



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:03 AM GMT

PDB ID : 2P5G
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

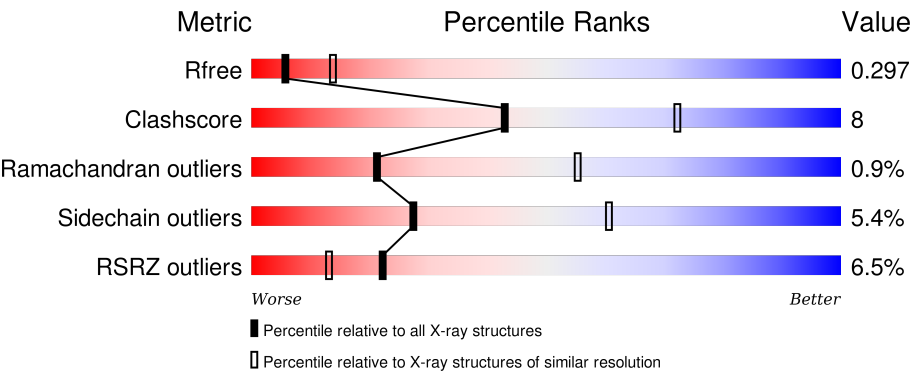
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	
1	G	21	
1	I	21	
1	K	21	
2	F	15	

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Mol	Chain	Length	Quality of chain
2	H	15	<div><div></div><div>33%33%60%7%</div></div>
2	J	15	<div><div></div><div>67%33%</div></div>
2	L	15	<div><div></div><div>13%47%33%7%13%</div></div>
3	A	903	<div><div></div><div>3%79%18%..</div></div>
3	B	903	<div><div></div><div>3%62%19%.16%</div></div>
3	C	903	<div><div></div><div>4%74%22%..</div></div>
3	D	903	<div><div></div><div>14%81%15%..</div></div>

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

There are 8 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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
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

3 Residue-property plots [i](#)

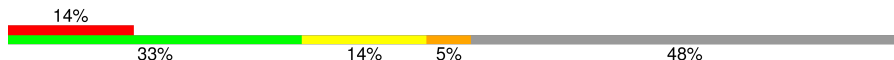
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: Template DNA

Chain E: 



- Molecule 1: Template DNA

Chain G: 



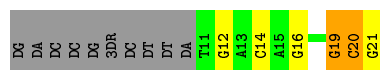
- Molecule 1: Template DNA

Chain I: 



- Molecule 1: Template DNA

Chain K: 



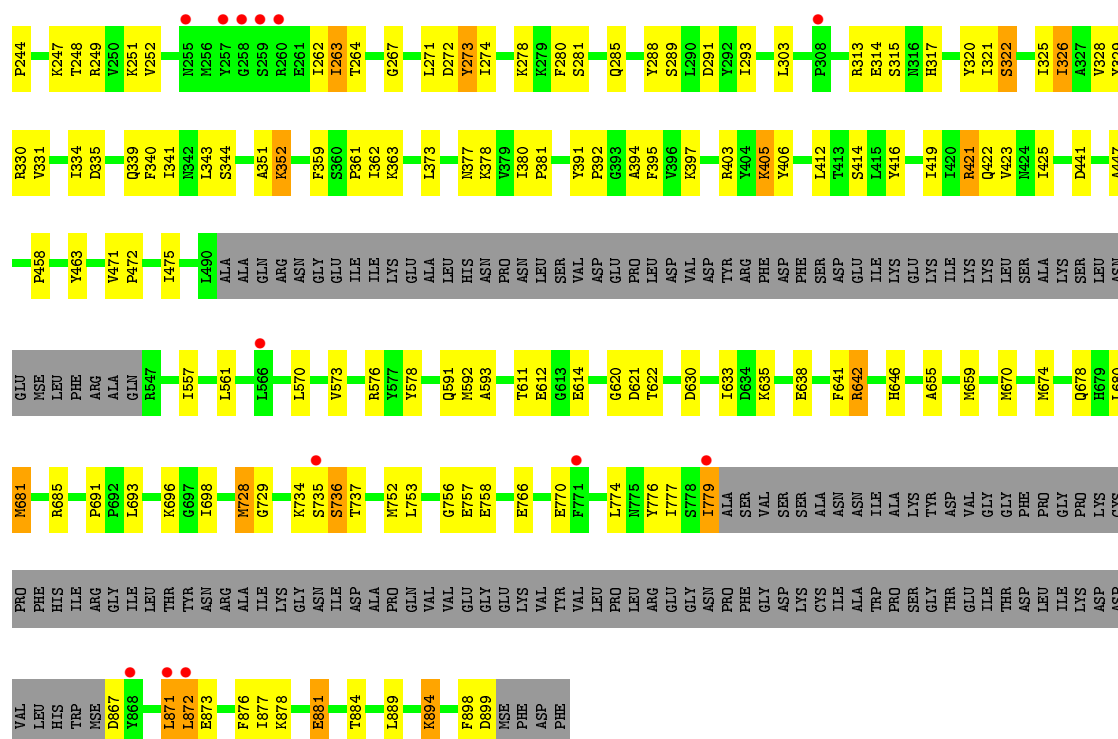
- Molecule 2: Primer DNA

Chain F: 

