



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 11:41 pm BST

PDB ID : 4OIQ
Title : Crystal structure of Thermus thermophilus transcription initiation complex soaked with GE23077 and rifampicin
Authors : Zhang, Y.; Ebright, R.H.; Arnold, E.
Deposited on : 2014-01-20
Resolution : 3.62 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

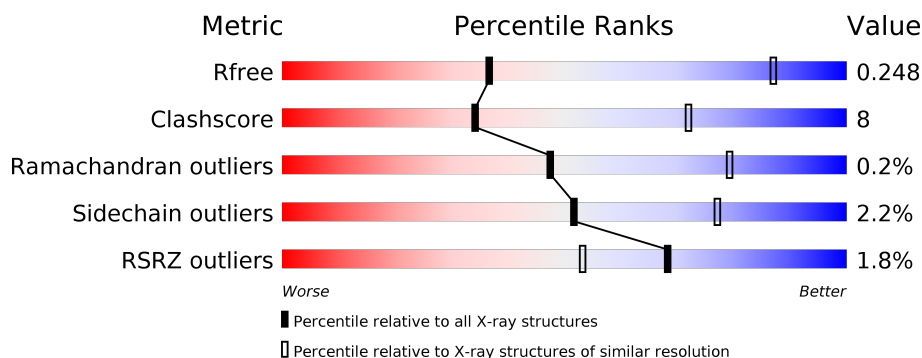
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.62 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.





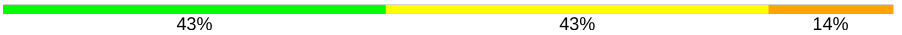
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1290 (3.74-3.50)
Clashscore	141614	1387 (3.74-3.50)
Ramachandran outliers	138981	1339 (3.74-3.50)
Sidechain outliers	138945	1339 (3.74-3.50)
RSRZ outliers	127900	1191 (3.74-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	315	<div> <div>2%</div> <div>59% 14% 27%</div> </div>
1	B	315	<div> <div>53% 17% 30%</div> </div>
2	C	1119	<div> <div>2%</div> <div>81% 17% ..</div> </div>
3	D	1524	<div> <div>2%</div> <div>73% 24% ..</div> </div>
4	E	99	<div> <div>4%</div> <div>77% 18% 5%</div> </div>
5	F	443	<div> <div>3%</div> <div>60% 18% 22%</div> </div>

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Mol	Chain	Length	Quality of chain
6	G	21	 48% 24% 5% 24%
7	H	27	 44% 30% 15% 11%
8	I	7	 43% 43% 14%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 28527 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1809	1155	315	337	2			
1	B	221	Total	C	N	O	S	0	0	0
			1741	1112	302	325	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1112	Total	C	N	O	S	0	0	0
			8774	5550	1565	1635	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1487	Total	C	N	O	S	0	1	0
			11754	7451	2071	2196	36			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			758	483	132	139	4			

- Molecule 5 is a protein called DNA directed RNA polymerase sigma factor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2807	1770	509	524	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	EXPRESSION TAG	UNP Q5SKW1
F	-18	GLY	-	EXPRESSION TAG	UNP Q5SKW1
F	-17	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	-16	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	-15	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-14	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-13	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-12	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-11	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-10	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-9	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	-8	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	-7	GLY	-	EXPRESSION TAG	UNP Q5SKW1
F	-6	LEU	-	EXPRESSION TAG	UNP Q5SKW1
F	-5	VAL	-	EXPRESSION TAG	UNP Q5SKW1
F	-4	PRO	-	EXPRESSION TAG	UNP Q5SKW1
F	-3	ARG	-	EXPRESSION TAG	UNP Q5SKW1
F	-2	GLY	-	EXPRESSION TAG	UNP Q5SKW1
F	-1	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	0	HIS	-	EXPRESSION TAG	UNP Q5SKW1

- Molecule 6 is a DNA chain called 5'-D(*CP*CP*T*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	16	Total	C	N	O	P	0	0	0
			328	156	63	94	15			

- Molecule 7 is a DNA chain called 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*C P*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	24	Total	C	N	O	P	0	0	0
			495	236	94	142	23			

- Molecule 8 is a protein called GE23077.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	I	7	Total	C	N	O	0	0	0
			50	26	9	15			

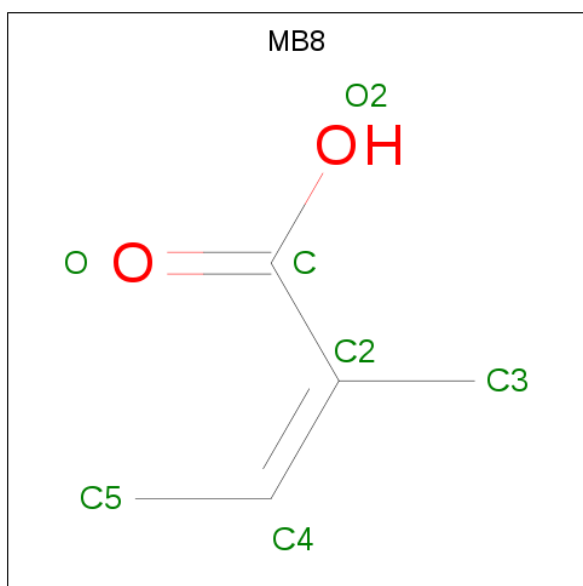
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total	Zn	0	0
			2	2		

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	3	Total	Mg	0	0
			3	3		
10	F	1	Total	Mg	0	0
			1	1		

- Molecule 11 is (2Z)-2-methylbut-2-enoic acid (three-letter code: MB8) (formula: C₅H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	I	1	Total	C	O	0	0
			2	1	1		

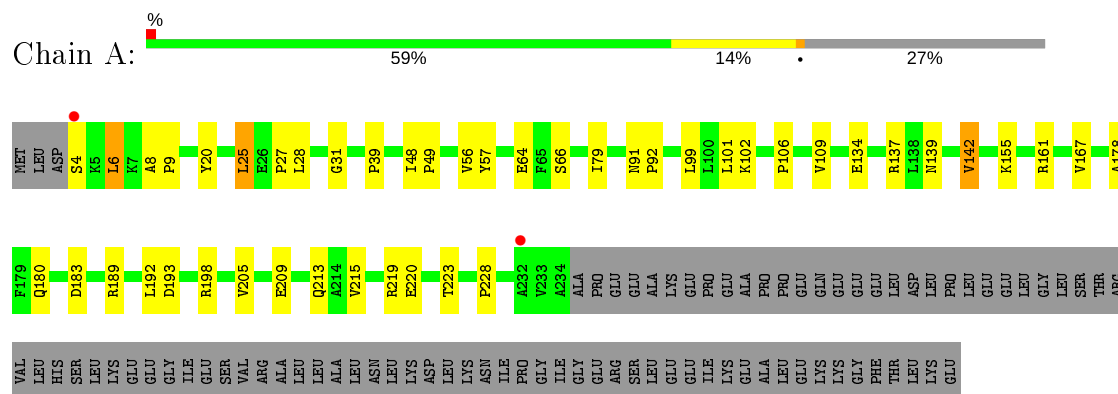
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	D	3	Total	O	0	0
			3	3		

