



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:48 PM UTC

PDB ID : 2P5G / pdb_00002p5g
Title : Crystal structure of RB69 gp43 in complex with DNA with dAMP opposite an abasic site analog in a 21mer template
Authors : Zahn, K.E.; Belrhali, H.; Wallace, S.S.; Doublié, S.
Deposited on : 2007-03-15
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

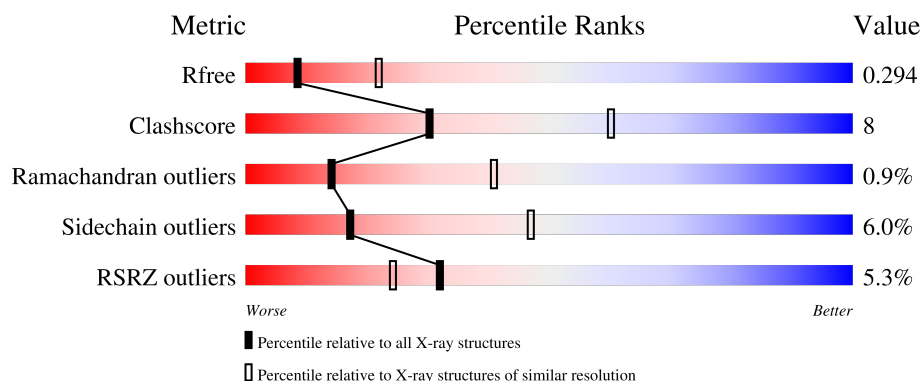
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	E	21	5% 52% 19% 29%
1	G	21	14% 43% 10% 48%
1	I	21	5% 62% 33% 5%
1	K	21	33% 19% 48%
2	F	15	67% 33%

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Mol	Chain	Length	Quality of chain
2	H	15	13% 40% 53% 7%
2	J	15	87% 13%
2	L	15	47% 40% 13%
3	A	903	2% 77% 20% ••
3	B	903	3% 61% 20% • 16%
3	C	903	2% 73% 23% ••
3	D	903	12% 80% 16% ••

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29179 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 DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	15	Total	C	N	O	P	0	0	0
			303	145	56	88	14			
1	G	11	Total	C	N	O	P	0	0	0
			223	106	44	63	10			
1	I	20	Total	C	N	O	P	0	0	0
			395	188	72	116	19			
1	K	11	Total	C	N	O	P	0	0	0
			226	106	44	65	11			

- Molecule 2 is a DNA chain called Primer DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	15	Total	C	N	O	P	0	0	0
			308	147	60	87	14			
2	H	15	Total	C	N	O	P	0	0	0
			308	147	60	87	14			
2	J	15	Total	C	N	O	P	0	0	0
			308	147	60	87	14			
2	L	13	Total	C	N	O	P	0	0	0
			265	127	50	76	12			

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	A	890	Total 7143	C 4588	N 1193	O 1331	S 8	Se 23	0	0	0
3	B	756	Total 6036	C 3877	N 998	O 1134	S 6	Se 21	0	0	0
3	C	885	Total 7113	C 4560	N 1180	O 1341	S 8	Se 24	0	0	0
3	D	875	Total 6148	C 3867	N 1039	O 1216	S 7	Se 19	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	engineered mutation	UNP Q38087
A	327	ALA	ASP	engineered mutation	UNP Q38087
B	222	ALA	ASP	engineered mutation	UNP Q38087
B	327	ALA	ASP	engineered mutation	UNP Q38087
C	222	ALA	ASP	engineered mutation	UNP Q38087
C	327	ALA	ASP	engineered mutation	UNP Q38087
D	222	ALA	ASP	engineered mutation	UNP Q38087
D	327	ALA	ASP	engineered mutation	UNP Q38087

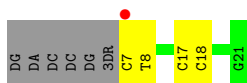
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	4	Total O 4 4	0	0
4	F	7	Total O 7 7	0	0
4	G	9	Total O 9 9	0	0
4	H	9	Total O 9 9	0	0
4	I	10	Total O 10 10	0	0
4	J	10	Total O 10 10	0	0
4	K	1	Total O 1 1	0	0
4	L	2	Total O 2 2	0	0
4	A	125	Total O 125 125	0	0
4	B	86	Total O 86 86	0	0
4	C	116	Total O 116 116	0	0
4	D	24	Total O 24 24	0	0

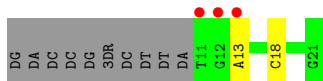
3 Residue-property plots [i](#)

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.

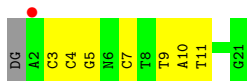
- Molecule 1: Template DNA



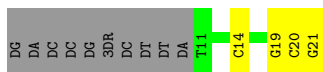
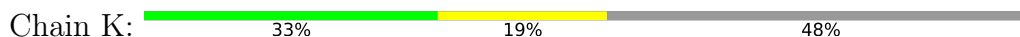
- Molecule 1: Template DNA



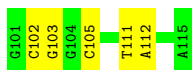
- Molecule 1: Template DNA



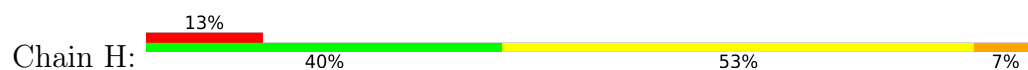
- Molecule 1: Template DNA



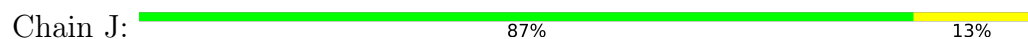
- Molecule 2: Primer DNA



- Molecule 2: Primer DNA



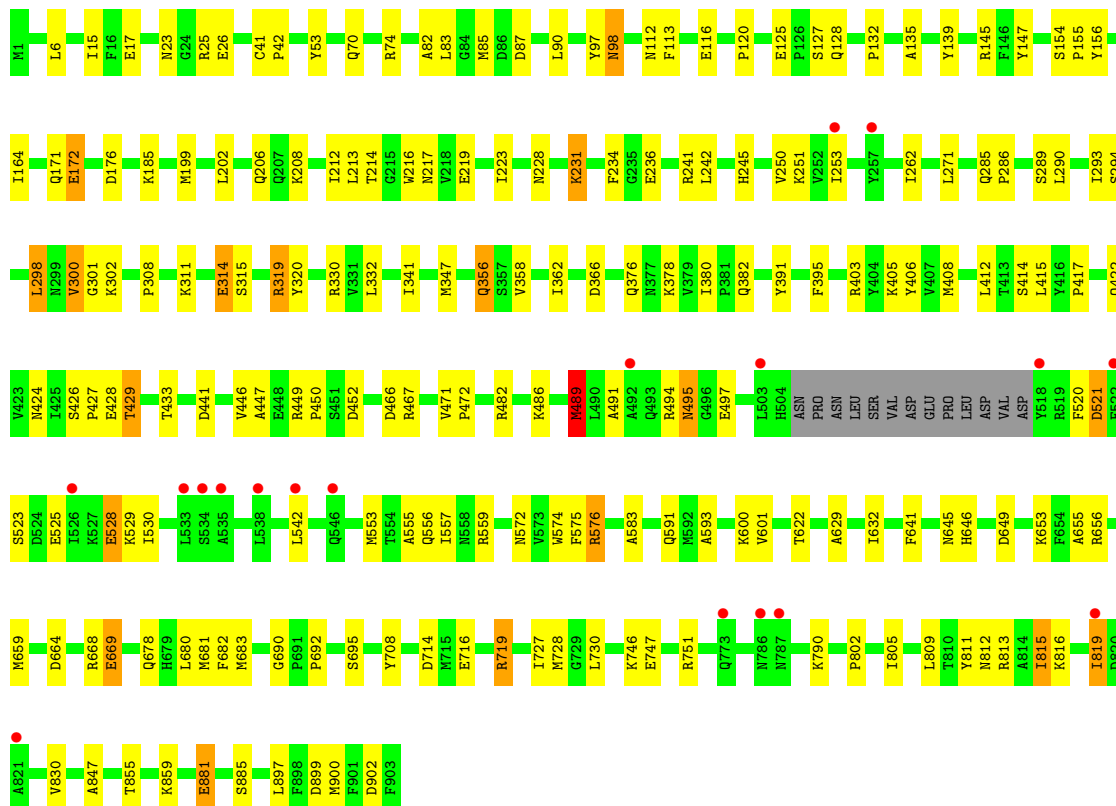
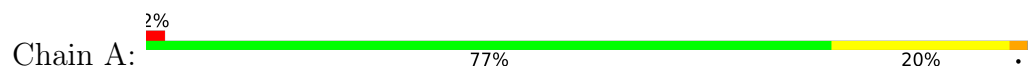
• Molecule 2: Primer DNA