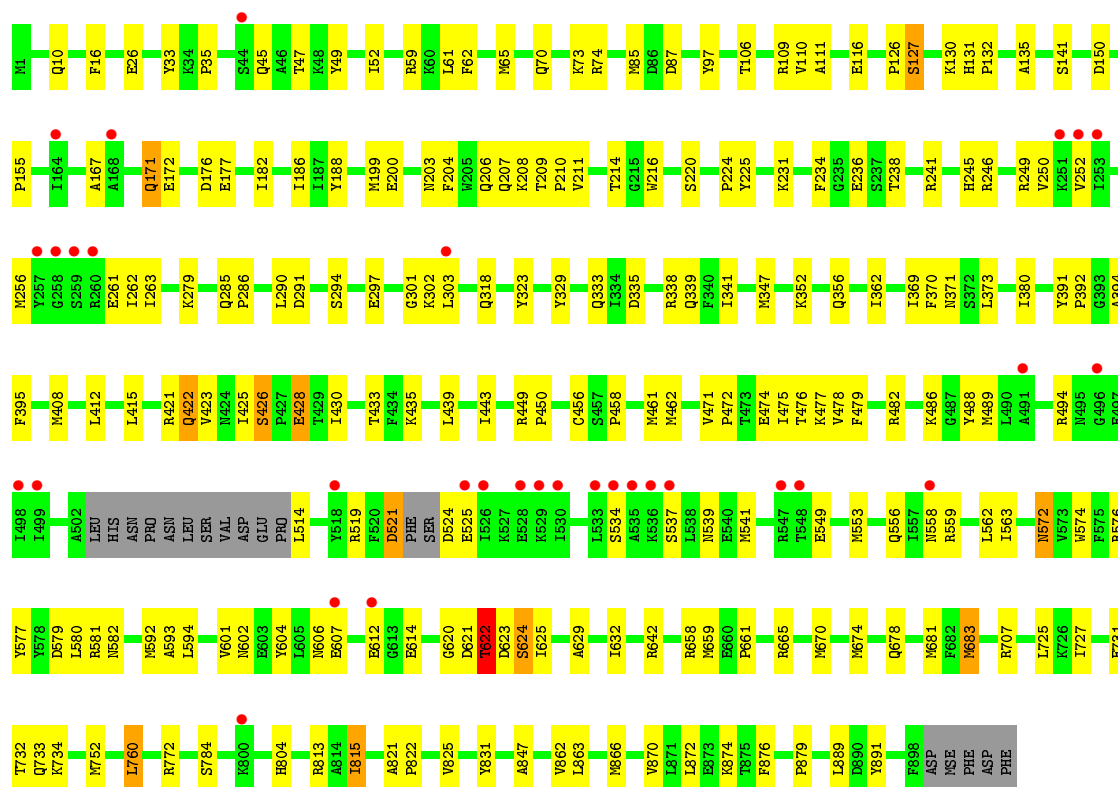
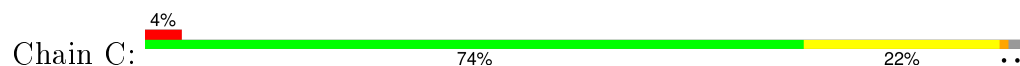


- Molecule 2: Primer DNA

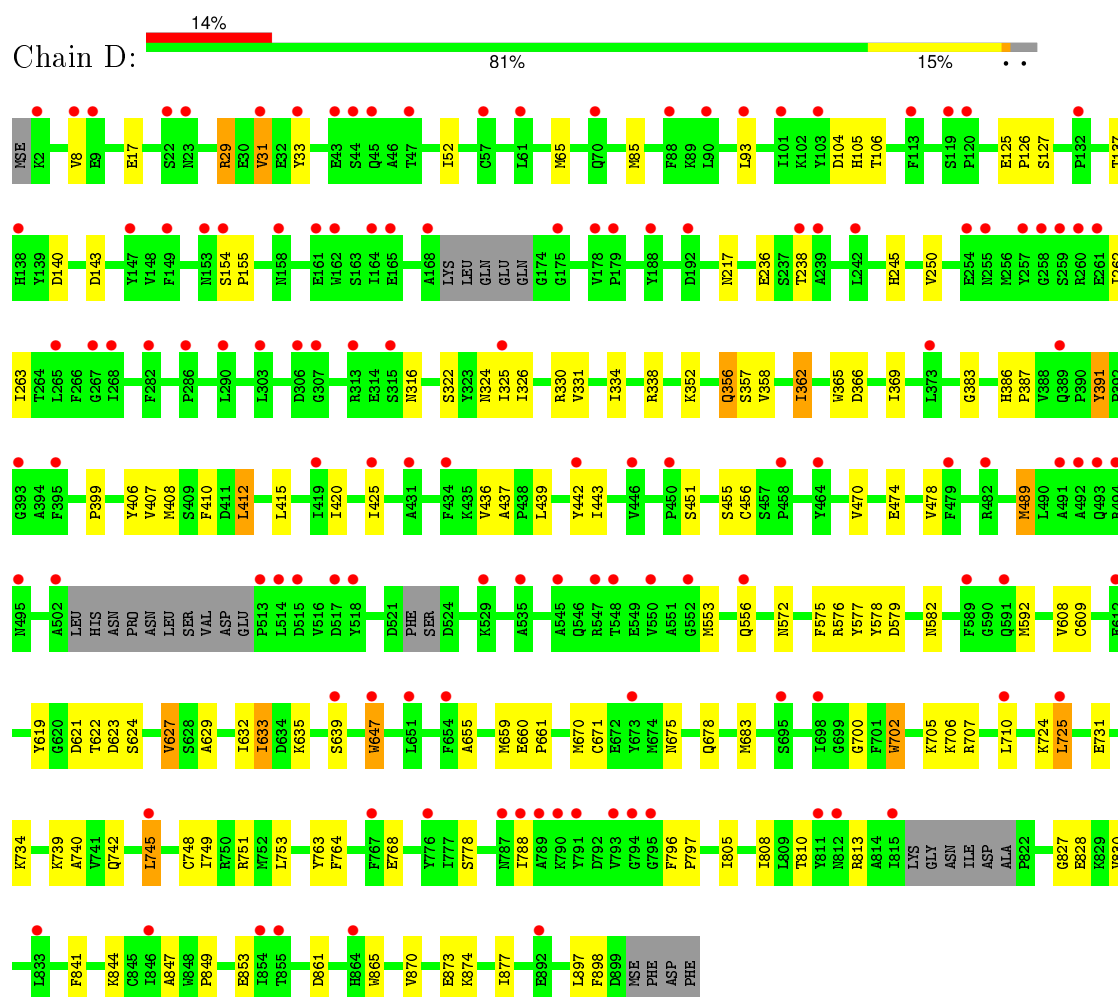
Chain H: 