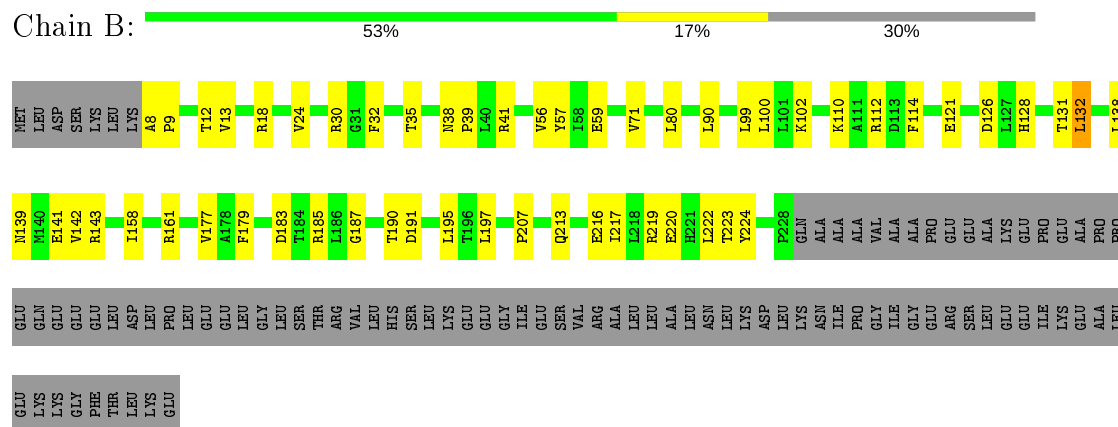
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

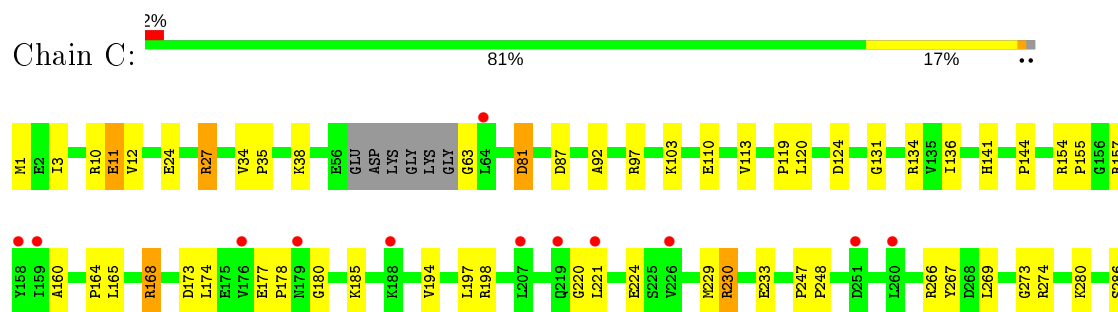
- Molecule 1: DNA-directed RNA polymerase subunit alpha

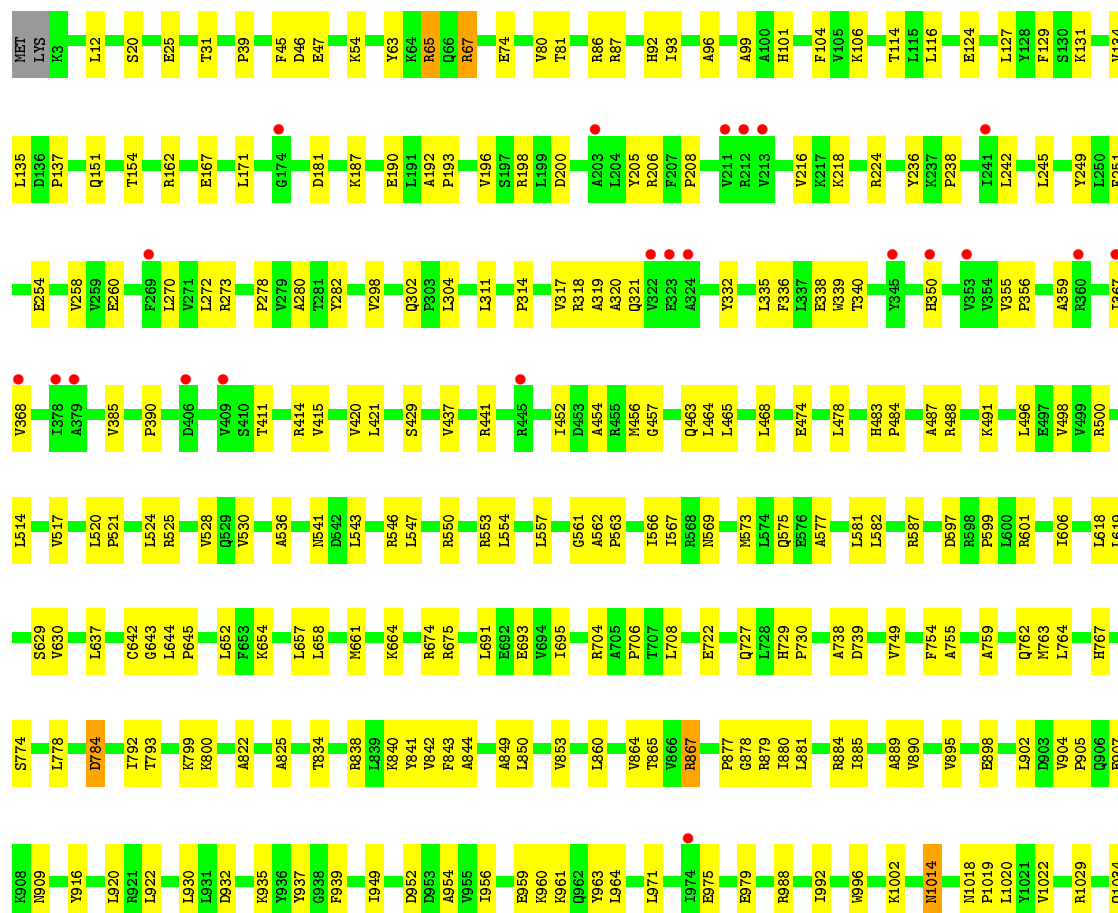


- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 2: DNA-directed RNA polymerase subunit beta





- Molecule 7: 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'

Chain H: 



- Molecule 8: GE23077

Chain I: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.84Å 104.18Å 295.32Å 90.00° 98.52° 90.00°	Depositor
Resolution (Å)	48.68 – 3.62 48.97 – 3.62	Depositor EDS
% Data completeness (in resolution range)	91.3 (48.68-3.62) 91.4 (48.97-3.62)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.199 , 0.248 0.203 , 0.248	Depositor DCC
R_{free} test set	1823 reflections (3.14%)	wwPDB-VP
Wilson B-factor (Å ²)	102.3	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28527	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: FGL, ZN, 2TL, DVA, MG, 2RA, DSN, MB8, 0QZ, R2T

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	0/1841	0.61	0/2504
1	B	0.37	0/1773	0.54	0/2413
2	C	0.41	0/8941	0.65	1/12092 (0.0%)
3	D	0.38	0/11963	0.54	0/16173
4	E	0.41	0/772	0.60	0/1040
5	F	0.36	0/2852	0.51	0/3837
6	G	0.70	0/368	1.29	5/567 (0.9%)
7	H	0.69	0/556	1.27	5/858 (0.6%)
All	All	0.40	0/29066	0.62	11/39484 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
8	I	0	1
All	All	0	2