• Molecule 2: Primer DNA

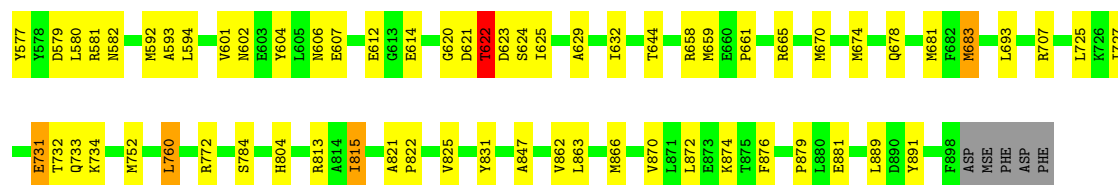


• Molecule 3: DNA polymerase

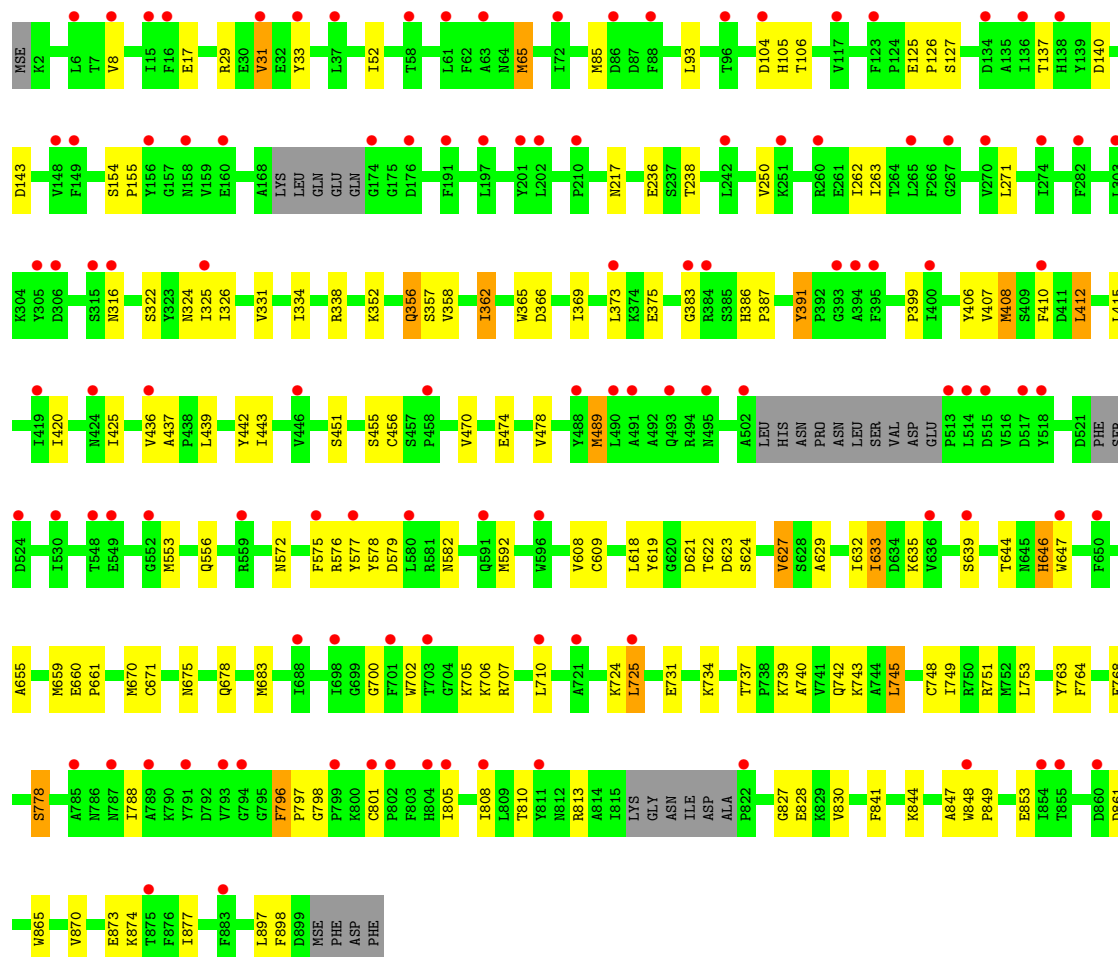
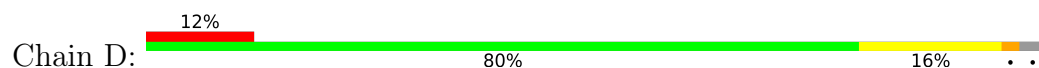


• Molecule 3: DNA polymerase





• Molecule 3: DNA polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	131.63Å 122.27Å 163.87Å 90.00° 96.45° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.4 (30.00-2.80) 91.5 (30.00-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.3.0011	Depositor
R, R_{free}	0.234 , 0.295 0.237 , 0.294	Depositor DCC
R_{free} test set	24078 reflections (9.64%)	wwPDB-VP
Wilson B-factor (Å ²)	62.2	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	29179	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: 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	E	0.28	0/339	0.85	0/521
1	G	0.33	0/250	0.93	0/384
1	I	0.32	0/429	0.97	0/657
1	K	0.27	0/253	0.92	0/388
2	F	0.28	0/346	0.96	2/533 (0.4%)
2	H	0.26	0/346	0.83	1/533 (0.2%)
2	J	0.33	0/346	1.05	0/533
2	L	0.24	0/297	0.77	0/457
3	A	0.49	0/7294	0.85	4/9830 (0.0%)
3	B	0.47	0/6163	0.82	4/8319 (0.0%)
3	C	0.49	0/7262	0.80	0/9788
3	D	0.46	0/6255	0.87	11/8520 (0.1%)
All	All	0.47	0/29580	0.84	22/40463 (0.1%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	801	CYS	CA-C-N	9.72	129.81	119.90
3	D	801	CYS	C-N-CA	9.72	129.81	119.90
3	D	848	TRP	CA-C-N	9.41	131.60	119.84
3	D	848	TRP	C-N-CA	9.41	131.60	119.84
3	D	796	PHE	CA-C-N	8.63	130.63	119.84
3	D	796	PHE	C-N-CA	8.63	130.63	119.84
3	D	646	HIS	N-CA-C	-6.71	106.29	114.75
3	B	178	VAL	CA-C-N	5.87	127.18	119.84
3	B	178	VAL	C-N-CA	5.87	127.18	119.84
3	D	798	GLY	CA-C-N	5.85	127.15	119.84
3	D	798	GLY	C-N-CA	5.85	127.15	119.84
3	B	457	SER	CA-C-N	5.50	126.72	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	457	SER	C-N-CA	5.50	126.72	119.84
2	F	105	DC	O4'-C1'-N1	5.48	116.62	108.40
2	H	111	DT	C1'-O4'-C4'	-5.45	101.52	109.70
3	A	125	GLU	CA-C-N	5.34	125.41	119.32
3	A	125	GLU	C-N-CA	5.34	125.41	119.32
3	D	737	THR	CA-C-N	5.18	125.19	119.90
3	D	737	THR	C-N-CA	5.18	125.19	119.90
3	A	223	ILE	CA-C-N	-5.18	113.58	119.28
3	A	223	ILE	C-N-CA	-5.18	113.58	119.28
2	F	105	DC	C1'-O4'-C4'	-5.03	102.16	109.70