• 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 49.61 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.4 (30.00-2.80) 96.1 (49.61-2.80)	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 0.241 , 0.297	Depositor DCC
R_{free} test set	12248 reflections (11.69%)	DCC
Wilson B-factor (Å ²)	62.2	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 249661 reflections	Xtriage
F_o, F_c correlation	0.91	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.71	0/339	1.37	2/521 (0.4%)
1	G	0.77	0/250	1.53	3/384 (0.8%)
1	I	0.75	1/429 (0.2%)	1.43	8/657 (1.2%)
1	K	0.70	0/253	1.46	5/388 (1.3%)
2	F	0.71	0/346	1.58	7/533 (1.3%)
2	H	0.71	0/346	1.39	3/533 (0.6%)
2	J	0.75	0/346	1.45	4/533 (0.8%)
2	L	0.69	0/297	1.25	1/457 (0.2%)
3	A	0.40	0/7294	0.54	0/9830
3	B	0.37	0/6163	0.52	0/8319
3	C	0.39	0/7262	0.52	0/9788
3	D	0.33	0/6255	0.47	0/8520
All	All	0.42	1/29580 (0.0%)	0.67	33/40463 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	11	DT	C3'-O3'	-5.08	1.37	1.44

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	105	DC	O4'-C1'-N1	12.32	116.62	108.00
2	J	114	DG	O4'-C1'-N9	11.08	115.76	108.00
2	H	111	DT	O4'-C1'-N1	10.57	115.40	108.00
1	K	20	DC	O4'-C1'-N1	9.93	114.95	108.00
1	G	13	DA	O4'-C1'-N9	9.26	114.48	108.00
2	H	111	DT	C1'-O4'-C4'	-8.58	101.52	110.10
1	I	7	DC	O4'-C1'-N1	8.15	113.71	108.00
2	F	105	DC	C1'-O4'-C4'	-7.94	102.16	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	9	DT	O4'-C4'-C3'	-7.64	101.41	106.00
1	I	20	DC	O4'-C1'-N1	6.76	112.73	108.00
2	H	101	DG	P-O3'-C3'	6.59	127.61	119.70
2	F	102	DC	O4'-C1'-N1	6.52	112.56	108.00
2	F	114	DG	O4'-C1'-N9	6.13	112.29	108.00
1	K	20	DC	C1'-O4'-C4'	-6.06	104.04	110.10
1	G	17	DC	O4'-C1'-N1	5.99	112.19	108.00
1	I	4	DC	P-O3'-C3'	5.77	126.62	119.70
1	K	12	DG	C1'-O4'-C4'	-5.70	104.40	110.10
1	K	19	DG	P-O3'-C3'	5.64	126.47	119.70
1	G	11	DT	O4'-C1'-N1	5.64	111.95	108.00
1	K	16	DG	O4'-C1'-N9	5.64	111.95	108.00
2	F	113	DA	C1'-O4'-C4'	-5.54	104.56	110.10
2	F	104	DG	C1'-O4'-C4'	-5.52	104.58	110.10
2	J	113	DA	P-O3'-C3'	5.49	126.29	119.70
1	I	3	DC	O4'-C1'-N1	5.46	111.83	108.00
2	J	105	DC	O4'-C1'-N1	5.44	111.81	108.00
2	F	112	DA	O4'-C4'-C3'	-5.41	102.33	104.50
1	I	8	DT	O4'-C1'-N1	5.21	111.65	108.00
2	J	114	DG	C1'-O4'-C4'	-5.21	104.89	110.10
1	I	4	DC	O4'-C1'-N1	5.20	111.64	108.00
2	L	109	DC	P-O3'-C3'	5.19	125.92	119.70
1	I	9	DT	O4'-C1'-N1	5.17	111.62	108.00
1	I	14	DC	C1'-O4'-C4'	-5.10	105.00	110.10
1	E	7	DC	O4'-C1'-N1	5.06	111.55	108.00

