O	2:C:163:ILE:HG22	2.15	0.47
3:D:1395:GLN:O	3:D:1399:ARG:HB2	2.15	0.47
3:D:1358:SER:OG	3:D:1359:TYR:N	2.48	0.46
3:D:1405:VAL:HG23	3:D:1507:ILE:HG23	1.96	0.46
2:C:78:ASN:ND2	3:D:1458:ARG:HB2	2.31	0.46
2:C:191:LEU:HA	2:C:238:ARG:HE	1.81	0.46
3:D:1359:TYR:HE1	3:D:1509:LYS:HG3	1.81	0.46
2:B:218:LEU:HG	2:B:256:GLN:HE22	1.79	0.46
2:B:133:GLU:OE1	2:B:178:SER:OG	2.33	0.46
3:A:1445:MET:HB2	3:A:1519:MET:CE	2.46	0.46
2:C:214:GLY:HA2	2:C:254:PRO:HG3	1.98	0.46
2:B:101:ALA:O	2:B:107:ARG:HG3	2.16	0.45
2:B:114:HIS:HB3	2:B:117:LEU:HD12	1.98	0.45
3:A:1355:PRO:HG2	3:A:1583:LEU:HD23	1.97	0.45
2:C:167:CYS:O	2:C:171:MET:HG3	2.16	0.45
3:D:1424:VAL:HG21	3:D:1441:ALA:HA	1.99	0.45
3:D:1427:ASP:OD1	3:D:1572:TYR:OH	2.32	0.45
3:D:1355:PRO:HG2	3:D:1583:LEU:HD22	1.98	0.45
3:D:1381:PRO:HB2	3:D:1487:MET:HB2	1.99	0.45
3:A:1389:LEU:HD21	3:A:1476:ALA:HB3	1.97	0.45
2:B:266:LEU:O	2:B:273:LYS:HD2	2.17	0.45
3:A:1442:HIS:O	3:A:1446[A]:ARG:HG3	2.17	0.45
3:D:1433:GLU:OE2	3:D:1433:GLU:HA	2.15	0.45
1:G:23:MK8:HB1A	1:G:26:GLU:HB2	1.99	0.45
2:B:141:GLY:HA3	4:B:301:BU1:H32	1.99	0.45
3:A:1364:VAL:HA	3:A:1506:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1526:GLU:HB3	3:A:1530:ARG:NH1	2.31	0.45
3:A:1470:LYS:HD3	3:A:1489:ASP:HA	1.98	0.44
2:B:110:PHE:CE1	2:B:116:PRO:HD3	2.52	0.44
3:A:1411:ARG:HG3	3:A:1411:ARG:HH11	1.82	0.44
3:A:1420:CYS:SG	3:A:1444:MET:HE3	2.57	0.44
3:A:1457[B]:CYS:O	3:A:1461:LEU:HB2	2.17	0.44
2:B:122:PHE:O	2:B:125:THR:OG1	2.33	0.44
3:A:1411:ARG:HG3	3:A:1411:ARG:NH1	2.33	0.44
2:C:92:ASN:O	2:C:96:LEU:HD12	2.16	0.44
2:C:43:SER:O	2:C:46:ARG:HD3	2.17	0.44
2:C:217:VAL:HG11	2:C:254:PRO:HB2	2.00	0.44
1:F:28:LEU:HD22	2:B:181:VAL:HG21	2.00	0.44
3:A:1483:GLN:O	3:A:1487:MET:HG3	2.18	0.44
2:B:157:PHE:CE1	2:B:161:THR:HG21	2.51	0.44
2:C:118:PHE:CZ	3:D:1448:LEU:HD13	2.52	0.43
2:C:278:GLN:OE1	2:C:278:GLN:HA	2.18	0.43
2:C:13:GLY:N	2:C:17:LEU:HD12	2.34	0.43
3:D:1428:PHE:CB	3:D:1437:MET:HE2	2.48	0.43
2:B:244:ARG:HD2	2:B:244:ARG:HA	1.71	0.43