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	E	303	0	170	2	0
1	G	223	0	124	2	0
1	I	395	0	222	5	0
1	K	226	0	123	4	0
2	F	308	0	170	2	0
2	H	308	0	170	9	0
2	J	308	0	170	4	0
2	L	265	0	148	5	0
3	A	7143	0	6923	117	0
3	B	6036	0	5779	119	0
3	C	7113	0	6872	127	0
3	D	6148	0	5083	76	0
4	A	125	0	0	2	0
4	B	86	0	0	5	0
4	C	116	0	0	3	0
4	D	24	0	0	1	0
4	E	4	0	0	0	0
4	F	7	0	0	1	0
4	G	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	9	0	0	1	0
4	I	10	0	0	1	0
4	J	10	0	0	0	0
4	K	1	0	0	0	0
4	L	2	0	0	0	0
All	All	29179	0	25954	461	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (461) 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:B:728:MSE:HG2	4:B:983:HOH:O	1.47	1.11
3:A:85:MSE:CE	3:A:87:ASP:HB3	1.82	1.08
3:A:85:MSE:HE3	3:A:87:ASP:HB3	1.10	1.04
3:A:85:MSE:HE3	3:A:87:ASP:CB	1.95	0.95
3:A:422:GLN:HG3	3:A:678:GLN:O	1.66	0.94
3:A:424:ASN:O	3:A:429:THR:HG21	1.68	0.93
3:C:461:MSE:HE2	4:C:945:HOH:O	1.70	0.90
3:A:422:GLN:NE2	3:A:680:LEU:H	1.72	0.88
3:B:441:ASP:HB3	3:B:447:ALA:HB2	1.56	0.87
3:C:85:MSE:HE2	3:C:87:ASP:HB3	1.56	0.85
3:D:365:TRP:O	3:D:369:ILE:HG22	1.78	0.84
3:B:87:ASP:OD2	3:B:363:LYS:HE3	1.80	0.82
3:C:380:ILE:HG23	3:C:576:ARG:HD3	1.59	0.82
3:A:112:ASN:HB3	4:A:1018:HOH:O	1.79	0.82
3:C:456:CYS:HB2	3:C:674:MSE:HE3	1.61	0.82
3:C:732:THR:HG23	3:C:733:GLN:OE1	1.80	0.81
3:B:458:PRO:HG3	3:B:592:MSE:SE	2.31	0.80
3:A:356:GLN:H	3:A:356:GLN:HE21	1.28	0.80
3:D:700:GLY:H	3:D:753:LEU:HD22	1.46	0.79
3:C:863:LEU:HA	3:C:866:MSE:HE2	1.65	0.79
2:H:110:DA:H2''	2:H:111:DT:H5''	1.63	0.78
3:B:873:GLU:HA	3:B:877:ILE:HG12	1.67	0.77
3:C:862:VAL:O	3:C:866:MSE:HG3	1.85	0.77
3:A:98:ASN:H	3:A:98:ASN:HD22	1.34	0.75
3:A:408:MSE:HE1	3:A:655:ALA:HB2	1.68	0.73
3:A:85:MSE:HE2	3:A:90:LEU:HD12	1.71	0.73
3:C:116:GLU:HB2	3:C:135:ALA:HB3	1.72	0.72
3:C:132:PRO:HG3	3:C:155:PRO:HD2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:212:ILE:HG23	3:A:271:LEU:HD12	1.71	0.71
3:B:98:ASN:H	3:B:98:ASN:HD22	1.36	0.71
3:B:394:ALA:HB1	3:B:622:THR:HB	1.72	0.71
3:D:725:LEU:HD23	3:D:725:LEU:H	1.56	0.71
1:E:17:DC:H2''	1:E:18:DC:H5'	1.73	0.70
3:C:85:MSE:HE2	3:C:87:ASP:CB	2.22	0.69
3:A:366:ASP:OD1	3:A:576:ARG:HD2	1.92	0.69
3:D:740:ALA:HB2	3:D:778:SER:HB2	1.74	0.69
3:D:137:THR:OG1	3:D:324:ASN:HB3	1.91	0.69
3:B:472:PRO:HA	3:B:475:ILE:HG22	1.74	0.69
3:C:203:ASN:O	3:C:207:GLN:HG2	1.92	0.69
3:B:71:TRP:NE1	3:B:75:MSE:HE3	2.08	0.69
3:C:167:ALA:HA	3:C:176:ASP:HB2	1.76	0.68
3:C:572:ASN:HD22	3:C:574:TRP:H	1.41	0.68
3:A:593:ALA:HB1	3:A:681:MSE:HE2	1.76	0.67
3:C:231:LYS:HG3	3:C:236:GLU:HA	1.76	0.67
3:A:356:GLN:H	3:A:356:GLN:NE2	1.93	0.67
3:D:408:MSE:HB3	3:D:627:VAL:HG23	1.76	0.67
3:A:395:PHE:HB2	3:A:591:GLN:HG3	1.77	0.66
3:D:702:TRP:CZ3	3:D:710:LEU:HD21	2.30	0.66
3:A:441:ASP:HB3	3:A:447:ALA:HB2	1.77	0.66
3:C:870:VAL:HG12	3:C:874:LYS:HD3	1.78	0.65
3:D:553:MSE:HA	3:D:556:GLN:HG2	1.79	0.65
3:C:110:VAL:H	3:C:141:SER:HB3	1.62	0.64
3:C:224:PRO:HB3	3:C:263:ILE:HG12	1.77	0.64
3:A:98:ASN:H	3:A:98:ASN:ND2	1.95	0.64
3:C:772:ARG:NH1	4:C:961:HOH:O	2.30	0.64
3:D:731:GLU:HA	3:D:734:LYS:HG3	1.78	0.64
3:D:621:ASP:HB3	3:D:624:SER:HB2	1.80	0.63
3:A:714:ASP:OD2	3:A:719:ARG:NH1	2.30	0.63
3:B:696:LYS:O	3:B:756:GLY:HA3	1.98	0.63
3:C:204:PHE:CE1	3:C:208:LYS:HD2	2.34	0.63
3:C:297:GLU:OE2	3:C:338:ARG:NH1	2.32	0.63
3:C:592:MSE:HE3	3:C:670:MSE:SE	2.49	0.62
3:D:407:VAL:HG11	3:D:710:LEU:HD22	1.81	0.62
3:C:85:MSE:CE	3:C:87:ASP:H	2.11	0.62
3:A:422:GLN:HE22	3:A:681:MSE:HG2	1.63	0.62
3:A:362:ILE:HD11	3:A:572:ASN:HB3	1.81	0.62
3:A:664:ASP:OD2	3:A:668:ARG:NH1	2.32	0.62
3:B:441:ASP:CB	3:B:447:ALA:HB2	2.29	0.61
3:B:641:PHE:HA	3:B:646:HIS:HD2	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:776:TYR:HA	3:B:779:ILE:HG22	1.83	0.61
3:B:328:VAL:O	3:B:331:VAL:HG12	2.01	0.61
3:C:303:LEU:HD11	3:C:323:TYR:HB2	1.82	0.61
3:C:478:VAL:HG13	3:C:559:ARG:HG3	1.83	0.61
3:C:97:TYR:O	3:C:352:LYS:HE2	2.01	0.61
3:A:422:GLN:HE21	3:A:680:LEU:H	1.49	0.60
3:C:579:ASP:HB3	3:C:582:ASN:HB2	1.83	0.60
3:D:870:VAL:HG22	3:D:874:LYS:HE2	1.83	0.60
3:C:471:VAL:HB	3:C:472:PRO:HD3	1.82	0.60
2:H:109:DC:H2'	2:H:110:DA:C8	2.36	0.60
3:B:381:PRO:HG2	3:B:576:ARG:HG2	1.84	0.60
3:A:245:HIS:HE1	4:A:923:HOH:O	1.83	0.59
3:A:649:ASP:OD1	3:A:719:ARG:NH2	2.35	0.59
3:B:458:PRO:CG	3:B:592:MSE:SE	3.00	0.59
3:A:899:ASP:HB2	3:A:900:MSE:HE2	1.85	0.59
3:B:280:PHE:HD2	3:B:343:LEU:HD23	1.68	0.59
3:B:145:ARG:HD3	3:B:187:ILE:HD11	1.84	0.59
3:C:294:SER:HB2	3:C:301:GLY:HA2	1.85	0.58
3:C:486:LYS:HA	3:C:489:MSE:HE3	1.84	0.58
3:A:212:ILE:CG2	3:A:271:LEU:HD12	2.32	0.58
3:A:802:PRO:HG2	3:A:805:ILE:HD12	1.85	0.58
3:A:356:GLN:HE21	3:A:356:GLN:N	1.98	0.58
3:C:347:MSE:HE2	3:C:558:ASN:HD22	1.68	0.57
3:D:410:PHE:O	3:D:624:SER:HA	2.04	0.57
3:B:331:VAL:HA	3:B:334:ILE:HD12	1.86	0.57
3:D:621:ASP:O	3:D:623:ASP:N	2.37	0.57
3:A:486:LYS:HA	3:A:489:MSE:HB3	1.86	0.57
3:D:154:SER:HB3	3:D:155:PRO:HD2	1.86	0.57
3:A:202:LEU:O	3:A:206:GLN:HG2	2.05	0.57
3:B:421:ARG:HD3	3:B:475:ILE:HG23	1.87	0.57
3:D:140:ASP:HB3	3:D:143:ASP:HB2	1.85	0.57
3:C:329:TYR:O	3:C:333:GLN:HG3	2.05	0.57
3:C:661:PRO:O	3:C:665:ARG:HB2	2.04	0.57
3:D:406:TYR:HD1	3:D:647:TRP:HZ2	1.53	0.57
3:A:251:LYS:HB3	3:A:262:ILE:HG13	1.86	0.56
3:C:395:PHE:HD2	3:C:594:LEU:HD23	1.70	0.56
4:F:117:HOH:O	3:A:802:PRO:HB3	2.05	0.56
3:A:593:ALA:CB	3:A:681:MSE:HE2	2.35	0.56
3:C:394:ALA:HB1	3:C:622:THR:HB	1.87	0.56
3:A:116:GLU:HB3	3:A:320:TYR:OH	2.06	0.56
3:B:273:TYR:OH	3:B:335:ASP:HA	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:458:PRO:HG3	3:C:592:MSE:SE	2.55	0.56
3:C:85:MSE:HE2	3:C:87:ASP:H	1.69	0.55
3:B:752:MSE:HE3	3:B:889:LEU:HD12	1.88	0.55
3:C:572:ASN:ND2	3:C:574:TRP:H	2.04	0.55
3:D:749:ILE:O	3:D:753:LEU:HG	2.06	0.55
2:F:111:DT:H2''	2:F:112:DA:H5''	1.89	0.55
3:A:6:LEU:CD1	3:A:26:GLU:HG3	2.36	0.55
3:C:489:MSE:HE2	3:C:553:MSE:HA	1.88	0.55
3:C:412:LEU:HD13	3:C:415:LEU:HD13	1.89	0.55
3:D:391:TYR:HD1	3:D:391:TYR:H	1.54	0.55
3:A:555:ALA:O	3:A:559:ARG:HG2	2.08	0.55
3:C:10:GLN:HG3	3:C:65:MSE:HE1	1.87	0.54
3:D:8:VAL:HG21	3:D:93:LEU:HD21	1.88	0.54
3:D:451:SER:HB3	3:D:456:CYS:SG	2.46	0.54
1:I:9:DT:H2''	1:I:10:DA:H5''	1.88	0.54
3:A:206:GLN:HG3	3:A:241:ARG:HH21	1.72	0.54
3:B:735:SER:HA	4:B:941:HOH:O	2.07	0.54
3:D:609:CYS:HA	3:D:635:LYS:HD2	1.87	0.54
3:B:71:TRP:CE2	3:B:75:MSE:HE3	2.41	0.54
3:C:870:VAL:CG1	3:C:874:LYS:HD3	2.36	0.54
3:A:231:LYS:HG3	3:A:236:GLU:HA	1.90	0.54
3:D:702:TRP:HZ3	3:D:710:LEU:HD21	1.72	0.54
3:D:412:LEU:HA	3:D:683:MSE:HA	1.90	0.54
3:D:629:ALA:HA	3:D:632:ILE:HD12	1.89	0.54
2:L:106:DT:H2''	2:L:107:DG:C8	2.43	0.54
2:L:111:DT:H2''	2:L:112:DA:C8	2.42	0.54
3:A:494:ARG:O	3:A:497:GLU:HG2	2.08	0.54
3:C:433:THR:O	3:C:462:MSE:HE2	2.07	0.54
3:C:370:PHE:HB2	3:C:380:ILE:HD11	1.89	0.54
2:H:113:DA:H5'	3:B:289:SER:HB2	1.90	0.53
3:A:830:VAL:CG1	3:A:847:ALA:HB1	2.38	0.53
3:C:59:ARG:HH12	3:C:61:LEU:HD13	1.74	0.53
3:B:288:TYR:HA	3:B:293:ILE:HD11	1.90	0.53
3:D:439:LEU:O	3:D:443:ILE:HG12	2.08	0.53
3:D:731:GLU:HA	3:D:734:LYS:CG	2.38	0.53
3:A:347:MSE:HG2	3:A:358:VAL:HG23	1.90	0.53