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	111	0
3	B	6036	0	5779	116	0
3	C	7113	0	6872	122	0
3	D	6148	0	5083	74	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
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	445	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 (445) 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:C:380:ILE:HG23	3:C:576:ARG:HD3	1.59	0.82
3:B:87:ASP:OD2	3:B:363:LYS:HE3	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:456:CYS:HB2	3:C:674:MSE:HE3	1.61	0.82
3:A:112:ASN:HB3	4:A:1018:HOH:O	1.79	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:HE21	3:A:356:GLN:H	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:C:862:VAL:O	3:C:866:MSE:HG3	1.85	0.77
3:B:873:GLU:HA	3:B:877:ILE:HG12	1.67	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
3:A:212:ILE:HG23	3:A:271:LEU:HD12	1.71	0.71
3:B:98:ASN:HD22	3:B:98:ASN:H	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:NE2	3:A:356:GLN:H	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:224:PRO:HB3	3:C:263:ILE:HG12	1.77	0.64
3:C:110:VAL:H	3:C:141:SER:HB3	1.62	0.64
3:A:98:ASN:H	3:A:98:ASN:ND2	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:B:776:TYR:HA	3:B:779:ILE:HG22	1.83	0.61
3:C:303:LEU:HD11	3:C:323:TYR:HB2	1.82	0.61
3:B:328:VAL:O	3:B:331:VAL:HG12	2.01	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:649:ASP:OD1	3:A:719:ARG:NH2	2.35	0.59
3:A:245:HIS:HE1	4:A:923:HOH:O	1.83	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:D:621:ASP:O	3:D:623:ASP:N	2.37	0.57
3:B:331:VAL:HA	3:B:334:ILE:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:421:ARG:HD3	3:B:475:ILE:HG23	1.87	0.57
3:A:202:LEU:O	3:A:206:GLN:HG2	2.05	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:D:406:TYR:HD1	3:D:647:TRP:HZ2	1.53	0.57
3:C:661:PRO:O	3:C:665:ARG:HB2	2.04	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:C:458:PRO:HG3	3:C:592:MSE:SE	2.55	0.56
3:B:273:TYR:OH	3:B:335:ASP:HA	2.06	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:D:749:ILE:O	3:D:753:LEU:HG	2.06	0.55
3:C:572:ASN:ND2	3:C:574:TRP:H	2.04	0.55
3:A:6:LEU:CD1	3:A:26:GLU:HG3	2.36	0.55
2:F:111:DT:H2"	2:F:112:DA:H5"	1.89	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:H	3:D:391:TYR:HD1	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
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
1:I:9:DT:H2"	1:I:10:DA:H5"	1.88	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:D:702:TRP:HZ3	3:D:710:LEU:HD21	1.72	0.54
3:A:231:LYS:HG3	3:A:236:GLU:HA	1.90	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
3:C:433:THR:O	3:C:462:MSE:HE2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:370:PHE:HB2	3:C:380:ILE:HD11	1.89	0.54
3:A:830:VAL:CG1	3:A:847:ALA:HB1	2.38	0.53
2:H:113:DA:H5'	3:B:289:SER:HB2	1.90	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:B:877:ILE:HG13	3:B:878:LYS:N	2.23	0.53
3:A:347:MSE:HG2	3:A:358:VAL:HG23	1.90	0.53
3:D:125:GLU:HG3	3:D:127:SER:H	1.73	0.53
3:C:475:ILE:HD11	3:C:563:ILE:HA	1.91	0.53
3:B:231:LYS:HA	3:B:239:ALA:HB2	1.92	0.52
3:C:422:GLN:HG2	3:C:678:GLN:O	2.09	0.52
3:D:655:ALA:HA	3:D:659:MSE:HB2	1.90	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
1:E:7:DC:H2'	1:E:8:DT:H72	1.92	0.52
3:B:11:ILE:HG12	3:B:247:LYS:HD2	1.91	0.52
3:A:819:ILE:H	3:A:819:ILE:HD13	1.74	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:D:455:SER:HA	3:D:675:ASN:O	2.11	0.51
3:C:731:GLU:HG3	3:C:879:PRO:HB3	1.93	0.51
3:C:391:TYR:HB2	3:C:392:PRO:HD2	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:109:ARG:HH21	3:C:208:LYS:HB3	1.75	0.50
3:B:391:TYR:HB2	3:B:392:PRO:HD2	1.93	0.50
3:A:314:GLU:HG2	3:A:315:SER:N	2.25	0.50
2:J:112:DA:H5'	3:C:734:LYS:HG2	1.93	0.50
3:D:437:ALA:HB3	3:D:442:TYR:CE2	2.46	0.50
3:A:127:SER:HA	3:A:228:ASN:ND2	2.27	0.50
3:C:602:ASN:O	3:C:606:ASN:ND2	2.39	0.50
3:C:214:THR:HG21	3:C:341:ILE:HD11	1.94	0.49
3:A:23:ASN:HD22	3:A:25:ARG:HH21	1.59	0.49
3:A:574:TRP:CE3	3:A:574:TRP:HA	2.46	0.49
3:B:222:ALA:O	3:B:226:VAL:HG23	2.12	0.49
3:B:193:ASN:HB3	3:B:196:GLU:HB2	1.93	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:471:VAL:HG11	3:B:570:LEU:HD11	1.95	0.49
3:B:149:PHE:HB3	3:B:197:LEU:HD21	1.95	0.49
3:B:734:LYS:HE2	3:B:736:SER:HB2	1.95	0.49
3:C:593:ALA:HB1	3:C:681:MSE:HE2	1.93	0.49
3:B:881:GLU:HA	3:B:884:THR:OG1	2.13	0.49
3:B:611:THR:HG22	3:B:612:GLU:H	1.78	0.49
3:A:391:TYR:CZ	3:A:583:ALA:HB1	2.48	0.49
3:B:592:MSE:HE1	3:B:674:MSE:HE3	1.95	0.48