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	17	DA	O4'-C1'-N9	9.26	114.48	108.00
7	H	13	DT	O4'-C4'-C3'	-8.88	100.67	106.00
6	G	5	DC	O4'-C4'-C3'	-8.73	100.76	106.00
2	C	513	VAL	CG1-CB-CG2	6.75	121.69	110.90
7	H	16	DC	O4'-C4'-C3'	-6.74	101.81	104.50
6	G	15	DT	C4-C5-C7	5.88	122.53	119.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	5	DC	C4'-C3'-C2'	-5.62	98.04	103.10
7	H	15	DT	O4'-C1'-N1	5.40	111.78	108.00
6	G	15	DT	C4'-C3'-C2'	-5.20	98.42	103.10
6	G	7	DT	N3-C4-O4	5.20	123.02	119.90
7	H	13	DT	N3-C4-O4	5.15	122.99	119.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	421	GLU	Peptide
8	I	5	2TL	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1809	0	1863	29	0
1	B	1741	0	1784	38	0
2	C	8774	0	8877	134	0
3	D	11754	0	11994	238	0
4	E	758	0	770	14	0
5	F	2807	0	2882	58	0
6	G	328	0	181	4	0
7	H	495	0	272	14	0
8	I	50	0	37	5	0
9	D	2	0	0	0	0
10	D	3	0	0	0	0
10	F	1	0	0	0	0
11	I	2	0	0	0	0
12	D	3	0	0	1	0
All	All	28527	0	28660	479	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 (479) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:628:PHE:H	2:C:638:ASP:HB3	1.32	0.93
2:C:418:LEU:HA	2:C:422:ARG:HH11	1.37	0.89
1:B:190:THR:HG21	3:D:722:GLU:HG3	1.65	0.77
2:C:758:ARG:HH21	2:C:788:THR:HB	1.50	0.77
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.66	0.77
2:C:81:ASP:OD1	2:C:81:ASP:N	2.20	0.74
3:D:134:VAL:HG22	3:D:151:GLN:H	1.52	0.72
3:D:739:ASP:OD2	12:D:2103:HOH:O	2.07	0.71
2:C:194:VAL:HG22	2:C:221:LEU:HD12	1.72	0.71
8:I:4:R2T:N	8:I:4:R2T:OG1	2.22	0.70
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.72	0.70
1:A:25:LEU:HD23	1:A:28:LEU:HD21	1.73	0.70
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.74	0.70
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.25	0.69
7:H:18:DC:H2'	7:H:19:DG:C8	2.28	0.69
3:D:1208:ASP:HB2	3:D:1215:VAL:HA	1.75	0.69
2:C:418:LEU:HA	2:C:422:ARG:NH1	2.09	0.68
2:C:3:ILE:HD13	2:C:900:ARG:HB2	1.77	0.67
1:B:59:GLU:OE1	1:B:139:ASN:ND2	2.29	0.66
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.29	0.66
2:C:165:LEU:HB2	2:C:168:ARG:HG3	1.78	0.66
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.76	0.66
1:A:220:GLU:O	1:A:223:THR:HB	1.97	0.65
2:C:428:ARG:NH2	2:C:447:ALA:O	2.29	0.65
2:C:501:THR:HG21	2:C:513:VAL:HG23	1.79	0.65
2:C:628:PHE:H	2:C:638:ASP:CB	2.07	0.65
2:C:1083:GLU:OE2	3:D:87:ARG:NH2	2.30	0.65
2:C:545:ASN:HB3	2:C:583:LEU:HD23	1.77	0.64
3:D:1198:TYR:OH	3:D:1432:LYS:NZ	2.26	0.64
3:D:273:ARG:HB3	3:D:278:PRO:HA	1.80	0.64
2:C:628:PHE:N	2:C:638:ASP:HB3	2.10	0.64
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.79	0.64
7:H:10:DA:H2''	7:H:11:DG:H5''	1.80	0.64
3:D:664:LYS:NZ	3:D:693:GLU:OE1	2.31	0.63
5:F:81:VAL:HG22	5:F:210:LEU:HD21	1.79	0.63
5:F:166:LEU:HD13	5:F:170:HIS:HB3	1.80	0.63
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.81	0.63
2:C:24:GLU:OE2	2:C:27:ARG:NH2	2.31	0.63
3:D:65:ARG:HB3	3:D:67:ARG:HG2	1.81	0.62
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.81	0.62
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.15	0.62
4:E:50:THR:HG22	4:E:53:GLY:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1349:VAL:HG22	3:D:1368:ILE:HG22	1.81	0.61
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.83	0.61
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.35	0.60
3:D:208:PRO:HA	3:D:390:PRO:HA	1.83	0.60
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.84	0.60
3:D:39:PRO:HG2	3:D:47:GLU:HG3	1.84	0.60
1:B:128:HIS:HE1	1:B:131:THR:HG23	1.65	0.60
5:F:208:SER:HB3	5:F:211:ASP:OD2	2.01	0.60
3:D:1462:LEU:HD22	3:D:1472:ILE:HB	1.84	0.59
3:D:63:TYR:OH	3:D:74:GLU:OE2	2.19	0.59
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.85	0.59
3:D:1111:ASP:OD1	3:D:1189:ARG:NH2	2.35	0.59
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.83	0.59
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.35	0.59
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.85	0.59
1:A:64:GLU:OE2	2:C:830:LYS:NZ	2.35	0.59
3:D:637:LEU:HD13	3:D:642:CYS:HA	1.85	0.59
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.85	0.58
3:D:1274:ILE:HD11	3:D:1334:GLN:HB3	1.85	0.58
3:D:657:LEU:HG	3:D:661:MET:HE2	1.83	0.58
1:B:128:HIS:CE1	1:B:131:THR:HG23	2.38	0.58
2:C:413:LEU:HD12	2:C:452:ILE:HD11	1.85	0.58
1:A:183:ASP:HA	2:C:938:LYS:HE3	1.84	0.58
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.32	0.57
3:D:954:ALA:O	3:D:1062:ARG:NH2	2.36	0.57
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.85	0.57
1:B:220:GLU:O	1:B:223:THR:OG1	2.20	0.57
3:D:864:VAL:HG22	3:D:865:THR:H	1.69	0.57
2:C:134:ARG:NH1	2:C:392:SER:OG	2.37	0.57
1:B:132:LEU:HD21	1:B:138:LEU:HB2	1.87	0.57
2:C:144:PRO:HB2	2:C:273:GLY:HA3	1.87	0.57
2:C:165:LEU:CB	2:C:168:ARG:HG3	2.34	0.57
2:C:97:ARG:NH2	2:C:110:GLU:OE2	2.36	0.57
3:D:1433:SER:O	3:D:1433:SER:OG	2.23	0.57
4:E:18:ARG:NH2	4:E:77:GLU:OE1	2.38	0.57
2:C:229:MET:HB3	2:C:233:GLU:HB2	1.87	0.56
3:D:171:LEU:HD12	3:D:390:PRO:HG2	1.87	0.56
2:C:445:GLU:OE1	8:I:4:R2T:OG1	2.23	0.56
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.87	0.56
3:D:1377:LYS:HE3	3:D:1378:TYR:CZ	2.41	0.56
5:F:135:ILE:HD11	5:F:178:ARG:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:971:LEU:HD21	3:D:992:ILE:HG23	1.88	0.56
3:D:988:ARG:NH2	3:D:1054:GLU:OE2	2.38	0.55
3:D:224:ARG:NE	3:D:254:GLU:OE2	2.31	0.55
3:D:840:LYS:HE3	3:D:841:TYR:OH	2.07	0.55
3:D:889:ALA:HB1	3:D:930:LEU:HA	1.88	0.55
1:A:25:LEU:HB3	1:A:28:LEU:HD11	1.87	0.55
2:C:197:LEU:HD12	2:C:221:LEU:HD11	1.89	0.55
2:C:678:PRO:HA	2:C:683:ASN:HD21	1.71	0.55
3:D:224:ARG:H	3:D:251:PHE:HE1	1.55	0.55
1:B:32:PHE:HA	1:B:35:THR:HB	1.88	0.54
3:D:543:LEU:HD13	3:D:581:LEU:HA	1.90	0.54
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.43	0.54
2:C:939:ARG:HG2	2:C:982:PRO:HD3	1.89	0.54
3:D:1209:LEU:HD11	3:D:1364:HIS:CD2	2.43	0.54
4:E:50:THR:HG23	4:E:52:GLU:N	2.24	0.53
5:F:284:ARG:NH2	5:F:290:GLU:OE2	2.42	0.53