3:B:877:ILE:HG13	3:B:878:LYS:N	2.23	0.53
3:C:475:ILE:HD11	3:C:563:ILE:HA	1.91	0.53
3:D:125:GLU:HG3	3:D:127:SER:H	1.73	0.53
3:D:608:VAL:O	3:D:635:LYS:NZ	2.41	0.52
3:B:231:LYS:HA	3:B:239:ALA:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:422:GLN:HG2	3:C:678:GLN:O	2.09	0.52
3:A:116:GLU:HB2	3:A:135:ALA:HB3	1.92	0.52
3:C:61:LEU:HG	3:C:62:PHE:H	1.74	0.52
3:D:655:ALA:HA	3:D:659:MSE:HB2	1.90	0.52
1:E:7:DC:H2'	1:E:8:DT:H72	1.92	0.52
3:A:819:ILE:H	3:A:819:ILE:HD13	1.74	0.52
3:B:11:ILE:HG12	3:B:247:LYS:HD2	1.91	0.52
3:B:317:HIS:CE1	3:B:321:ILE:HD11	2.45	0.52
3:B:359:PHE:O	3:B:361:PRO:HD3	2.10	0.52
3:B:17:GLU:OE1	3:B:29:ARG:NH1	2.40	0.52
3:B:373:LEU:HB3	3:B:378:LYS:HB2	1.91	0.52
3:D:250:VAL:HA	3:D:263:ILE:HA	1.93	0.51
3:A:424:ASN:O	3:A:429:THR:CG2	2.50	0.51
3:B:162:TRP:HB2	3:B:321:ILE:HD12	1.92	0.51
2:L:110:DA:H2''	2:L:111:DT:H5''	1.91	0.51
3:A:811:TYR:O	3:A:815:ILE:HB	2.11	0.51
2:J:111:DT:H2''	2:J:112:DA:H8	1.75	0.51
3:B:214:THR:HG21	3:B:341:ILE:HD11	1.92	0.51
3:C:391:TYR:HB2	3:C:392:PRO:HD2	1.91	0.51
3:C:731:GLU:HG3	3:C:879:PRO:HB3	1.93	0.51
3:D:455:SER:HA	3:D:675:ASN:O	2.11	0.51
2:H:112:DA:H2''	2:H:113:DA:C8	2.45	0.51
3:C:593:ALA:CB	3:C:681:MSE:HE2	2.41	0.51
2:H:108:DT:H2''	2:H:109:DC:H5''	1.91	0.51
3:D:764:PHE:O	3:D:768:GLU:HG2	2.11	0.51
3:C:604:TYR:OH	3:C:658:ARG:HG3	2.11	0.51
3:A:412:LEU:HD13	3:A:415:LEU:HD13	1.93	0.50
3:B:391:TYR:HB2	3:B:392:PRO:HD2	1.93	0.50
3:C:109:ARG:HH21	3:C:208:LYS:HB3	1.75	0.50
3:A:314:GLU:HG2	3:A:315:SER:N	2.25	0.50
3:A:528:GLU:C	3:A:530:ILE:H	2.18	0.50
2:J:112:DA:H5'	3:C:734:LYS:HG2	1.93	0.50
3:A:172:GLU:H	3:A:172:GLU:CD	2.18	0.50
3:A:127:SER:HA	3:A:228:ASN:ND2	2.27	0.50
3:D:437:ALA:HB3	3:D:442:TYR:CE2	2.46	0.50
3:C:602:ASN:O	3:C:606:ASN:ND2	2.39	0.50
3:A:23:ASN:HD22	3:A:25:ARG:HH21	1.59	0.49
3:A:574:TRP:HA	3:A:574:TRP:CE3	2.46	0.49
3:C:214:THR:HG21	3:C:341:ILE:HD11	1.94	0.49
3:D:356:GLN:C	3:D:358:VAL:H	2.20	0.49
3:B:193:ASN:HB3	3:B:196:GLU:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:222:ALA:O	3:B:226:VAL:HG23	2.12	0.49
3:B:272:ASP:OD1	3:B:274:ILE:HG22	2.11	0.49
3:B:291:ASP:HA	4:B:946:HOH:O	2.12	0.49
3:B:573:VAL:HG12	3:B:578:TYR:CZ	2.48	0.49
3:C:111:ALA:HB3	3:C:210:PRO:HB3	1.95	0.49
3:C:216:TRP:CD2	3:C:290:LEU:HD23	2.47	0.49
3:B:149:PHE:HB3	3:B:197:LEU:HD21	1.95	0.49
3:B:471:VAL:HG11	3:B:570:LEU:HD11	1.95	0.49
3:B:734:LYS:HE2	3:B:736:SER:HB2	1.95	0.49
3:A:391:TYR:CZ	3:A:583:ALA:HB1	2.48	0.49
3:B:611:THR:HG22	3:B:612:GLU:H	1.78	0.49
3:B:881:GLU:HA	3:B:884:THR:OG1	2.13	0.49
3:C:593:ALA:HB1	3:C:681:MSE:HE2	1.93	0.49
3:C:426:SER:C	3:C:582:ASN:HD21	2.20	0.48
3:A:747:GLU:HG3	3:A:751:ARG:HD2	1.95	0.48
3:B:592:MSE:HE1	3:B:674:MSE:HE3	1.95	0.48
3:A:17:GLU:OE2	3:A:97:TYR:OH	2.20	0.48
3:A:70:GLN:O	3:A:74:ARG:HB2	2.13	0.48
3:C:412:LEU:HG	3:C:683:MSE:HE3	1.93	0.48
3:A:414:SER:O	3:A:417:PRO:HD2	2.13	0.48
3:A:466:ASP:OD1	3:A:467:ARG:N	2.46	0.48
3:B:642:ARG:HE	3:B:646:HIS:CG	2.31	0.48
1:I:11:DT:H4'	3:C:707:ARG:HD3	1.95	0.48
3:A:495:ASN:OD1	3:A:495:ASN:C	2.56	0.48
3:A:897:LEU:O	3:A:900:MSE:HG2	2.13	0.48
3:B:313:ARG:HH11	3:B:314:GLU:HG3	1.79	0.48
3:C:285:GLN:HG3	3:C:286:PRO:HD2	1.96	0.48
3:C:369:ILE:HG12	3:C:474:GLU:HG3	1.96	0.48
3:C:423:VAL:HB	3:C:425:ILE:HG13	1.94	0.48
3:A:449:ARG:HH12	3:A:452:ASP:HB3	1.78	0.48
3:D:386:HIS:HB3	3:D:387:PRO:HD2	1.95	0.48
3:D:841:PHE:HZ	3:D:861:ASP:HB3	1.79	0.48
3:A:290:LEU:HB3	3:A:302:LYS:HD2	1.96	0.48
3:C:130:LYS:HG3	3:C:131:HIS:CD2	2.49	0.48
3:D:322:SER:HA	3:D:325:ILE:HD12	1.96	0.48
3:A:489:MSE:HE1	3:A:553:MSE:HG2	1.94	0.48
3:A:553:MSE:HE3	3:A:557:ILE:HD11	1.95	0.48
3:B:2:LYS:HA	4:B:966:HOH:O	2.13	0.48
3:C:291:ASP:CG	3:C:302:LYS:HB2	2.39	0.48
3:A:199:MSE:HE3	3:A:234:PHE:CE2	2.49	0.48
3:A:406:TYR:HB3	3:A:629:ALA:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:291:ASP:OD2	3:C:302:LYS:HB2	2.14	0.48
3:B:898:PHE:N	4:B:925:HOH:O	2.45	0.47
3:D:406:TYR:CE2	3:D:633:ILE:HG21	2.49	0.47
2:J:112:DA:C5'	3:C:734:LYS:HG2	2.44	0.47
3:C:127:SER:HA	3:C:261:GLU:OE1	2.14	0.47
3:A:471:VAL:HB	3:A:472:PRO:HD3	1.95	0.47
3:C:61:LEU:HG	3:C:62:PHE:N	2.30	0.47
1:I:7:DC:H1'	4:I:65:HOH:O	2.14	0.47
3:B:728:MSE:HE2	3:B:729:GLY:H	1.78	0.47
3:D:104:ASP:C	3:D:106:THR:H	2.23	0.47
3:A:881:GLU:O	3:A:885:SER:HB3	2.14	0.47
3:C:760:LEU:HD13	3:C:891:TYR:HA	1.95	0.47
3:C:813:ARG:C	3:C:815:ILE:H	2.23	0.47
3:C:831:TYR:O	3:C:847:ALA:HA	2.15	0.47
3:A:120:PRO:HG3	3:A:156:TYR:CE1	2.50	0.47
3:B:249:ARG:HB3	3:B:264:THR:HB	1.97	0.47
3:C:126:PRO:HA	3:C:225:TYR:CD2	2.50	0.47
3:C:439:LEU:O	3:C:443:ILE:HG13	2.15	0.47
3:B:48:LYS:HG3	3:B:377:ASN:HD22	1.80	0.47
3:C:199:MSE:HG2	3:C:234:PHE:CZ	2.50	0.47
3:C:629:ALA:HA	3:C:632:ILE:HD12	1.96	0.47
3:D:29:ARG:HG3	3:D:31:VAL:HG12	1.97	0.47
3:B:303:LEU:HD23	3:B:326:ILE:HD13	1.97	0.47
3:C:494:ARG:HD2	3:C:521:ASP:OD2	2.15	0.47
3:A:308:PRO:HG2	3:A:311:LYS:HG2	1.96	0.46
3:C:422:GLN:HE21	3:C:422:GLN:HB3	1.56	0.46
3:C:727:ILE:HD13	3:C:732:THR:HG21	1.97	0.46
3:D:705:LYS:C	3:D:707:ARG:H	2.24	0.46
3:A:82:ALA:O	3:A:382:GLN:HB2	2.15	0.46
3:B:38:PHE:CE2	3:B:59:ARG:HB2	2.50	0.46
3:B:406:TYR:CD2	3:B:633:ILE:HG13	2.51	0.46
1:K:14:DC:OP1	3:D:874:LYS:HD2	2.14	0.46
3:A:113:PHE:CE1	3:A:213:LEU:HD11	2.50	0.46
3:B:182:ILE:HD11	3:B:329:TYR:CD2	2.50	0.46
3:B:395:PHE:HB2	3:B:591:GLN:HG2	1.97	0.46
3:A:251:LYS:HD3	3:A:262:ILE:HD11	1.97	0.46
3:B:373:LEU:HD12	3:B:380:ILE:HG22	1.98	0.46
3:B:621:ASP:OD1	3:B:622:THR:HG22	2.14	0.46
3:B:872:LEU:HD22	3:B:876:PHE:HB3	1.97	0.46
3:B:25:ARG:HH11	3:B:25:ARG:HB3	1.80	0.46
3:B:635:LYS:HG2	3:D:898:PHE:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:250:VAL:HG22	3:C:263:ILE:HD12	1.97	0.46
3:C:534:SER:HB2	3:C:537:SER:HB2	1.96	0.46
3:D:725:LEU:H	3:D:725:LEU:CD2	2.26	0.46
3:C:16:PHE:HB3	3:C:245:HIS:CE1	2.51	0.46
3:D:621:ASP:O	3:D:624:SER:N	2.43	0.46
3:D:660:GLU:N	3:D:661:PRO:HD2	2.31	0.46
1:K:19:DG:H2''	1:K:20:DC:OP2	2.16	0.46
2:L:106:DT:H2''	2:L:107:DG:H8	1.81	0.46
3:A:53:TYR:CE2	3:A:428:GLU:HA	2.51	0.46
3:A:171:GLN:HE22	3:A:319:ARG:HH12	1.64	0.46
3:A:298:LEU:HB2	3:A:300:VAL:HG12	1.97	0.46
3:B:149:PHE:HB3	3:B:197:LEU:CD2	2.46	0.46
3:B:421:ARG:HB3	3:B:680:LEU:CD1	2.45	0.46
3:A:145:ARG:HG3	3:A:185:LYS:O	2.16	0.46
3:B:129:ALA:HB1	3:B:225:TYR:CZ	2.51	0.46
3:C:488:TYR:HB3	3:C:519:ARG:HG2	1.98	0.46
3:D:474:GLU:O	3:D:478:VAL:HG23	2.16	0.46
3:A:641:PHE:HA	3:A:646:HIS:ND1	2.31	0.45
3:A:812:ASN:HA	3:A:815:ILE:HG22	1.97	0.45
3:B:405:LYS:HB3	3:B:630:ASP:OD1	2.16	0.45
3:C:111:ALA:CB	3:C:210:PRO:HB3	2.46	0.45
3:C:614:GLU:HA	3:C:614:GLU:OE1	2.16	0.45
3:D:420:ILE:HG23	3:D:425:ILE:HB	1.97	0.45
3:A:132:PRO:HG3	3:A:155:PRO:HD2	1.97	0.45
3:B:123:PHE:HA	3:B:124:PRO:HD3	1.82	0.45
3:B:322:SER:HA	3:B:325:ILE:HD12	1.97	0.45
3:A:629:ALA:HA	3:A:632:ILE:HD12	1.97	0.45
3:D:52:ILE:HD11	3:D:470:VAL:HB	1.97	0.45
3:B:117:VAL:HG12	3:B:118:THR:N	2.31	0.45
1:G:13:DA:H61	2:H:108:DT:H3	1.65	0.45
3:A:176:ASP:HA	3:A:319:ARG:NH2	2.32	0.45
3:B:263:ILE:HD13	3:B:263:ILE:H	1.81	0.45
3:B:326:ILE:H	3:B:326:ILE:HG13	1.53	0.45