3:A:747:GLU:HG3	3:A:751:ARG:HD2	1.95	0.48
3:C:412:LEU:HG	3:C:683:MSE:HE3	1.93	0.48
3:A:70:GLN:O	3:A:74:ARG:HB2	2.13	0.48
3:B:642:ARG:HE	3:B:646:HIS:CG	2.31	0.48
3:A:466:ASP:OD1	3:A:467:ARG:N	2.46	0.48
3:A:414:SER:O	3:A:417:PRO:HD2	2.13	0.48
1:I:11:DT:H4'	3:C:707:ARG:HD3	1.95	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:423:VAL:HB	3:C:425:ILE:HG13	1.94	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:D:841:PHE:HZ	3:D:861:ASP:HB3	1.79	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:C:130:LYS:HG3	3:C:131:HIS:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:290:LEU:HB3	3:A:302:LYS:HD2	1.96	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:OD2	3:C:302:LYS:HB2	2.14	0.48
3:A:406:TYR:HB3	3:A:629:ALA:HB3	1.95	0.48
3:A:199:MSE:HE3	3:A:234:PHE:CE2	2.49	0.48
3:D:406:TYR:CE2	3:D:633:ILE:HG21	2.49	0.47
3:B:898:PHE:N	4:B:925:HOH:O	2.45	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
3:B:728:MSE:HE2	3:B:729:GLY:H	1.78	0.47
1:I:7:DC:H1'	4:I:65:HOH:O	2.14	0.47
3:C:831:TYR:O	3:C:847:ALA:HA	2.15	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:A:120:PRO:HG3	3:A:156:TYR:CE1	2.50	0.47
3:C:126:PRO:HA	3:C:225:TYR:CD2	2.50	0.47
3:B:249:ARG:HB3	3:B:264:THR:HB	1.97	0.47
3:C:439:LEU:O	3:C:443:ILE:HG13	2.15	0.47
3:C:199:MSE:HG2	3:C:234:PHE:CZ	2.50	0.47
3:B:48:LYS:HG3	3:B:377:ASN:HD22	1.80	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:C:494:ARG:HD2	3:C:521:ASP:OD2	2.15	0.47
3:B:303:LEU:HD23	3:B:326:ILE:HD13	1.97	0.47
3:C:727:ILE:HD13	3:C:732:THR:HG21	1.97	0.46
3:C:422:GLN:HB3	3:C:422:GLN:HE21	1.56	0.46
3:A:308:PRO:HG2	3:A:311:LYS:HG2	1.96	0.46
3:B:406:TYR:CD2	3:B:633:ILE:HG13	2.51	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
1:K:14:DC:OP1	3:D:874:LYS:HD2	2.14	0.46
3:B:182:ILE:HD11	3:B:329:TYR:CD2	2.50	0.46
3:A:113:PHE:CE1	3:A:213:LEU:HD11	2.50	0.46
3:B:395:PHE:HB2	3:B:591:GLN:HG2	1.97	0.46
3:B:621:ASP:OD1	3:B:622:THR:HG22	2.14	0.46
3:A:251:LYS:HD3	3:A:262:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:373:LEU:HD12	3:B:380:ILE:HG22	1.98	0.46
3:B:872:LEU:HD22	3:B:876:PHE:HB3	1.97	0.46
3:D:725:LEU:CD2	3:D:725:LEU:H	2.26	0.46
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:B:635:LYS:HG2	3:D:898:PHE:CE2	2.51	0.46
3:B:25:ARG:HB3	3:B:25:ARG:HH11	1.80	0.46
3:D:621:ASP:O	3:D:624:SER:N	2.43	0.46
3:C:16:PHE:HB3	3:C:245:HIS:CE1	2.51	0.46
3:D:660:GLU:N	3:D:661:PRO:HD2	2.31	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:298:LEU:HB2	3:A:300:VAL:HG12	1.97	0.46
3:A:171:GLN:HE22	3:A:319:ARG:HH12	1.64	0.46
1:K:19:DG:H2"	1:K:20:DC:OP2	2.16	0.46
3:B:421:ARG:HB3	3:B:680:LEU:CD1	2.45	0.46
3:B:149:PHE:HB3	3:B:197:LEU:CD2	2.46	0.46
3:C:488:TYR:HB3	3:C:519:ARG:HG2	1.98	0.46
3:B:129:ALA:HB1	3:B:225:TYR:CZ	2.51	0.46
3:A:145:ARG:HG3	3:A:185:LYS:O	2.16	0.46
3:D:474:GLU:O	3:D:478:VAL:HG23	2.16	0.46
3:A:812:ASN:HA	3:A:815:ILE:HG22	1.97	0.45
3:C:111:ALA:CB	3:C:210:PRO:HB3	2.46	0.45
3:A:528:GLU:C	3:A:530:ILE:H	2.18	0.45
3:A:641:PHE:HA	3:A:646:HIS:ND1	2.31	0.45
3:D:420:ILE:HG23	3:D:425:ILE:HB	1.97	0.45
3:C:614:GLU:OE1	3:C:614:GLU:HA	2.16	0.45
3:B:405:LYS:HB3	3:B:630:ASP:OD1	2.16	0.45
3:A:132:PRO:HG3	3:A:155:PRO:HD2	1.97	0.45
3:B:322:SER:HA	3:B:325:ILE:HD12	1.97	0.45
3:B:123:PHE:HA	3:B:124:PRO:HD3	1.82	0.45
3:A:629:ALA:HA	3:A:632:ILE:HD12	1.97	0.45
3:A:172:GLU:CD	3:A:172:GLU:H	2.18	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:H	3:B:263:ILE:HD13	1.81	0.45
3:C:85:MSE:HE3	3:C:87:ASP:H	1.80	0.45
3:B:326:ILE:H	3:B:326:ILE:HG13	1.53	0.45
3:C:752:MSE:HE3	3:C:889:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:356:GLN:C	3:D:358:VAL:H	2.20	0.45
3:D:579:ASP:HB3	3:D:582:ASN:HB2	1.99	0.45
3:C:109:ARG:HB3	3:C:211:VAL:HG23	1.99	0.45
3:B:423:VAL:HB	3:B:425:ILE:HG13	1.99	0.45
3:A:112:ASN:HB2	3:A:139:TYR:HB3	1.99	0.45
3:D:608:VAL:O	3:D:635:LYS:NZ	2.41	0.45
3:B:412:LEU:HD22	3:B:681:MSE:HG3	1.98	0.45
3:C:49:TYR:CZ	3:C:59:ARG:HD3	2.52	0.44
3:B:655:ALA:HA	3:B:659:MSE:HB2	1.99	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: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
3:A:727:ILE:HG23	3:A:730:LEU:HD12	1.98	0.44
3:D:399:PRO:HG3	3:D:702:TRP:CD1	2.52	0.44
3:C:421:ARG:HD2	3:C:476:THR:OG1	2.16	0.44
2:F:102:DC:H2"	2:F:103:DG:C8	2.53	0.44
3:B:98:ASN:HD22	3:B:98:ASN:N	2.11	0.44
3:B:394:ALA:CB	3:B:622:THR:HB	2.42	0.44
3:D:751:ARG:CZ	3:D:763:TYR:HB2	2.48	0.44
3:B:351:ALA:O	3:B:352:LYS:HB2	2.18	0.44
3:D:619:TYR:OH	3:D:706:LYS:N	2.50	0.44