5:F:326:ASP:OD2	6:G:18:DA:N6	2.42	0.53
3:D:563:PRO:HD2	3:D:566:ILE:HD12	1.88	0.53
3:D:437:VAL:HG11	5:F:175:HIS:CD2	2.44	0.53
5:F:88:ILE:HD11	5:F:192:LEU:HD13	1.91	0.53
1:A:57:TYR:CG	1:A:161:ARG:HD2	2.44	0.53
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.91	0.53
1:A:106:PRO:HG3	1:A:134:GLU:HG2	1.91	0.53
2:C:612:VAL:HG22	2:C:622:GLU:HG3	1.89	0.53
2:C:630:ARG:NH1	2:C:705:ILE:O	2.32	0.53
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.91	0.53
8:I:2:DSN:O	8:I:5:2TL:OG1	2.27	0.53
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.44	0.53
1:B:100:LEU:HG	1:B:141:GLU:HG2	1.91	0.53
1:B:41:ARG:HA	1:B:177:VAL:HG11	1.90	0.52
2:C:784:ASP:N	2:C:784:ASP:OD1	2.37	0.52
1:A:25:LEU:HD11	1:B:224:TYR:O	2.09	0.52
2:C:35:PRO:HG2	2:C:38:LYS:HD2	1.91	0.52
2:C:168:ARG:O	2:C:267:TYR:HA	2.09	0.52
2:C:726:ILE:HD11	2:C:757:GLY:HA3	1.91	0.52
3:D:272:LEU:HB2	3:D:280:ALA:HB3	1.90	0.52
4:E:45:ARG:NH1	4:E:56:ASP:OD2	2.43	0.52
3:D:956:ILE:HD11	3:D:1062:ARG:HD2	1.91	0.52
1:A:209:GLU:O	1:A:213:GLN:HG2	2.10	0.52
2:C:405:ARG:HD2	2:C:442:GLU:OE2	2.09	0.52
3:D:840:LYS:HE3	3:D:841:TYR:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:963:TYR:HE2	3:D:1002:LYS:HD3	1.74	0.52
3:D:904:VAL:HG22	3:D:905:PRO:HD2	1.91	0.52
2:C:280:LYS:HE3	2:C:309:TYR:CZ	2.45	0.51
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.92	0.51
2:C:11:GLU:OE1	2:C:537:LYS:HE2	2.10	0.51
3:D:1093:TYR:CZ	3:D:1097:LYS:HE3	2.45	0.51
2:C:177:GLU:HG3	2:C:178:PRO:HD2	1.93	0.51
2:C:937:ASP:OD1	2:C:939:ARG:HD3	2.10	0.51
3:D:652:LEU:HB3	3:D:749:VAL:HG21	1.92	0.51
3:D:658:LEU:HA	3:D:661:MET:HE3	1.91	0.51
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.31	0.51
3:D:569:ASN:ND2	5:F:214:GLN:OE1	2.44	0.51
2:C:435:TYR:OH	2:C:533:ASP:OD2	2.23	0.51
3:D:704:ARG:HD2	3:D:738:ALA:HB2	1.91	0.51
3:D:759:ALA:HA	3:D:763:MET:HB2	1.92	0.51
3:D:1225:ALA:O	3:D:1229:ILE:HG13	2.10	0.51
3:D:99:ALA:HB1	3:D:575:GLN:HE22	1.76	0.51
3:D:1020:LEU:HB3	3:D:1035:ILE:HD12	1.92	0.51
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.93	0.50
5:F:144:ILE:HB	5:F:147:LEU:HD13	1.93	0.50
3:D:1305:LEU:HD13	3:D:1309:ALA:HB3	1.93	0.50
3:D:500:ARG:NH1	3:D:1388:ARG:O	2.43	0.50
3:D:844:ALA:HB1	3:D:867:ARG:HH21	1.76	0.50
3:D:1093:TYR:OH	3:D:1441:GLN:NE2	2.40	0.50
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.94	0.50
2:C:136:ILE:HB	2:C:336:VAL:HG13	1.94	0.50
3:D:784:ASP:HB2	3:D:939:PHE:CE2	2.47	0.50
3:D:792:ILE:HG13	3:D:793:THR:HG23	1.94	0.50
3:D:799:LYS:NZ	3:D:1014:ASN:HA	2.27	0.50
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.94	0.50
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.94	0.49
3:D:31:THR:HG21	5:F:257:THR:HG22	1.94	0.49
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.94	0.49
3:D:1048:PRO:O	3:D:1079:LYS:NZ	2.43	0.49
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.93	0.49
3:D:561:GLY:HA3	5:F:132:ARG:HD3	1.93	0.49
3:D:784:ASP:HB2	3:D:939:PHE:HE2	1.77	0.49
3:D:134:VAL:HG12	3:D:454:ALA:HB2	1.94	0.49
2:C:1048:THR:HG22	3:D:755:ALA:HB1	1.93	0.49
2:C:422:ARG:NH2	7:H:14:DG:P	2.85	0.49
3:D:93:ILE:HD12	3:D:547:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:16:LYS:O	4:E:19:LEU:HB3	2.12	0.49
3:D:190:GLU:HA	3:D:196:VAL:HA	1.94	0.49
5:F:386:VAL:HB	5:F:397:ILE:HG12	1.95	0.49
3:D:960:LYS:NZ	3:D:1063:GLU:OE2	2.37	0.49
2:C:422:ARG:HH21	7:H:14:DG:P	2.36	0.49
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.94	0.49
3:D:135:LEU:HD23	3:D:463:GLN:HG2	1.94	0.49
5:F:395:GLU:OE2	5:F:398:ARG:NH2	2.46	0.49
1:B:71:VAL:HG22	1:B:132:LEU:HD23	1.94	0.49
3:D:483:HIS:CE1	3:D:488:ARG:HD3	2.48	0.49
2:C:764:GLU:OE2	3:D:54:LYS:HE2	2.11	0.49
1:A:99:LEU:HB2	1:A:142:VAL:HG22	1.94	0.49
2:C:911:GLU:O	2:C:915:LYS:HG2	2.13	0.49
3:D:1065:LEU:HD23	3:D:1069:GLU:HB3	1.94	0.48
2:C:878:SER:HA	3:D:1034:GLN:OE1	2.13	0.48
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.96	0.48
3:D:1282:ARG:NH2	3:D:1295:GLU:OE2	2.46	0.48
3:D:706:PRO:HB3	6:G:15:DT:H1'	1.95	0.48
6:G:8:DC:N4	7:H:19:DG:O6	2.46	0.48
1:A:228:PRO:HB3	1:B:13:VAL:HG21	1.96	0.48
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.41	0.48
2:C:324:ASP:OD2	2:C:431:HIS:NE2	2.36	0.48
3:D:691:LEU:O	3:D:695:ILE:HG23	2.13	0.48
5:F:193:ARG:HB2	7:H:6:DT:H1'	1.96	0.48
1:A:56:VAL:HG23	1:A:167:VAL:HG21	1.96	0.48
2:C:460:ARG:HD2	2:C:485:TYR:CZ	2.48	0.48
3:D:1486:VAL:HG21	4:E:22:VAL:HG13	1.96	0.48
7:H:16:DC:H2'	7:H:17:DA:C8	2.49	0.48
1:B:90:LEU:HD21	1:B:121:GLU:HB2	1.95	0.48
2:C:229:MET:O	2:C:233:GLU:HB2	2.13	0.48
3:D:129:PHE:CD1	3:D:456:MET:HB3	2.49	0.48
2:C:768:THR:O	2:C:771:GLU:N	2.46	0.48
1:B:110:LYS:HD3	1:B:128:HIS:HA	1.96	0.48
2:C:1035:MET:HG2	2:C:1038:TRP:CZ3	2.48	0.48
2:C:154:ARG:NH1	2:C:178:PRO:HG3	2.28	0.48
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.67	0.48
2:C:607:ASP:HB3	2:C:610:ARG:H	1.78	0.48
3:D:101:HIS:CE1	3:D:582:LEU:HD13	2.49	0.48
3:D:411:THR:O	5:F:178:ARG:NH1	2.45	0.48
2:C:882:LEU:HD11	3:D:1038:LEU:HD22	1.94	0.47
3:D:258:VAL:HG12	3:D:273:ARG:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:774:SER:HB2	3:D:1362:LYS:HG2	1.96	0.47
3:D:116:LEU:HD21	3:D:465:LEU:HD23	1.95	0.47
5:F:96:LEU:O	5:F:100:VAL:HG23	2.13	0.47
3:D:557:LEU:HD13	3:D:566:ILE:HG22	1.96	0.47
3:D:1103:HIS:ND1	3:D:1463:LYS:HG3	2.28	0.47
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.48	0.47
3:D:601:ARG:NH1	3:D:606:ILE:HG12	2.29	0.47
3:D:961:LYS:HE3	3:D:961:LYS:HB2	1.71	0.47
1:B:179:PHE:HB3	1:B:197:LEU:HD13	1.95	0.47
1:B:216:GLU:OE1	1:B:219:ARG:NH2	2.46	0.47
2:C:351:LEU:HD11	2:C:373:VAL:HG13	1.95	0.47
3:D:1103:HIS:CG	3:D:1463:LYS:HG3	2.50	0.47
1:A:180:GLN:HE22	2:C:929:ARG:NH1	2.13	0.47
2:C:773:LEU:O	2:C:777:ILE:HG13	2.14	0.47
2:C:548:PRO:O	2:C:843:HIS:HE1	1.97	0.47
3:D:514:LEU:HD13	3:D:517:VAL:HG22	1.97	0.47
2:C:930:LYS:NZ	2:C:935:GLY:HA2	2.30	0.47
3:D:116:LEU:HD23	3:D:468:LEU:HD11	1.96	0.47
2:C:119:PRO:HG2	2:C:386:PHE:CD1	2.49	0.47