3:C:85:MSE:HE3	3:C:87:ASP:H	1.80	0.45
3:C:752:MSE:HE3	3:C:889:LEU:HD12	1.99	0.45
3:D:579:ASP:HB3	3:D:582:ASN:HB2	1.99	0.45
3:B:423:VAL:HB	3:B:425:ILE:HG13	1.99	0.45
3:C:109:ARG:HB3	3:C:211:VAL:HG23	1.99	0.45
3:A:112:ASN:HB2	3:A:139:TYR:HB3	1.99	0.45
3:B:412:LEU:HD22	3:B:681:MSE:HG3	1.98	0.45
3:B:655:ALA:HA	3:B:659:MSE:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:49:TYR:CZ	3:C:59:ARG:HD3	2.52	0.44
3:A:692:PRO:O	3:A:695:SER:OG	2.33	0.44
3:B:218:VAL:N	3:B:272:ASP:OD2	2.50	0.44
3:B:281:SER:HA	3:B:340:PHE:HZ	1.83	0.44
3:A:680:LEU:HA	3:A:682:PHE:CZ	2.52	0.44
3:B:206:GLN:HE21	3:B:241:ARG:HH21	1.65	0.44
3:C:33:TYR:O	3:C:35:PRO:HD3	2.16	0.44
3:A:727:ILE:HG23	3:A:730:LEU:HD12	1.98	0.44
3:B:274:ILE:O	3:B:278:LYS:HB2	2.18	0.44
3:B:638:GLU:O	3:B:693:LEU:HD11	2.17	0.44
2:F:102:DC:H2''	2:F:103:DG:C8	2.53	0.44
3:C:421:ARG:HD2	3:C:476:THR:OG1	2.16	0.44
3:D:399:PRO:HG3	3:D:702:TRP:CD1	2.52	0.44
3:B:98:ASN:HD22	3:B:98:ASN:N	2.11	0.44
3:B:351:ALA:O	3:B:352:LYS:HB2	2.18	0.44
3:B:394:ALA:CB	3:B:622:THR:HB	2.42	0.44
3:D:619:TYR:OH	3:D:706:LYS:N	2.50	0.44
3:D:751:ARG:CZ	3:D:763:TYR:HB2	2.48	0.44
3:B:194:GLU:HG2	3:B:229:ARG:HH21	1.83	0.44
3:B:634:ASP:C	3:B:636:VAL:H	2.26	0.44
3:D:373:LEU:C	3:D:375:GLU:H	2.26	0.44
3:A:414:SER:O	3:A:415:LEU:C	2.60	0.44
3:A:216:TRP:CD2	3:A:290:LEU:HD13	2.53	0.43
3:B:25:ARG:HD2	3:B:25:ARG:HA	1.74	0.43
3:B:757:GLU:HB2	3:B:889:LEU:HD22	2.00	0.43
3:C:621:ASP:O	3:C:623:ASP:N	2.51	0.43
3:A:294:SER:HB3	3:A:301:GLY:HA2	2.00	0.43
3:A:523:SER:C	3:A:525:GLU:H	2.26	0.43
3:C:347:MSE:HE2	3:C:558:ASN:ND2	2.33	0.43
3:D:331:VAL:HA	3:D:334:ILE:HD12	1.99	0.43
3:A:809:LEU:O	3:A:813:ARG:HG3	2.18	0.43
3:A:593:ALA:HB1	3:A:681:MSE:CE	2.47	0.43
3:D:808:ILE:HA	3:D:847:ALA:HB3	2.00	0.43
1:G:18:DC:H42	2:H:103:DG:H1	1.67	0.43
2:H:115:DA:O3'	3:B:117:VAL:O	2.36	0.43
3:B:98:ASN:H	3:B:98:ASN:ND2	2.11	0.43
3:C:428:GLU:H	3:C:428:GLU:HG3	1.52	0.43
3:C:482:ARG:HE	3:C:556:GLN:NE2	2.16	0.43
3:D:369:ILE:HG21	3:D:577:TYR:CE1	2.54	0.43
3:D:406:TYR:CD1	3:D:647:TRP:HZ2	2.33	0.43
3:D:739:LYS:HA	3:D:742:GLN:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:199:MSE:HE2	3:A:199:MSE:HA	2.01	0.43
3:B:165:GLU:H	3:B:165:GLU:CD	2.27	0.43
3:C:872:LEU:HD12	3:C:876:PHE:HB3	2.01	0.43
3:D:873:GLU:HA	3:D:877:ILE:HB	1.99	0.43
3:C:110:VAL:HB	3:C:141:SER:HB2	2.01	0.43
3:C:413:THR:O	3:C:414:SER:C	2.61	0.43
3:C:486:LYS:HB2	3:C:556:GLN:HG3	2.01	0.43
3:C:577:TYR:HA	4:C:993:HOH:O	2.18	0.43
3:B:35:PRO:HG3	3:B:65:MSE:HG2	1.99	0.43
3:B:271:LEU:HD21	3:B:344:SER:HB3	2.00	0.43
3:D:412:LEU:HD13	3:D:415:LEU:HD13	2.01	0.43
3:D:788:ILE:HA	3:D:805:ILE:HD11	2.00	0.43
3:A:139:TYR:CG	3:A:332:LEU:HD11	2.54	0.43
3:A:449:ARG:NH1	3:A:452:ASP:HB3	2.33	0.43
3:A:489:MSE:C	3:A:491:ALA:H	2.26	0.43
3:B:249:ARG:HG2	3:B:251:LYS:HG3	1.99	0.43
3:D:408:MSE:HE3	3:D:659:MSE:HE2	2.01	0.43
3:C:206:GLN:NE2	3:C:241:ARG:O	2.51	0.42
3:C:514:LEU:HB3	3:C:541:MSE:SE	2.68	0.42
3:B:244:PRO:HG2	3:B:267:GLY:HA3	2.02	0.42
3:B:766:GLU:HG2	3:B:770:GLU:OE2	2.18	0.42
3:C:731:GLU:CG	3:C:879:PRO:HB3	2.48	0.42
3:A:412:LEU:HG	3:A:683:MSE:HG2	2.00	0.42
3:B:422:GLN:HG3	3:B:678:GLN:O	2.19	0.42
1:I:3:DC:H4'	3:C:87:ASP:HB2	2.02	0.42
3:A:482:ARG:HE	3:A:556:GLN:HG2	1.84	0.42
3:B:209:THR:HA	3:B:210:PRO:HD3	1.83	0.42
3:C:449:ARG:HA	3:C:450:PRO:HD3	1.87	0.42
3:A:708:TYR:CZ	3:A:728:MSE:HG3	2.53	0.42
3:B:249:ARG:HD3	3:B:251:LYS:HE3	2.02	0.42
3:B:779:ILE:HG12	3:B:871:LEU:HG	2.01	0.42
3:C:45:GLN:O	3:C:47:THR:HG23	2.20	0.42
3:C:209:THR:HA	3:C:210:PRO:HD3	1.79	0.42
3:D:362:ILE:O	3:D:366:ASP:HB2	2.19	0.42
3:D:489:MSE:HE3	3:D:489:MSE:HB3	2.01	0.42
3:A:285:GLN:HA	3:A:286:PRO:HD3	1.94	0.42
3:A:376:GLN:HG3	3:A:378:LYS:HG3	2.01	0.42
3:B:145:ARG:CZ	3:B:145:ARG:HB3	2.49	0.42
3:C:302:LYS:HD3	3:C:323:TYR:CE1	2.54	0.42
3:C:601:VAL:HG13	3:C:659:MSE:HE1	2.01	0.42
3:B:263:ILE:H	3:B:263:ILE:CD1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:644:THR:C	3:D:646:HIS:H	2.27	0.42
3:C:356:GLN:CD	3:C:356:GLN:H	2.28	0.42
3:A:600:LYS:NZ	3:A:669:GLU:OE1	2.36	0.42
3:B:593:ALA:HA	3:B:670:MSE:SE	2.70	0.42
3:A:415:LEU:HD11	3:A:681:MSE:HE1	2.02	0.42
3:A:653:LYS:HG2	3:A:656:ARG:NH2	2.35	0.42
3:B:698:ILE:HG13	3:B:753:LEU:HD23	2.01	0.42
3:C:352:LYS:HB2	3:C:371:ASN:HD21	1.84	0.42
3:C:456:CYS:CB	3:C:674:MSE:HE3	2.43	0.42
2:H:106:DT:H5''	4:H:124:HOH:O	2.20	0.41
3:C:154:SER:C	3:C:156:TYR:H	2.27	0.41
3:D:412:LEU:HD12	3:D:412:LEU:H	1.85	0.41
3:A:719:ARG:HH11	3:A:719:ARG:HB2	1.85	0.41
3:B:335:ASP:O	3:B:339:GLN:HA	2.20	0.41
3:B:425:ILE:HG12	3:B:463:TYR:CE1	2.54	0.41
3:C:620:GLY:HA2	3:C:624:SER:O	2.19	0.41
3:A:23:ASN:ND2	3:A:25:ARG:NH2	2.68	0.41
3:A:147:TYR:OH	3:A:208:LYS:NZ	2.53	0.41
3:B:85:MSE:SE	3:B:87:ASP:H	2.53	0.41
3:D:125:GLU:HA	3:D:126:PRO:HD3	1.88	0.41
3:D:575:PHE:HB3	3:D:578:TYR:HB2	2.02	0.41
3:A:362:ILE:HG23	3:A:575:PHE:HD1	1.84	0.41
3:A:449:ARG:HA	3:A:450:PRO:HD3	1.94	0.41
3:B:416:TYR:HD1	3:B:419:ILE:HD12	1.85	0.41
3:B:894:LYS:HE2	3:B:894:LYS:HB3	1.89	0.41
3:A:41:CYS:HB2	3:A:42:PRO:CD	2.50	0.41
3:C:150:ASP:HB2	3:C:188:TYR:HE1	1.85	0.41
3:A:405:LYS:O	3:A:690:GLY:HA2	2.20	0.41
3:B:119:SER:HA	3:B:120:PRO:HD2	1.90	0.41
3:B:405:LYS:O	3:B:691:PRO:HD3	2.21	0.41
3:D:334:ILE:O	3:D:338:ARG:N	2.52	0.41
1:I:4:DC:H2'	1:I:5:DG:C5	2.55	0.41
3:B:3:GLU:HG2	3:B:21:ASP:HA	2.03	0.41
3:B:131:HIS:HA	3:B:132:PRO:HD3	1.89	0.41
3:C:52:ILE:HB	3:C:428:GLU:HG2	2.03	0.41
3:C:171:GLN:H	3:C:177:GLU:HG2	1.86	0.41
3:C:182:ILE:O	3:C:186:ILE:HG13	2.19	0.41
3:C:335:ASP:O	3:C:339:GLN:N	2.49	0.41
3:C:461:MSE:HE1	3:C:581:ARG:HD2	2.02	0.41
3:D:592:MSE:HE3	3:D:670:MSE:SE	2.71	0.41
3:D:745:LEU:HA	3:D:748:CYS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:810:THR:HG23	3:D:813:ARG:HH22	1.86	0.41
1:K:21:DG:O6	3:A:380:ILE:HG12	2.21	0.40
3:B:557:ILE:O	3:B:561:LEU:HG	2.21	0.40
3:C:813:ARG:C	3:C:815:ILE:N	2.79	0.40
3:D:830:VAL:HA	3:D:849:PRO:HA	2.03	0.40
3:B:330:ARG:O	3:B:334:ILE:HG13	2.22	0.40
3:B:413:THR:O	3:B:414:SER:C	2.65	0.40
3:B:611:THR:HG21	3:B:614:GLU:OE1	2.21	0.40
3:C:150:ASP:HB2	3:C:188:TYR:CE1	2.57	0.40
3:C:784:SER:O	3:C:804:HIS:CD2	2.75	0.40
3:D:33:TYR:HD2	3:D:65:MSE:HE1	1.86	0.40
2:J:111:DT:H2''	2:J:112:DA:C8	2.54	0.40
2:L:109:DC:H2'	2:L:110:DA:C8	2.56	0.40
3:A:214:THR:HG21	3:A:341:ILE:HD11	2.03	0.40
3:A:289:SER:O	3:A:293:ILE:HG12	2.22	0.40
3:A:426:SER:O	3:A:427:PRO:C	2.63	0.40
3:A:601:VAL:HG13	3:A:659:MSE:HE1	2.03	0.40
3:B:116:GLU:HG2	3:B:320:TYR:CZ	2.56	0.40
3:C:70:GLN:O	3:C:74:ARG:HB2	2.19	0.40
1:K:14:DC:H4'	4:D:920:HOH:O	2.20	0.40
3:B:397:LYS:HB3	3:B:620:GLY:H	1.86	0.40
3:C:644:THR:HG1	3:C:693:LEU:H	1.67	0.40
3:C:821:ALA:HA	3:C:822:PRO:HD3	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	886/903 (98%)	828 (94%)	51 (6%)	7 (1%)	16	44
3	B	750/903 (83%)	683 (91%)	61 (8%)	6 (1%)	16	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	879/903 (97%)	816 (93%)	58 (7%)	5 (1%)	21	51
3	D	865/903 (96%)	750 (87%)	101 (12%)	14 (2%)	7	27
All	All	3380/3612 (94%)	3077 (91%)	271 (8%)	32 (1%)	14	41