2:C:107:ARG:NH2	2:C:151:GLU:OE2	2.51	0.43
3:D:1465:ILE:HG21	3:D:1496:ALA:HA	2.00	0.43
3:D:1485:ARG:HG3	3:D:1485:ARG:HH11	1.83	0.43
2:B:114:HIS:O	2:B:117:LEU:HB2	2.19	0.43
2:C:255:ASP:OD2	2:C:255:ASP:N	2.50	0.43
3:D:1430:LEU:HD13	3:D:1561:VAL:HA	2.00	0.43
2:B:27:ASN:ND2	3:A:1556:GLN:O	2.36	0.43
3:A:1473:PHE:CB	3:A:1488:MET:HG2	2.47	0.43
3:D:1357:TYR:CE2	3:D:1502:LEU:HB2	2.54	0.43
1:F:20:ASN:O	1:F:24:NLE:HB3	2.18	0.43
2:C:234:ARG:HD2	2:C:234:ARG:HA	1.65	0.43
3:A:1559:LEU:HD23	3:A:1559:LEU:HA	1.79	0.43
2:B:235:CYS:O	2:B:239:LEU:HG	2.20	0.42
2:B:238:ARG:HA	2:B:238:ARG:HD2	1.80	0.42
2:C:72:ASN:N	2:C:72:ASN:HD22	2.18	0.42
2:B:132:PHE:HB3	2:B:136:ARG:HH21	1.85	0.42
3:D:1555:GLU:HG2	3:D:1558:ARG:HH21	1.84	0.42
2:C:218:LEU:HA	2:C:256:GLN:HE21	1.84	0.42
2:B:49:VAL:CG1	2:B:52:LEU:HB2	2.49	0.42
2:C:77:ILE:HG12	2:C:132:PHE:HE1	1.84	0.42
2:C:121:PRO:HB3	3:D:1455:ILE:HG21	2.01	0.42
3:D:1428:PHE:HB3	3:D:1437:MET:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:19:MK8:HDA	1:F:23:MK8:HDA	1.77	0.42
3:D:1485:ARG:HD2	3:D:1485:ARG:C	2.45	0.42
3:D:1461:LEU:HD23	3:D:1461:LEU:HA	1.84	0.42
3:D:1531:LYS:O	3:D:1535:GLN:HG2	2.20	0.42
2:B:206:PHE:C	2:B:206:PHE:CD2	2.98	0.41
2:C:66:LEU:HD13	2:C:97:LEU:HG	2.01	0.41
3:A:1398:GLU:HA	3:A:1401:VAL:HG12	2.01	0.41
3:A:1489:ASP:OD1	3:A:1489:ASP:N	2.53	0.41
3:D:1460:PRO:O	3:D:1464:SER:HB2	2.20	0.41
1:G:19:MK8:HB1A	1:G:22:LYS:HB2	2.03	0.41
2:C:249:LEU:HD23	2:C:249:LEU:HA	1.87	0.41
2:C:191:LEU:HA	2:C:238:ARG:NE	2.36	0.41
2:C:276:LEU:HD12	2:C:276:LEU:O	2.20	0.41
3:D:1424:VAL:HG11	3:D:1441:ALA:HB2	2.01	0.41
1:F:23:MK8:HG	4:F:101:BU1:H31	2.03	0.41
2:B:115:ILE:N	2:B:116:PRO:HD2	2.36	0.41
2:C:171:MET:O	2:C:216:MET:HE3	2.20	0.41
1:F:20:ASN:HA	1:F:23:MK8:CD	2.51	0.41
2:B:276:LEU:O	2:B:280:VAL:HG23	2.21	0.40
3:D:1409:VAL:HG22	3:D:1511:ALA:HB2	2.03	0.40
2:B:70:ILE:HG23	2:B:122:PHE:CZ	2.57	0.40
2:C:246:ARG:HG2	2:C:283:LEU:CD2	2.51	0.40
2:C:79:PRO:HA	2:C:80:PRO:HD3	1.98	0.40
3:D:1432:SER:OG	3:D:1540:TYR:N	2.54	0.40