2:C:627:ARG:HA	2:C:638:ASP:HB2	1.97	0.47
2:C:890:LEU:HD13	2:C:914:ILE:HG23	1.97	0.47
2:C:640:ARG:HE	2:C:642:ARG:HH22	1.62	0.47
2:C:910:LYS:O	2:C:914:ILE:HG13	2.15	0.47
3:D:1144:LEU:O	3:D:1147:ARG:HG3	2.15	0.47
2:C:1067:TYR:CE2	2:C:1071:ILE:HD13	2.50	0.47
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.68	0.47
3:D:137:PRO:HA	3:D:452:ILE:HG13	1.96	0.47
3:D:975:GLU:O	3:D:979:GLU:HG2	2.15	0.47
3:D:134:VAL:CG2	3:D:151:GLN:H	2.26	0.46
3:D:916:TYR:CE2	3:D:920:LEU:HD21	2.51	0.46
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.96	0.46
5:F:368:VAL:HG21	5:F:400:ILE:HD11	1.98	0.46
1:A:4:SER:O	1:A:189:ARG:NH2	2.39	0.46
2:C:1019:GLN:HG3	2:C:1058:ASP:HB3	1.96	0.46
2:C:286:SER:OG	2:C:301:GLU:OE2	2.23	0.46
3:D:167:GLU:OE2	3:D:198:ARG:NH1	2.47	0.46
4:E:68:LEU:HA	4:E:68:LEU:HD12	1.75	0.46
1:A:20:TYR:OH	1:A:198:ARG:HD2	2.15	0.46
2:C:63:GLY:O	2:C:103:LYS:HG2	2.15	0.46
2:C:571:LEU:HD23	2:C:702:SER:HB3	1.98	0.46
3:D:1350:GLU:O	3:D:1354:LYS:HG3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:114:THR:HG21	3:D:498:VAL:HG21	1.97	0.46
3:D:853:VAL:HG11	3:D:860:LEU:HG	1.97	0.46
5:F:321:ILE:HD12	5:F:332:PHE:CE1	2.51	0.46
8:I:4:R2T:OB1	8:I:4:R2T:NE2	2.49	0.46
1:A:101:LEU:HD21	1:A:109:VAL:HG11	1.98	0.46
1:A:27:PRO:HB2	1:A:192:LEU:HD13	1.98	0.46
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.15	0.46
3:D:181:ASP:HB2	3:D:205:TYR:HD1	1.79	0.46
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.51	0.46
3:D:916:TYR:O	3:D:920:LEU:HG	2.16	0.46
2:C:327:HIS:CE1	2:C:433:THR:HG21	2.51	0.46
2:C:401:LEU:HD21	2:C:543:ASN:ND2	2.31	0.46
3:D:1347:TYR:CZ	3:D:1351:GLU:HG3	2.51	0.46
2:C:224:GLU:CD	2:C:224:GLU:H	2.19	0.45
3:D:841:TYR:HB2	3:D:864:VAL:CG2	2.46	0.45
2:C:445:GLU:OE2	8:I:6:0QZ:N	2.49	0.45
3:D:270:LEU:HD13	3:D:304:LEU:HD13	1.98	0.45
3:D:487:ALA:O	3:D:491:LYS:HG2	2.15	0.45
5:F:81:VAL:HG22	5:F:210:LEU:CD2	2.46	0.45
1:B:213:GLN:O	1:B:217:ILE:HG13	2.17	0.45
1:B:216:GLU:CD	1:B:219:ARG:HH21	2.20	0.45
2:C:367:LEU:HD13	2:C:372:LEU:HD21	1.98	0.45
4:E:50:THR:HG23	4:E:52:GLU:H	1.81	0.45
3:D:483:HIS:CG	3:D:484:PRO:HD2	2.52	0.45
5:F:229:TYR:CZ	5:F:230:LYS:HD3	2.52	0.45
2:C:1038:TRP:NE1	3:D:1099:VAL:HG11	2.31	0.45
3:D:1465:ASN:OD1	3:D:1470:ARG:NH1	2.50	0.45
3:D:996:TRP:CE2	3:D:1056:PRO:HG3	2.50	0.45
1:B:143:ARG:NH1	1:B:158:ILE:HD12	2.31	0.45
2:C:952:LEU:HD12	2:C:952:LEU:HA	1.77	0.45
3:D:963:TYR:CE2	3:D:1002:LYS:HD3	2.51	0.45
3:D:1488:ASP:OD1	3:D:1488:ASP:N	2.43	0.45
3:D:520:LEU:HD11	3:D:524:LEU:HD12	1.98	0.45
3:D:298:VAL:HG12	3:D:302:GLN:NE2	2.32	0.45
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.66	0.45
1:B:18:ARG:O	1:B:207:PRO:HD3	2.17	0.45
3:D:1237:THR:HG22	3:D:1238:MET:N	2.31	0.45
1:A:215:VAL:HG13	1:B:222:LEU:HB3	1.98	0.45
3:D:39:PRO:HB3	3:D:45:PHE:O	2.17	0.45
1:A:31:GLY:N	1:A:193:ASP:OD1	2.49	0.45
2:C:771:GLU:O	2:C:775:ARG:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:317:VAL:HG23	3:D:339:TRP:HB3	1.98	0.44
3:D:45:PHE:O	3:D:86:ARG:NH2	2.50	0.44
5:F:417:LYS:HB3	5:F:418:LEU:HD12	1.99	0.44
5:F:193:ARG:HB3	7:H:7:DG:H5"	1.99	0.44
1:B:99:LEU:HB3	1:B:114:PHE:CD1	2.52	0.44
3:D:1491:THR:O	3:D:1495:ILE:HG13	2.17	0.44
3:D:654:LYS:O	3:D:658:LEU:HG	2.18	0.44
5:F:172:ARG:O	5:F:176:ILE:HG12	2.17	0.44
2:C:674:VAL:HG12	2:C:869:VAL:HB	2.00	0.44
2:C:1043:TYR:CD1	3:D:763:MET:HG2	2.52	0.44
2:C:583:LEU:HD12	2:C:583:LEU:O	2.16	0.44
3:D:1383:ASP:HB3	3:D:1416:ALA:HB3	1.99	0.44
3:D:236:TYR:HB2	3:D:319:ALA:HB3	1.99	0.44
3:D:932:ASP:O	3:D:935:LYS:HB3	2.18	0.44
3:D:959:GLU:HB3	3:D:963:TYR:CE1	2.53	0.44
3:D:550:ARG:HD2	3:D:577:ALA:HB2	1.99	0.44
3:D:675:ARG:HH22	5:F:420:ASP:HB3	1.83	0.44
3:D:879:ARG:HD3	3:D:902:LEU:O	2.18	0.44
3:D:573:MET:SD	5:F:210:LEU:HB3	2.58	0.44
5:F:333:ILE:HA	5:F:334:PRO:HD3	1.80	0.44
2:C:266:ARG:NH1	7:H:11:DG:O6	2.38	0.44
1:A:155:LYS:HD2	1:A:155:LYS:HA	1.79	0.44
2:C:198:ARG:NH1	2:C:230:ARG:HA	2.32	0.44
2:C:396:ASP:OD2	2:C:402:SER:HB3	2.18	0.44
3:D:1209:LEU:HD11	3:D:1364:HIS:HD2	1.83	0.44
2:C:1015:LEU:HD11	3:D:528:VAL:HG21	1.98	0.44
2:C:124:ASP:HB3	2:C:592:LEU:HD12	1.99	0.43
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.53	0.43
3:D:1168:MET:O	3:D:1171:VAL:HB	2.18	0.43
3:D:1296:SER:OG	3:D:1297:GLU:N	2.51	0.43
3:D:916:TYR:CE1	3:D:920:LEU:HD11	2.53	0.43
5:F:321:ILE:O	5:F:327:SER:HB3	2.18	0.43
5:F:383:LEU:HD13	5:F:398:ARG:HB2	2.00	0.43
3:D:1106:VAL:O	3:D:1108:ARG:HG3	2.18	0.43
2:C:1067:TYR:OH	3:D:674[A]:ARG:NH1	2.50	0.43
4:E:44:GLU:O	4:E:66:LYS:NZ	2.45	0.43
1:B:110:LYS:HD2	1:B:126:ASP:O	2.18	0.43
3:D:1433:SER:HG	3:D:1436:SER:HB3	1.83	0.43
2:C:164:PRO:HA	2:C:269:LEU:HD23	2.00	0.43
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.99	0.43
3:D:764:LEU:HD23	3:D:767:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:45:ARG:HA	4:E:46:PRO:HD3	1.91	0.43
5:F:153:PRO:HA	5:F:156:VAL:HG22	2.00	0.43
1:B:190:THR:CG2	3:D:722:GLU:HG3	2.42	0.43
3:D:729:HIS:HA	3:D:730:PRO:HD3	1.90	0.43
3:D:907:GLU:OE1	3:D:909:ASN:N	2.50	0.43
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	2.01	0.43
3:D:478:LEU:HD21	3:D:500:ARG:NH2	2.33	0.43
3:D:536:ALA:HA	5:F:315:VAL:O	2.18	0.43
2:C:422:ARG:HA	7:H:15:DT:O4'	2.19	0.43
2:C:878:SER:CB	3:D:1029:ARG:HD2	2.49	0.43
3:D:1323:GLN:HA	3:D:1324:PRO:HD3	1.94	0.43
3:D:355:VAL:HG11	3:D:385:VAL:HG21	2.01	0.43
1:B:12:THR:HB	1:B:24:VAL:HB	2.01	0.43
3:D:1402:ALA:O	3:D:1405:GLU:HG2	2.18	0.43
1:B:185:ARG:NH1	1:B:187:GLY:O	2.52	0.43
3:D:963:TYR:CE2	3:D:1002:LYS:HB3	2.53	0.43
3:D:236:TYR:CE1	3:D:242:LEU:HD12	2.54	0.43
5:F:187:LEU:HD23	5:F:224:VAL:HG13	2.00	0.43
5:F:88:ILE:HD11	5:F:192:LEU:CD1	2.48	0.43
2:C:92:ALA:HB2	2:C:120:LEU:HD11	2.00	0.42
3:D:251:PHE:HZ	3:D:282:TYR:CD1	2.37	0.42
3:D:706:PRO:HB2	3:D:708:LEU:HD21	2.00	0.42
1:B:38:ASN:ND2	2:C:979:THR:HG22	2.34	0.42
2:C:557:ARG:HA	2:C:557:ARG:HD2	1.81	0.42
2:C:862:PRO:HD2	2:C:925:TYR:OH	2.19	0.42
3:D:1047:LYS:HG2	3:D:1053:PHE:CZ	2.54	0.42