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	622	THR
3	D	622	THR
3	D	796	PHE
3	A	521	ASP
3	A	622	THR
3	A	716	GLU
3	B	352	LYS
3	A	816	LYS
3	B	262	ILE
3	C	256	MSE
3	D	797	PRO
3	A	529	LYS
3	B	315	SER
3	D	105	HIS
3	D	316	ASN
3	D	357	SER
3	D	436	VAL
3	D	828	GLU
3	D	897	LEU
3	A	489	MSE
3	C	252	VAL
3	A	300	VAL
3	B	172	GLU
3	B	179	PRO
3	C	525	GLU
3	D	352	LYS
3	D	383	GLY
3	B	777	ILE
3	D	827	GLY
3	C	430	ILE
3	D	262	ILE
3	D	31	VAL

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	
3	A	752/775 (97%)	712 (95%)	40 (5%)	20	52
3	B	632/775 (82%)	591 (94%)	41 (6%)	15	43
3	C	752/775 (97%)	705 (94%)	47 (6%)	16	45
3	D	518/775 (67%)	488 (94%)	30 (6%)	18	49
All	All	2654/3100 (86%)	2496 (94%)	158 (6%)	17	47

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	15	ILE
3	A	83	LEU
3	A	98	ASN
3	A	128	GLN
3	A	154	SER
3	A	164	ILE
3	A	172	GLU
3	A	217	ASN
3	A	219	GLU
3	A	231	LYS
3	A	242	LEU
3	A	250	VAL
3	A	253	ILE
3	A	298	LEU
3	A	314	GLU
3	A	319	ARG
3	A	330	ARG
3	A	356	GLN
3	A	403	ARG
3	A	429	THR
3	A	433	THR
3	A	446	VAL
3	A	489	MSE
3	A	495	ASN