All (1) 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)
3:D:1391:GLN:O	3:D:1391:GLN:NE2[6_554]	2.18	0.02

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	F	12/19 (63%)	12 (100%)	0	0	100	100
1	G	11/19 (58%)	11 (100%)	0	0	100	100
2	B	273/273 (100%)	264 (97%)	8 (3%)	1 (0%)	30	42
2	C	274/273 (100%)	265 (97%)	8 (3%)	1 (0%)	30	42
3	A	236/244 (97%)	233 (99%)	3 (1%)	0	100	100
3	D	229/244 (94%)	218 (95%)	9 (4%)	2 (1%)	14	21
All	All	1035/1072 (96%)	1003 (97%)	28 (3%)	4 (0%)	30	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	1470	LYS
2	C	80	PRO
2	B	50	PRO
3	D	1355	PRO

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	F	12/12 (100%)	12 (100%)	0	100	100
1	G	12/12 (100%)	12 (100%)	0	100	100
2	B	248/246 (101%)	244 (98%)	4 (2%)	55	73
2	C	249/246 (101%)	246 (99%)	3 (1%)	63	78
3	A	205/210 (98%)	199 (97%)	6 (3%)	37	57
3	D	201/210 (96%)	193 (96%)	8 (4%)	28	45
All	All	927/936 (99%)	906 (98%)	21 (2%)	44	65

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	73	ILE
2	B	115	ILE
2	B	129	THR
2	B	209	VAL
3	A	1462	LEU
3	A	1466	SER
3	A	1467	THR
3	A	1568	GLN
3	A	1571	VAL
3	A	1585	THR
2	C	129	THR
2	C	170	ILE
2	C	268	ASP
3	D	1362	ILE
3	D	1379	THR
3	D	1380	ILE
3	D	1434	GLU
3	D	1547	THR
3	D	1559	LEU
3	D	1567	LYS
3	D	1569	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	124	HIS
2	B	152	GLN
2	B	201	GLN
3	A	1386	HIS
3	A	1395	GLN
3	A	1422	GLN
3	A	1442	HIS
3	A	1494	GLN
3	A	1532	HIS
2	C	72	ASN
3	D	1356	GLN
3	D	1377	ASN
3	D	1578	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	$\# Z > 2$
1	NLE	G	31	1	6,7,8	0.50	0	2,7,9	0.37	0
1	MK8	G	19	1	5,8,9	0.73	0	6,10,12	1.19	0
1	MK8	G	23	1	5,8,9	0.75	0	6,10,12	1.11	1 (16%)
1	NLE	F	24	1	6,7,8	0.47	0	2,7,9	0.41	0
1	MK8	F	19	1	5,8,9	0.74	0	6,10,12	1.23	0
1	NLE	G	24	1	6,7,8	0.49	0	2,7,9	0.33	0
1	NLE	F	31	1	6,7,8	0.54	0	2,7,9	0.45	0
1	MK8	F	23	1	5,8,9	0.72	0	6,10,12	1.67	1 (16%)

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
1	NLE	G	31	1	-	0/5/6/8	-
1	MK8	G	19	1	-	4/6/8/11	-
1	MK8	G	23	1	-	1/6/8/11	-
1	NLE	F	24	1	-	4/5/6/8	-
1	MK8	F	19	1	-	1/6/8/11	-
1	NLE	G	24	1	-	0/5/6/8	-
1	NLE	F	31	1	-	1/5/6/8	-
1	MK8	F	23	1	-	1/6/8/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	23	MK8	CB1-CA-CB	-3.14	105.80	110.97
1	G	23	MK8	CB1-CA-CB	-2.21	107.33	110.97

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	G	19	MK8	N-CA-CB-CG
1	G	19	MK8	CB1-CA-CB-CG
1	F	24	NLE	N-CA-CB-CG
1	F	24	NLE	C-CA-CB-CG
1	G	19	MK8	CA-CB-CG-CD
1	F	19	MK8	CA-CB-CG-CD
1	F	24	NLE	CA-CB-CG-CD
1	F	24	NLE	CE-CD-CG-CB
1	G	19	MK8	C-CA-CB-CG
1	F	23	MK8	CA-CB-CG-CD
1	G	23	MK8	CE-CD-CG-CB
1	F	31	NLE	CE-CD-CG-CB