3:D:127:LEU:HA	3:D:457:GLY:HA2	2.00	0.42
3:D:1302:GLU:OE1	3:D:1304:LYS:HE3	2.19	0.42
3:D:192:ALA:HB1	3:D:193:PRO:HD2	2.01	0.42
5:F:264:MET:HB2	5:F:264:MET:HE2	1.85	0.42
2:C:154:ARG:HA	2:C:155:PRO:HD3	1.85	0.42
3:D:1107:VAL:HB	3:D:1218:GLY:H	1.83	0.42
3:D:1267:ARG:HA	3:D:1268:PRO:HD3	1.83	0.42
3:D:350:HIS:HE1	5:F:232:ARG:HB3	1.85	0.42
3:D:597:ASP:O	3:D:599:PRO:HD3	2.19	0.42
3:D:131:LYS:O	3:D:456:MET:HG2	2.19	0.42
3:D:619:LEU:HD11	3:D:1439:SER:HB2	2.01	0.42
3:D:860:LEU:HD23	3:D:877:PRO:HB2	2.01	0.42
3:D:964:LEU:HA	3:D:964:LEU:HD23	1.95	0.42
5:F:276:ARG:O	5:F:279:GLN:HG3	2.19	0.42
5:F:364:ARG:HG3	5:F:390:PHE:CE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:15:DT:H2''	7:H:16:DC:O4'	2.19	0.42
1:A:178:ALA:HB2	2:C:864:GLY:HA3	2.02	0.42
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.20	0.42
3:D:1192:LEU:HG	3:D:1369:GLU:HB3	2.01	0.42
3:D:1366:LYS:O	3:D:1370:ILE:HG12	2.20	0.42
3:D:1372:VAL:HA	3:D:1375:MET:HE3	2.01	0.42
5:F:370:LYS:O	5:F:376:ILE:HG12	2.19	0.42
1:B:57:TYR:CG	1:B:161:ARG:HD2	2.55	0.42
3:D:1435:LEU:HB2	3:D:1457:ASP:OD2	2.20	0.42
3:D:834:THR:OG1	3:D:838:ARG:HD2	2.19	0.42
3:D:843:PHE:HE1	3:D:864:VAL:HG21	1.84	0.42
2:C:595:LEU:HD11	2:C:623:TYR:HB3	2.01	0.42
3:D:224:ARG:HB2	3:D:332:TYR:HD1	1.85	0.42
3:D:245:LEU:HD23	3:D:249:TYR:HB3	2.02	0.42
5:F:181:GLU:O	5:F:185:GLN:HG2	2.20	0.42
1:A:6:LEU:HD11	1:A:27:PRO:HG2	2.02	0.42
2:C:1118:LYS:HE2	3:D:20:SER:O	2.20	0.42
2:C:693:GLU:OE1	2:C:696:LYS:HD2	2.20	0.42
2:C:878:SER:HB3	3:D:1029:ARG:HD2	2.02	0.42
2:C:877:PRO:HG2	3:D:1029:ARG:HB3	2.01	0.42
3:D:525:ARG:HD2	3:D:541:ASN:OD1	2.19	0.42
3:D:557:LEU:HB3	3:D:567:ILE:HD11	2.01	0.42
2:C:1019:GLN:HG2	2:C:1057:SER:OG	2.19	0.42
2:C:180:GLY:O	2:C:220:GLY:HA3	2.20	0.42
2:C:617:ASP:HB2	2:C:619:ARG:HG2	2.00	0.42
3:D:1197:ARG:HB2	3:D:1398:TRP:CH2	2.55	0.42
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.55	0.42
3:D:99:ALA:HB1	3:D:575:GLN:NE2	2.33	0.42
7:H:16:DC:H2''	7:H:17:DA:O5'	2.19	0.42
1:A:91:ASN:HA	1:A:92:PRO:HD3	1.88	0.41
1:B:110:LYS:NZ	1:B:128:HIS:HB2	2.34	0.41
3:D:1018:ASN:O	3:D:1022:VAL:HG23	2.20	0.41
3:D:421:LEU:HD11	3:D:429:SER:HB2	2.02	0.41
5:F:101:GLU:O	5:F:105:LYS:HG3	2.20	0.41
5:F:88:ILE:HA	5:F:88:ILE:HD12	1.77	0.41
3:D:877:PRO:O	3:D:880:ILE:HB	2.20	0.41
1:B:8:ALA:HA	1:B:9:PRO:HA	1.88	0.41
2:C:34:VAL:HA	2:C:35:PRO:HD2	1.85	0.41
2:C:598:GLU:O	2:C:651:LYS:NZ	2.45	0.41
2:C:691:SER:HA	2:C:858:MET:HE1	2.02	0.41
3:D:367:ILE:HG22	3:D:368:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:234:LYS:HB3	5:F:234:LYS:HE2	1.77	0.41
1:B:30:ARG:HB2	1:B:191:ASP:HB3	2.02	0.41
3:D:520:LEU:HD12	3:D:521:PRO:HD2	2.03	0.41
3:D:949:ILE:HA	3:D:949:ILE:HD13	1.84	0.41
2:C:173:ASP:HB2	2:C:185:LYS:HB3	2.02	0.41
2:C:540:PHE:HB3	2:C:544:THR:HB	2.03	0.41
2:C:693:GLU:O	2:C:697:ARG:HG2	2.20	0.41
3:D:1433:SER:HB2	3:D:1457:ASP:OD1	2.20	0.41
2:C:896:PHE:HB2	2:C:921:ALA:HB1	2.01	0.41
3:D:629:SER:OG	3:D:630:VAL:N	2.52	0.41
2:C:157:ARG:HA	2:C:157:ARG:HD3	1.87	0.41
3:D:1486:VAL:CG2	4:E:22:VAL:HG13	2.50	0.41
2:C:729:LEU:HD23	2:C:729:LEU:HA	1.94	0.41
3:D:187:LYS:N	3:D:200:ASP:OD1	2.45	0.41
5:F:123:ASP:OD2	5:F:125:ASP:HB2	2.21	0.41
3:D:553:ARG:HG3	5:F:218:GLN:NE2	2.36	0.41
5:F:365:GLU:HB2	5:F:404:ALA:HB2	2.02	0.41
7:H:16:DC:H3'	7:H:17:DA:H2'	2.03	0.41
2:C:586:ARG:HD2	2:C:586:ARG:HA	1.85	0.41
3:D:216:VAL:HA	3:D:340:THR:HG22	2.02	0.41
3:D:644:LEU:HD12	3:D:645:PRO:HD2	2.01	0.41
3:D:800:LYS:HB3	3:D:822:ALA:HB2	2.03	0.41
1:B:24:VAL:HA	1:B:195:LEU:O	2.21	0.41
3:D:162:ARG:O	3:D:414:ARG:NH1	2.53	0.41
3:D:562:ALA:O	5:F:140:ARG:NH1	2.46	0.41
4:E:57:ASP:HA	4:E:58:PRO:HD3	1.89	0.41
5:F:157:GLU:O	5:F:161:GLN:HG2	2.21	0.41
5:F:338:LEU:HA	5:F:339:PRO:HD3	1.88	0.41
1:A:48:ILE:HA	1:A:49:PRO:HD3	1.92	0.41
1:A:64:GLU:HG3	1:A:79:ILE:HD12	2.02	0.41
2:C:578:VAL:HG23	2:C:671:ASN:CG	2.41	0.41
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.21	0.41
3:D:844:ALA:O	3:D:867:ARG:HB3	2.20	0.41
3:D:860:LEU:HD22	3:D:878:GLY:HA2	2.03	0.41
3:D:881:LEU:O	3:D:885:ILE:HG13	2.21	0.41
3:D:895:VAL:O	3:D:898:GLU:N	2.54	0.41
3:D:959:GLU:HB3	3:D:963:TYR:HE1	1.86	0.41
1:A:102:LYS:HE2	1:A:139:ASN:OD1	2.21	0.40
2:C:957:LYS:HB3	2:C:961:GLU:HB2	2.02	0.40
3:D:464:LEU:HD23	3:D:464:LEU:HA	1.89	0.40
3:D:849:ALA:O	3:D:853:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:885:ILE:HD13	3:D:937:TYR:CG	2.56	0.40
4:E:52:GLU:OE1	4:E:52:GLU:N	2.48	0.40
5:F:369:LEU:HD22	5:F:404:ALA:HB1	2.03	0.40
1:A:219:ARG:HG2	1:B:219:ARG:HG3	2.02	0.40
2:C:442:GLU:OE1	2:C:543:ASN:HB2	2.21	0.40
3:D:850:LEU:HD12	3:D:884:ARG:NH2	2.36	0.40
3:D:964:LEU:HD22	3:D:1058:ARG:NH2	2.36	0.40
3:D:25:GLU:HB2	3:D:92:HIS:CE1	2.57	0.40
3:D:46:ASP:OD1	3:D:47:GLU:N	2.54	0.40
3:D:546:ARG:O	3:D:550:ARG:HG3	2.21	0.40
3:D:952:ASP:HA	3:D:1062:ARG:NH1	2.37	0.40
5:F:120:THR:HG22	5:F:122:LEU:HD13	2.02	0.40
5:F:89:GLY:HA2	5:F:193:ARG:NH2	2.36	0.40
1:B:102:LYS:HG2	1:B:139:ASN:OD1	2.21	0.40
1:B:57:TYR:CD1	1:B:161:ARG:HD2	2.56	0.40
2:C:317:VAL:HA	2:C:318:PRO:HD3	1.85	0.40
2:C:926:PHE:CE2	2:C:930:LYS:HD3	2.56	0.40
3:D:106:LYS:HD2	3:D:106:LYS:HA	1.83	0.40
3:D:321:GLN:HB2	3:D:336:PHE:CD2	2.57	0.40
3:D:822:ALA:HB3	3:D:825:ALA:HB2	2.03	0.40
5:F:386:VAL:HG12	5:F:397:ILE:HD11	2.04	0.40
7:H:12:DC:H2''	7:H:13:DT:C5	2.57	0.40
2:C:858:MET:HG2	2:C:867:VAL:O	2.22	0.40
3:D:1018:ASN:HA	3:D:1019:PRO:HD3	1.89	0.40
3:D:1348:LEU:HD23	3:D:1348:LEU:HA	1.84	0.40
5:F:79:ASP:HA	5:F:80:PRO:HD3	1.88	0.40
6:G:11:DT:H2'	6:G:11:DT:H6	1.76	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	
1	A	229/315 (73%)	227 (99%)	2 (1%)	0	100	100
1	B	219/315 (70%)	205 (94%)	14 (6%)	0	100	100
2	C	1108/1119 (99%)	1081 (98%)	24 (2%)	3 (0%)	41	74
3	D	1484/1524 (97%)	1410 (95%)	70 (5%)	4 (0%)	41	74
4	E	92/99 (93%)	90 (98%)	2 (2%)	0	100	100
5	F	344/443 (78%)	339 (98%)	5 (2%)	0	100	100
All	All	3476/3815 (91%)	3352 (96%)	117 (3%)	7 (0%)	47	79