3:B:194:GLU:HG2	3:B:229:ARG:HH21	1.83	0.44
3:C:426:SER:C	3:C:582:ASN:HD21	2.20	0.44
3:B:757:GLU:HB2	3:B:889:LEU:HD22	2.00	0.43
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:C:621:ASP:O	3:C:623:ASP:N	2.51	0.43
3:C:347:MSE:HE2	3:C:558:ASN:ND2	2.33	0.43
3:A:294:SER:HB3	3:A:301:GLY:HA2	2.00	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:495:ASN:OD1	3:A:495:ASN:C	2.56	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
3:D:369:ILE:HG21	3:D:577:TYR:CE1	2.54	0.43
3:B:98:ASN:ND2	3:B:98:ASN:H	2.11	0.43
3:C:482:ARG:HE	3:C:556:GLN:NE2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:406:TYR:CD1	3:D:647:TRP:HZ2	2.33	0.43
2:H:115:DA:O3'	3:B:117:VAL:O	2.36	0.43
1:G:18:DC:H42	2:H:103:DG:H1	1.67	0.43
3:C:428:GLU:HG3	3:C:428:GLU:H	1.52	0.43
3:D:739:LYS:HA	3:D:742:GLN:HB2	2.00	0.43
3:C:291:ASP:CG	3:C:302:LYS:HB2	2.39	0.43
3:A:199:MSE:HA	3:A:199:MSE:HE2	2.01	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: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:D:412:LEU:HD13	3:D:415:LEU:HD13	2.01	0.43
3:B:271:LEU:HD21	3:B:344:SER:HB3	2.00	0.43
3:B:35:PRO:HG3	3:B:65:MSE:HG2	1.99	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:D:408:MSE:HE3	3:D:659:MSE:HE2	2.01	0.43
3:A:449:ARG:NH1	3:A:452:ASP:HB3	2.33	0.43
3:B:249:ARG:HG2	3:B:251:LYS:HG3	1.99	0.43
3:C:514:LEU:HB3	3:C:541:MSE:SE	2.68	0.42
3:C:206:GLN:NE2	3:C:241:ARG:O	2.51	0.42
3:C:731:GLU:CG	3:C:879:PRO:HB3	2.48	0.42
3:D:104:ASP:C	3:D:106:THR:H	2.23	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: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:C:449:ARG:HA	3:C:450:PRO:HD3	1.87	0.42
3:B:209:THR:HA	3:B:210:PRO:HD3	1.83	0.42
3:B:779:ILE:HG12	3:B:871:LEU:HG	2.01	0.42
3:C:209:THR:HA	3:C:210:PRO:HD3	1.79	0.42
3:B:249:ARG:HD3	3:B:251:LYS:HE3	2.02	0.42
3:A:708:TYR:CZ	3:A:728:MSE:HG3	2.53	0.42
3:C:45:GLN:O	3:C:47:THR:HG23	2.20	0.42
3:D:489:MSE:HE3	3:D:489:MSE:HB3	2.01	0.42
3:D:362:ILE:O	3:D:366:ASP:HB2	2.19	0.42
3:C:302:LYS:HD3	3:C:323:TYR:CE1	2.54	0.42
3:B:145:ARG:HB3	3:B:145:ARG:CZ	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:376:GLN:HG3	3:A:378:LYS:HG3	2.01	0.42
3:A:285:GLN:HA	3:A:286:PRO:HD3	1.94	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
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:C:456:CYS:CB	3:C:674:MSE:HE3	2.43	0.42
3:C:352:LYS:HB2	3:C:371:ASN:HD21	1.84	0.42
3:B:698:ILE:HG13	3:B:753:LEU:HD23	2.01	0.42
3:A:653:LYS:HG2	3:A:656:ARG:NH2	2.35	0.42
3:D:705:LYS:C	3:D:707:ARG:H	2.24	0.42
3:D:412:LEU:HD12	3:D:412:LEU:H	1.85	0.41
2:H:106:DT:H5"	4:H:124:HOH:O	2.20	0.41
3:A:719:ARG:HB2	3:A:719:ARG:HH11	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: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:A:23:ASN:ND2	3:A:25:ARG:NH2	2.68	0.41
3:D:575:PHE:HB3	3:D:578:TYR:HB2	2.02	0.41
3:A:147:TYR:OH	3:A:208:LYS:NZ	2.53	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:HB3	3:B:894:LYS:HE2	1.89	0.41
3:A:41:CYS:HB2	3:A:42:PRO:CD	2.50	0.41
3:C:813:ARG:C	3:C:815:ILE:H	2.23	0.41
3:C:150:ASP:HB2	3:C:188:TYR:HE1	1.85	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
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:3:GLU:HG2	3:B:21:ASP:HA	2.03	0.41
1:I:4:DC:H2'	1:I:5:DG:C5	2.55	0.41
3:C:461:MSE:HE1	3:C:581:ARG:HD2	2.02	0.41
3:C:52:ILE:HB	3:C:428:GLU:HG2	2.03	0.41
3:D:592:MSE:HE3	3:D:670:MSE:SE	2.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:131:HIS:HA	3:B:132:PRO:HD3	1.89	0.41
3:C:335:ASP:O	3:C:339:GLN:N	2.49	0.41
3:D:810:THR:HG23	3:D:813:ARG:HH22	1.86	0.41
3:D:745:LEU:HA	3:D:748:CYS:HB2	2.03	0.41
3:D:830:VAL:HA	3:D:849:PRO:HA	2.03	0.40
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:B:330:ARG:O	3:B:334:ILE:HG13	2.22	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:D:33:TYR:HD2	3:D:65:MSE:HE1	1.86	0.40
3:C:784:SER:O	3:C:804:HIS:CD2	2.75	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:601:VAL:HG13	3:A:659:MSE:HE1	2.03	0.40
3:C:70:GLN:O	3:C:74:ARG:HB2	2.19	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:B:116:GLU:HG2	3:B:320:TYR:CZ	2.56	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: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%)	24	58
3	B	750/903 (83%)	683 (91%)	61 (8%)	6 (1%)	24	58
3	C	879/903 (97%)	816 (93%)	58 (7%)	5 (1%)	30	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	865/903 (96%)	750 (87%)	101 (12%)	14 (2%)	12	38
All	All	3380/3612 (94%)	3077 (91%)	271 (8%)	32 (1%)	21	55