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Mol	Chain	Res	Type
3	A	520	PHE
3	A	521	ASP
3	A	528	GLU
3	A	542	LEU
3	A	576	ARG
3	A	645	ASN
3	A	669	GLU
3	A	719	ARG
3	A	746	LYS
3	A	790	LYS
3	A	815	ILE
3	A	819	ILE
3	A	855	THR
3	A	859	LYS
3	A	881	GLU
3	A	902	ASP
3	B	22	SER
3	B	25	ARG
3	B	48	LYS
3	B	98	ASN
3	B	112	ASN
3	B	113	PHE
3	B	116	GLU
3	B	131	HIS
3	B	134	ASP
3	B	136	ILE
3	B	159	VAL
3	B	161	GLU
3	B	164	ILE
3	B	165	GLU
3	B	212	ILE
3	B	231	LYS
3	B	248	THR
3	B	252	VAL
3	B	263	ILE
3	B	322	SER
3	B	326	ILE
3	B	362	ILE
3	B	403	ARG
3	B	405	LYS
3	B	414	SER
3	B	421	ARG

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Mol	Chain	Res	Type
3	B	436	VAL
3	B	627	VAL
3	B	681	MSE
3	B	685	ARG
3	B	728	MSE
3	B	737	THR
3	B	758	GLU
3	B	774	LEU
3	B	779	ILE
3	B	867	ASP
3	B	871	LEU
3	B	872	LEU
3	B	877	ILE
3	B	881	GLU
3	B	894	LYS
3	C	15	ILE
3	C	20	ILE
3	C	26	GLU
3	C	73	LYS
3	C	106	THR
3	C	127	SER
3	C	171	GLN
3	C	172	GLU
3	C	220	SER
3	C	238	THR
3	C	246	ARG
3	C	249	ARG
3	C	256	MSE
3	C	262	ILE
3	C	279	LYS
3	C	290	LEU
3	C	299	ASN
3	C	318	GLN
3	C	356	GLN
3	C	362	ILE
3	C	373	LEU
3	C	380	ILE
3	C	408	MSE
3	C	422	GLN
3	C	428	GLU
3	C	435	LYS
3	C	477	LYS

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Mol	Chain	Res	Type
3	C	479	PHE
3	C	483	LYS
3	C	521	ASP
3	C	539	ASN
3	C	540	GLU
3	C	549	GLU
3	C	562	LEU
3	C	572	ASN
3	C	580	LEU
3	C	607	GLU
3	C	612	GLU
3	C	622	THR
3	C	625	ILE
3	C	683	MSE
3	C	725	LEU
3	C	731	GLU
3	C	760	LEU
3	C	815	ILE
3	C	825	VAL
3	C	881	GLU
3	D	17	GLU
3	D	65	MSE
3	D	85	MSE
3	D	217	ASN
3	D	236	GLU
3	D	238	THR
3	D	271	LEU
3	D	326	ILE
3	D	356	GLN
3	D	362	ILE
3	D	391	TYR
3	D	408	MSE
3	D	412	LEU
3	D	489	MSE
3	D	572	ASN
3	D	576	ARG
3	D	618	LEU
3	D	627	VAL
3	D	633	ILE
3	D	639	SER
3	D	671	CYS
3	D	678	GLN