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	19	MK8	1	0
1	G	23	MK8	1	0
1	F	24	NLE	1	0
1	F	19	MK8	2	0
1	F	23	MK8	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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
4	BU1	A	1602	-	5,5,5	0.33	0	4,4,4	0.55	0
4	BU1	B	302	-	5,5,5	0.37	0	4,4,4	0.50	0
4	BU1	F	101	-	5,5,5	0.34	0	4,4,4	0.64	0
4	BU1	B	301	-	5,5,5	0.33	0	4,4,4	0.51	0
4	BU1	C	301	-	5,5,5	0.31	0	4,4,4	0.59	0
4	BU1	A	1601	-	5,5,5	0.35	0	4,4,4	0.53	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
4	BU1	A	1602	-	-	1/3/3/3	-
4	BU1	B	302	-	-	1/3/3/3	-
4	BU1	F	101	-	-	1/3/3/3	-
4	BU1	B	301	-	-	1/3/3/3	-
4	BU1	C	301	-	-	1/3/3/3	-
4	BU1	A	1601	-	-	2/3/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	101	BU1	O5-C1-C2-C3
4	A	1601	BU1	O5-C1-C2-C3
4	B	301	BU1	O5-C1-C2-C3
4	B	302	BU1	O5-C1-C2-C3
4	A	1602	BU1	O5-C1-C2-C3
4	C	301	BU1	C2-C3-C4-O6
4	A	1601	BU1	C2-C3-C4-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	101	BU1	1	0
4	B	301	BU1	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	301	BU1	1	0

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	F	13/19 (68%)	-0.13	0	100	100	32, 43, 56, 84	0
1	G	13/19 (68%)	-0.00	0	100	100	40, 57, 79, 81	0
2	B	273/273 (100%)	-0.30	1 (0%)	88	87	15, 42, 72, 132	2 (0%)
2	C	273/273 (100%)	-0.09	3 (1%)	78	75	22, 58, 101, 129	3 (1%)
3	A	235/244 (96%)	-0.18	1 (0%)	88	87	12, 43, 76, 97	3 (1%)
3	D	233/244 (95%)	0.43	16 (6%)	23	19	31, 76, 142, 158	0
All	All	1040/1072 (97%)	-0.05	21 (2%)	65	61	12, 52, 112, 158	8 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1393	VAL	4.6
3	D	1588	LEU	3.9
3	D	1387	PRO	3.8
3	D	1389	LEU	3.6
3	D	1383	PHE	3.4
3	A	1588	LEU	3.4
3	D	1353	PRO	3.3
3	D	1482	PRO	2.6
3	D	1355	PRO	2.4
3	D	1491	ALA	2.4
3	D	1496	ALA	2.3
2	C	13	GLY	2.2
2	C	266	LEU	2.2
3	D	1474	ALA	2.1
3	D	1479	THR	2.1
3	D	1382	LEU	2.1
3	D	1385	ALA	2.1
3	D	1376	LEU	2.1
2	B	244	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
2	C	283	LEU	2.0
3	D	1583	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	MK8	F	19	9/10	0.92	0.09	29,44,53,60	0
1	MK8	F	23	9/10	0.93	0.12	30,43,60,62	0
1	NLE	G	24	8/9	0.93	0.11	45,50,55,55	0
1	MK8	G	19	9/10	0.95	0.07	43,49,68,75	0
1	NLE	F	24	8/9	0.95	0.15	22,38,50,55	0
1	MK8	G	23	9/10	0.96	0.08	28,43,51,54	0
1	NLE	G	31	8/9	0.96	0.10	44,53,59,59	0
1	NLE	F	31	8/9	0.96	0.09	30,36,43,51	0

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(Å ²)	Q<0.9
4	BU1	A	1601	6/6	0.75	0.21	42,45,52,53	0
4	BU1	B	302	6/6	0.78	0.20	69,73,84,89	0
4	BU1	A	1602	6/6	0.85	0.15	59,69,73,82	0
4	BU1	F	101	6/6	0.88	0.13	34,52,55,67	0
4	BU1	B	301	6/6	0.89	0.23	48,59,64,64	0
4	BU1	C	301	6/6	0.89	0.16	63,77,80,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.