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%)	723 (96%)	29 (4%)	39	74
3	B	632/775 (82%)	590 (93%)	42 (7%)	21	51
3	C	752/775 (97%)	710 (94%)	42 (6%)	26	59
3	D	518/775 (67%)	489 (94%)	29 (6%)	26	59
All	All	2654/3100 (86%)	2512 (95%)	142 (5%)	27	60

All (142) 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	250	VAL
3	A	273	TYR
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	489	MSE
3	A	495	ASN
3	A	520	PHE
3	A	521	ASP
3	A	528	GLU
3	A	542	LEU
3	A	576	ARG
3	A	719	ARG
3	A	746	LYS
3	A	790	LYS

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Mol	Chain	Res	Type
3	A	819	ILE
3	A	855	THR
3	A	881	GLU
3	A	885	SER
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	123	PHE
3	B	131	HIS
3	B	134	ASP
3	B	136	ILE
3	B	145	ARG
3	B	159	VAL
3	B	165	GLU
3	B	231	LYS
3	B	248	THR
3	B	252	VAL
3	B	263	ILE
3	B	273	TYR
3	B	285	GLN
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
3	B	642	ARG
3	B	681	MSE
3	B	685	ARG
3	B	728	MSE
3	B	736	SER
3	B	737	THR
3	B	758	GLU
3	B	774	LEU
3	B	779	ILE
3	B	867	ASP

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Mol	Chain	Res	Type
3	B	871	LEU
3	B	872	LEU
3	B	881	GLU
3	B	894	LYS
3	B	899	ASP
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	200	GLU
3	C	220	SER
3	C	238	THR
3	C	246	ARG
3	C	249	ARG
3	C	262	ILE
3	C	279	LYS
3	C	318	GLN
3	C	356	GLN
3	C	362	ILE
3	C	373	LEU
3	C	408	MSE
3	C	422	GLN
3	C	426	SER
3	C	428	GLU
3	C	435	LYS
3	C	477	LYS
3	C	479	PHE
3	C	521	ASP
3	C	524	ASP
3	C	539	ASN
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	624	SER
3	C	625	ILE
3	C	642	ARG

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Mol	Chain	Res	Type
3	C	683	MSE
3	C	725	LEU
3	C	760	LEU
3	C	815	ILE
3	C	825	VAL
3	D	17	GLU
3	D	29	ARG
3	D	85	MSE
3	D	217	ASN
3	D	236	GLU
3	D	238	THR
3	D	245	HIS
3	D	326	ILE
3	D	330	ARG
3	D	356	GLN
3	D	362	ILE
3	D	391	TYR
3	D	412	LEU
3	D	489	MSE
3	D	572	ASN
3	D	576	ARG
3	D	627	VAL
3	D	633	ILE
3	D	639	SER
3	D	647	TRP
3	D	671	CYS
3	D	678	GLN
3	D	702	TRP
3	D	724	LYS
3	D	725	LEU
3	D	745	LEU
3	D	844	LYS
3	D	853	GLU
3	D	865	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	23	ASN
3	A	98	ASN
3	A	171	GLN
3	A	356	GLN

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Mol	Chain	Res	Type
3	A	386	HIS
3	A	422	GLN
3	B	98	ASN
3	B	112	ASN
3	B	153	ASN
3	B	173	GLN
3	B	206	GLN
3	B	217	ASN
3	B	285	GLN
3	B	377	ASN
3	B	444	ASN
3	B	646	HIS
3	C	153	ASN
3	C	171	GLN
3	C	245	HIS
3	C	324	ASN
3	C	386	HIS
3	C	539	ASN
3	C	556	GLN
3	C	558	ASN
3	C	572	ASN
3	C	595	GLN
3	C	645	ASN
3	C	675	ASN
3	C	864	HIS
3	D	128	GLN
3	D	558	ASN
3	D	572	ASN
3	D	733	GLN
3	D	742	GLN
3	D	754	GLN
3	D	761	GLN

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	7,11,12	0.44	0	8,14,17	0.58	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	-	0/3/15/16	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates 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 ⓘ

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%)	-0.01	0 100 100	50, 71, 97, 100	0
1	G	11/21 (52%)	1.41	3 (27%) 1 0	68, 102, 119, 121	0
1	I	19/21 (90%)	0.20	2 (10%) 8 4	42, 52, 136, 139	0
1	K	11/21 (52%)	0.40	0 100 100	49, 104, 111, 112	0
2	F	15/15 (100%)	0.26	1 (6%) 21 12	64, 85, 111, 114	0
2	H	15/15 (100%)	1.63	5 (33%) 0 0	88, 116, 121, 124	0
2	J	15/15 (100%)	-0.19	0 100 100	39, 65, 82, 90	0
2	L	13/15 (86%)	0.92	2 (15%) 3 1	115, 119, 124, 124	0
3	A	865/903 (95%)	0.23	23 (2%) 58 45	39, 54, 100, 124	0
3	B	734/903 (81%)	0.38	28 (3%) 44 32	42, 66, 109, 115	0
3	C	861/903 (95%)	0.33	32 (3%) 45 33	35, 62, 99, 126	0
3	D	852/903 (94%)	0.79	127 (14%) 3 2	98, 118, 133, 141	0
All	All	3426/3756 (91%)	0.43	223 (6%) 22 13	35, 69, 127, 141	0