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Mol	Chain	Res	Type
3	D	724	LYS
3	D	725	LEU
3	D	743	LYS
3	D	745	LEU
3	D	778	SER
3	D	844	LYS
3	D	853	GLU
3	D	865	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	23	ASN
3	A	98	ASN
3	A	112	ASN
3	A	171	GLN
3	A	299	ASN
3	A	324	ASN
3	A	339	GLN
3	A	356	GLN
3	A	386	HIS
3	A	422	GLN
3	A	424	ASN
3	A	485	HIS
3	A	839	ASN
3	B	45	GLN
3	B	64	ASN
3	B	98	ASN
3	B	173	GLN
3	B	206	GLN
3	B	217	ASN
3	B	299	ASN
3	B	354	GLN
3	B	377	ASN
3	B	386	HIS
3	B	444	ASN
3	B	646	HIS
3	C	10	GLN
3	C	153	ASN
3	C	207	GLN
3	C	228	ASN
3	C	245	HIS

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Mol	Chain	Res	Type
3	C	324	ASN
3	C	371	ASN
3	C	389	GLN
3	C	485	HIS
3	C	539	ASN
3	C	556	GLN
3	C	558	ASN
3	C	572	ASN
3	C	645	ASN
3	C	675	ASN
3	D	10	GLN
3	D	112	ASN
3	D	128	GLN
3	D	558	ASN
3	D	572	ASN
3	D	646	HIS
3	D	733	GLN
3	D	742	GLN
3	D	754	GLN
3	D	761	GLN
3	D	812	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	3DR	I	6	1	8,11,12	0.46	0	7,14,17	0.88	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
1	3DR	I	6	1	-	2/3/15/16	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	I	6	3DR	O4'-C4'-C5'-O5'
1	I	6	3DR	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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	E	15/21 (71%)	-0.06	1 (6%) 24 17	50, 71, 97, 100	0
1	G	11/21 (52%)	1.32	3 (27%) 1 1	68, 102, 119, 120	0
1	I	19/21 (90%)	-0.04	1 (5%) 32 24	42, 52, 136, 139	0
1	K	11/21 (52%)	0.48	0 100 100	49, 104, 111, 112	0
2	F	15/15 (100%)	0.29	0 100 100	64, 85, 111, 114	0
2	H	15/15 (100%)	1.09	2 (13%) 7 5	88, 116, 121, 124	0
2	J	15/15 (100%)	-0.15	0 100 100	39, 65, 82, 90	0
2	L	13/15 (86%)	0.74	0 100 100	115, 119, 124, 124	0
3	A	865/903 (95%)	0.06	18 (2%) 63 54	39, 54, 100, 124	0
3	B	734/903 (81%)	0.36	25 (3%) 48 39	42, 66, 109, 115	0
3	C	861/903 (95%)	0.21	20 (2%) 61 51	35, 62, 99, 126	0
3	D	852/903 (94%)	1.04	112 (13%) 7 6	98, 118, 133, 141	0
All	All	3426/3756 (91%)	0.42	182 (5%) 32 24	35, 69, 127, 141	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	518	TYR	4.7
3	C	253	ILE	4.4
3	D	791	TYR	4.3
3	D	647	TRP	4.0
3	C	535	ALA	3.9
3	C	150	ASP	3.8
3	C	252	VAL	3.7
3	C	526	ILE	3.7
3	D	801	CYS	3.7
3	D	15	ILE	3.6
3	A	533	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
3	C	303	LEU	3.6
3	D	242	LEU	3.6
3	B	260	ARG	3.5
3	D	518	TYR	3.5
3	D	138	HIS	3.4
3	D	31	VAL	3.4
3	D	491	ALA	3.4
3	D	61	LEU	3.4
3	D	316	ASN	3.3
3	A	538	LEU	3.3
3	D	303	LEU	3.3
3	D	848	TRP	3.3
3	B	123	PHE	3.2
3	D	156	TYR	3.2
3	D	33	TYR	3.2
3	D	419	ILE	3.2
3	B	303	LEU	3.2
3	D	174	GLY	3.2
3	D	265	LEU	3.2
3	D	805	ILE	3.2
3	A	503	LEU	3.1
3	D	854	ILE	3.1
3	D	855	THR	3.1
3	D	446	VAL	3.1
3	C	44	SER	3.1
3	D	176	ASP	3.1
3	A	786	ASN	3.0
3	D	548	THR	3.0
3	B	309	ILE	3.0
3	D	787	ASN	3.0
3	D	202	LEU	3.0
3	D	524	ASP	3.0
3	B	160	GLU	2.9
3	D	650	PHE	2.9
3	A	522	PHE	2.9
3	D	88	PHE	2.9
3	B	156	TYR	2.9
3	D	515	ASP	2.8
3	B	257	TYR	2.8
3	C	495	ASN	2.8
3	D	315	SER	2.8
3	D	636	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	529	LYS	2.7
3	C	532	LYS	2.7
1	I	2	DA	2.7
3	D	160	GLU	2.7
3	D	270	VAL	2.7
3	B	198	LEU	2.7
3	B	290	LEU	2.7
3	D	86	ASP	2.7
3	C	538	LEU	2.7
3	D	514	LEU	2.7
3	D	305	TYR	2.7
3	D	134	ASP	2.7
3	D	490	LEU	2.7
3	D	210	PRO	2.6
3	D	580	LEU	2.6
3	D	274	ILE	2.6
3	D	282	PHE	2.6
3	D	577	TYR	2.6
3	D	698	ILE	2.6
3	B	259	SER	2.6
3	C	530	ILE	2.6
3	D	395	PHE	2.6
3	B	298	LEU	2.5
3	D	393	GLY	2.5
3	D	793	VAL	2.5
3	D	149	PHE	2.5
3	D	37	LEU	2.5
3	B	191	PHE	2.5
3	B	137	THR	2.5
3	D	785	ALA	2.5
3	B	178	VAL	2.4
1	G	11	DT	2.4
3	D	789	ALA	2.4
3	A	526	ILE	2.4
3	D	400	ILE	2.4
3	C	456	CYS	2.4
3	D	458	PRO	2.4
3	D	63	ALA	2.4
3	D	808	ILE	2.4
3	D	424	ASN	2.4
3	D	148	VAL	2.4
3	B	135	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	6	LEU	2.3
3	D	197	LEU	2.3
3	D	488	TYR	2.3
3	B	155	PRO	2.3
3	A	787	ASN	2.3
3	D	123	PHE	2.3
3	D	306	ASP	2.3
3	D	517	ASP	2.3
3	D	591	GLN	2.3
3	D	799	PRO	2.3
3	D	158	ASN	2.3
3	D	549	GLU	2.3
3	D	251	LYS	2.3
3	D	596	TRP	2.3
3	D	811	TYR	2.3
3	A	535	ALA	2.3
3	D	8	VAL	2.3
3	A	253	ILE	2.2
3	D	436	VAL	2.2
3	D	383	GLY	2.2
3	D	493	GLN	2.2
3	D	688	ILE	2.2
3	D	384	ARG	2.2
3	D	58	THR	2.2
3	B	127	SER	2.2
3	D	639	SER	2.2
3	D	16	PHE	2.2
3	D	104	ASP	2.2
3	B	132	PRO	2.2
3	B	174	GLY	2.2
3	B	305	TYR	2.2
3	B	308	PRO	2.2
3	C	516	VAL	2.2
3	D	117	VAL	2.2
3	D	703	THR	2.2
3	D	267	GLY	2.2
3	D	410	PHE	2.2
3	D	721	ALA	2.2
3	A	546	GLN	2.1
3	D	860	ASP	2.1
3	C	542	LEU	2.1
3	D	201	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	155	PRO	2.1
3	D	513	PRO	2.1
3	B	152	LEU	2.1
3	D	191	PHE	2.1
3	D	725	LEU	2.1
3	A	257	TYR	2.1
3	A	821	ALA	2.1
3	D	136	ILE	2.1
3	D	530	ILE	2.1
3	A	773	GLN	2.1
3	C	151	LEU	2.1
3	D	794	GLY	2.1
3	D	875	THR	2.1
3	D	883	PHE	2.1
3	B	253	ILE	2.1
3	D	325	ILE	2.1
3	B	735	SER	2.1
3	C	35	PRO	2.1
3	D	822	PRO	2.1
1	E	7	DC	2.1
3	D	373	LEU	2.1
3	D	710	LEU	2.1
3	D	552	GLY	2.1
3	D	701	PHE	2.1
3	A	534	SER	2.0
2	H	106	DT	2.0
3	D	804	HIS	2.0
3	D	802	PRO	2.0
1	G	13	DA	2.0
3	D	495	ASN	2.0
3	D	575	PHE	2.0
3	A	819	ILE	2.0
3	D	502	ALA	2.0
1	G	12	DG	2.0
3	A	542	LEU	2.0
3	C	198	LEU	2.0
3	B	228	ASN	2.0
3	D	260	ARG	2.0
3	D	559	ARG	2.0
2	H	112	DA	2.0
3	D	72	ILE	2.0
3	A	492	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
3	D	96	THR	2.0
3	D	394	ALA	2.0
3	C	201	TYR	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	3DR	I	6	11/12	0.89	0.12	94,99,110,110	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.