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	422	ARG
3	D	320	ALA
2	C	230	ARG
2	C	446	GLY
3	D	154	THR
3	D	1205	TYR
3	D	1166	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	200/273 (73%)	194 (97%)	6 (3%)	41	71
1	B	194/273 (71%)	191 (98%)	3 (2%)	65	83
2	C	936/941 (100%)	909 (97%)	27 (3%)	42	71
3	D	1255/1279 (98%)	1230 (98%)	25 (2%)	55	79
4	E	82/88 (93%)	81 (99%)	1 (1%)	71	86
5	F	301/388 (78%)	297 (99%)	4 (1%)	69	86
All	All	2968/3242 (92%)	2902 (98%)	66 (2%)	52	77

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	25	LEU
1	A	66	SER
1	A	137	ARG
1	A	142	VAL
1	A	205	VAL
1	B	112	ARG
1	B	132	LEU
1	B	183	ASP
2	C	1	MET
2	C	10	ARG
2	C	11	GLU
2	C	27	ARG
2	C	81	ASP
2	C	113	VAL
2	C	141	HIS
2	C	168	ARG
2	C	274	ARG
2	C	513	VAL
2	C	528	GLU
2	C	557	ARG
2	C	562	SER
2	C	610	ARG
2	C	617	ASP
2	C	670	GLN
2	C	764	GLU
2	C	771	GLU
2	C	775	ARG
2	C	784	ASP
2	C	807	ARG
2	C	815	LEU
2	C	929	ARG
2	C	952	LEU
2	C	1076	VAL
2	C	1078	GLU
2	C	1080	SER
3	D	65	ARG
3	D	67	ARG
3	D	80	VAL
3	D	81	THR
3	D	206	ARG
3	D	335	LEU
3	D	415	VAL