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	259	SER	7.7
3	C	535	ALA	7.4
3	B	257	TYR	6.8
3	D	491	ALA	6.6
3	D	514	LEU	6.3
3	D	513	PRO	6.2
3	C	252	VAL	6.0
3	B	259	SER	5.7
3	B	174	GLY	5.5
3	A	535	ALA	5.2
3	D	168	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
3	D	788	ILE	5.1
3	D	787	ASN	4.9
3	D	811	TYR	4.6
3	D	446	VAL	4.6
3	D	179	PRO	4.5
3	A	903	PHE	4.5
3	C	303	LEU	4.5
3	D	61	LEU	4.5
3	D	434	PHE	4.5
3	D	161	GLU	4.4
3	D	103	TYR	4.4
3	D	239	ALA	4.4
3	B	308	PRO	4.2
2	H	109	DC	4.2
3	B	155	PRO	4.2
3	D	175	GLY	4.2
2	H	107	DG	4.2
3	D	265	LEU	4.1
3	D	257	TYR	4.1
3	D	192	ASP	4.0
3	D	492	ALA	4.0
3	A	542	LEU	4.0
3	B	260	ARG	4.0
3	D	647	TRP	4.0
2	H	112	DA	3.9
3	D	815	ILE	3.9
3	C	44	SER	3.8
3	D	178	VAL	3.8
3	A	530	ILE	3.8
3	B	779	ILE	3.7
3	D	44	SER	3.7
3	A	501	GLU	3.7
3	D	138	HIS	3.7
3	D	789	ALA	3.7
3	C	530	ILE	3.6
3	D	450	PRO	3.5
3	C	498	ILE	3.5
3	D	282	PHE	3.4
3	D	147	TYR	3.4
3	D	286	PRO	3.4
3	A	502	ALA	3.4
3	D	307	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
3	C	253	ILE	3.3
3	B	258	GLY	3.3
3	D	548	THR	3.3
3	D	790	LYS	3.3
3	D	162	TRP	3.3
1	I	3	DC	3.3
3	D	315	SER	3.3
3	D	639	SER	3.3
3	D	47	THR	3.3
3	D	591	GLN	3.3
3	D	303	LEU	3.3
3	B	871	LEU	3.3
3	D	552	GLY	3.2
3	D	88	PHE	3.2
3	A	492	ALA	3.2
3	D	442	TYR	3.2
3	C	496	GLY	3.1
3	D	550	VAL	3.1
3	D	793	VAL	3.1
3	D	260	ARG	3.1
3	A	253	ILE	3.1
3	D	132	PRO	3.1
3	B	123	PHE	3.0
3	D	482	ARG	3.0
3	D	254	GLU	3.0
3	D	479	PHE	3.0
3	D	791	TYR	3.0
3	A	786	ASN	3.0
3	A	787	ASN	3.0
3	A	534	SER	2.9
3	B	128	GLN	2.9
2	H	108	DT	2.9
3	D	855	THR	2.9
3	D	846	ILE	2.9
3	D	70	GLN	2.9
3	B	234	PHE	2.9
1	G	12	DG	2.9
3	D	325	ILE	2.9
3	D	864	HIS	2.9
3	A	537	SER	2.8
3	D	493	GLN	2.8
3	A	902	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	518	TYR	2.8
3	D	43	GLU	2.8
3	D	120	PRO	2.8
3	C	533	LEU	2.8
3	D	812	ASN	2.8
1	G	13	DA	2.8
3	D	515	ASP	2.7
3	C	257	TYR	2.7
3	D	33	TYR	2.7
3	A	500	LYS	2.7
3	D	502	ALA	2.7
3	D	31	VAL	2.7
3	A	529	LYS	2.7
3	D	854	ILE	2.7
3	D	258	GLY	2.7
3	D	267	GLY	2.7
3	C	529	LYS	2.7
3	D	419	ILE	2.7
3	D	795	GLY	2.6
3	D	892	GLU	2.6
3	C	499	ILE	2.6
3	D	695	SER	2.6
3	D	673	TYR	2.6
3	A	497	GLU	2.6
3	D	101	ILE	2.6
3	B	137	THR	2.6
3	D	158	ASN	2.6
3	B	180	SER	2.6
3	C	525	GLU	2.6
3	D	165	GLU	2.6
3	B	191	PHE	2.5
3	D	164	ILE	2.5
3	D	393	GLY	2.5
3	C	536	LYS	2.5
3	C	537	SER	2.5
3	B	868	TYR	2.5
3	D	776	TYR	2.5
3	D	794	GLY	2.5
3	D	9	GLU	2.5
3	B	182	ILE	2.5
2	H	110	DA	2.5
3	D	119	SER	2.5

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Mol	Chain	Res	Type	RSRZ
3	D	529	LYS	2.5
3	A	793	VAL	2.5
3	D	149	PHE	2.5
3	D	425	ILE	2.4
3	D	23	ASN	2.4
3	C	251	LYS	2.4
3	A	799	PRO	2.4
3	D	431	ALA	2.4
3	C	526	ILE	2.4
3	D	2	LYS	2.4
3	D	545	ALA	2.4
3	A	498	ILE	2.4
3	C	164	ILE	2.4
3	D	8	VAL	2.4
3	C	168	ALA	2.4
3	A	818	ASN	2.4
3	D	535	ALA	2.3
3	D	306	ASP	2.3
3	C	548	THR	2.3
3	C	547	ARG	2.3
3	C	800	LYS	2.3
3	D	833	LEU	2.3
3	D	654	PHE	2.3
3	D	547	ARG	2.3
3	A	543	PHE	2.3
3	D	589	PHE	2.3
3	D	494	ARG	2.3
3	B	44	SER	2.3
3	B	255	ASN	2.3
3	D	113	PHE	2.3
3	D	154	SER	2.3
3	D	698	ILE	2.3
3	B	872	LEU	2.3
3	D	57	CYS	2.2
3	D	90	LEU	2.2
3	C	534	SER	2.2
3	B	160	GLU	2.2
3	D	261	GLU	2.2
1	I	2	DA	2.2
3	D	389	GLN	2.2
3	A	788	ILE	2.2
3	D	22	SER	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	238	THR	2.2
3	D	458	PRO	2.2
3	C	558	ASN	2.2
3	D	268	ILE	2.2
3	D	373	LEU	2.2
3	D	745	LEU	2.2
3	B	735	SER	2.2
3	C	259	SER	2.1
3	D	651	LEU	2.1
3	B	156	TYR	2.1
3	C	528	GLU	2.1
3	D	45	GLN	2.1
3	D	556	GLN	2.1
3	D	188	TYR	2.1
2	F	101	DG	2.1
3	C	258	GLY	2.1
3	D	290	LEU	2.1
3	C	260	ARG	2.1
3	D	517	ASP	2.1
3	B	566	LEU	2.1
3	D	313	ARG	2.1
2	L	109	DC	2.1
3	B	173	GLN	2.1
3	D	93	LEU	2.1
3	D	725	LEU	2.1
2	L	106	DT	2.1
3	A	536	LYS	2.1
3	C	612	GLU	2.1
3	D	612	GLU	2.1
3	D	495	ASN	2.0
3	B	46	ALA	2.0
3	C	491	ALA	2.0
3	D	395	PHE	2.0
3	C	607	GLU	2.0
1	G	16	DG	2.0
3	D	153	ASN	2.0
3	D	242	LEU	2.0
3	B	771	PHE	2.0
3	D	767	PHE	2.0
3	D	464	TYR	2.0
3	D	518	TYR	2.0
3	D	710	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
3	B	175	GLY	2.0
3	D	255	ASN	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	3DR	I	6	11/12	0.92	0.18	-	94,99,110,110	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.