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Mol	Chain	Res	Type
3	D	420	VAL
3	D	530	VAL
3	D	618	LEU
3	D	754	PHE
3	D	762	GLN
3	D	778	LEU
3	D	784	ASP
3	D	867	ARG
3	D	1014	ASN
3	D	1041	LEU
3	D	1055	VAL
3	D	1062	ARG
3	D	1100	ASP
3	D	1188	VAL
3	D	1207	TYR
3	D	1238	MET
3	D	1307	LYS
3	D	1433	SER
4	E	93	TYR
5	F	88	ILE
5	F	205	ARG
5	F	210	LEU
5	F	310	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	38	ASN
1	B	128	HIS
1	B	188	GLN
1	B	212	ASN
2	C	506	ASN
3	D	66	GLN
3	D	696	HIS
3	D	1124	GLN
3	D	1172	HIS
3	D	1441	GLN
5	F	83	GLN
5	F	381	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 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	$\# Z > 2$
8	0QZ	I	6	8	4,5,6	1.61	1 (25%)	2,5,7	0.28	0
8	2TL	I	5	8	5,6,7	1.18	0	6,7,9	1.30	0
8	R2T	I	4	8	8,10,11	1.96	1 (12%)	6,13,15	0.72	0
8	FGL	I	7	8	2,6,7	0.74	0	0,7,9	0.00	-
8	2RA	I	1	11,8	3,5,6	0.49	0	1,5,7	0.28	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
8	0QZ	I	6	8	-	2/3/4/6	-
8	2TL	I	5	8	-	5/5/6/8	-
8	R2T	I	4	8	-	6/13/14/16	-
8	FGL	I	7	8	-	0/0/6/8	-
8	2RA	I	1	11,8	-	2/2/4/6	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	4	R2T	CD-NE2	4.51	1.44	1.32
8	I	6	0QZ	OB-CA	-3.09	1.38	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	5	2TL	N-CA-CB-OG1
8	I	5	2TL	N-CA-CB-CG2
8	I	5	2TL	C-CA-CB-OG1
8	I	5	2TL	C-CA-CB-CG2
8	I	5	2TL	O-C-CA-CB
8	I	6	0QZ	N-C1-CA-C
8	I	6	0QZ	O-C-CA-C1
8	I	4	R2T	OB1-CB-CG-CD
8	I	4	R2T	OE1-CD-CG-OG1
8	I	4	R2T	NE2-CD-CG-OG1
8	I	1	2RA	C-CA-CB-NG
8	I	1	2RA	N-CA-CB-NG
8	I	4	R2T	OB1-CB-CG-OG1
8	I	4	R2T	CA-CB-CG-CD
8	I	4	R2T	CA-CB-CG-OG1

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	6	0QZ	1	0
8	I	5	2TL	1	0
8	I	4	R2T	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
11	MB8	I	101	8	0,1,6	0.00	-	-		

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.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	231/315 (73%)	-0.07	2 (0%) 84 73	26, 54, 80, 125	0
1	B	221/315 (70%)	-0.22	0 100 100	26, 58, 87, 115	0
2	C	1112/1119 (99%)	-0.07	18 (1%) 72 58	12, 50, 121, 145	0
3	D	1487/1524 (97%)	-0.07	29 (1%) 65 50	11, 50, 112, 141	0
4	E	94/99 (94%)	0.22	4 (4%) 35 23	26, 60, 110, 115	0
5	F	346/443 (78%)	-0.06	12 (3%) 44 29	24, 70, 139, 155	0
6	G	16/21 (76%)	0.45	0 100 100	84, 107, 178, 180	0
7	H	24/27 (88%)	-0.06	0 100 100	65, 125, 181, 192	0
8	I	0/7	-	-	-	-
All	All	3531/3870 (91%)	-0.07	65 (1%) 68 53	11, 55, 121, 192	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	390	PHE	5.0
2	C	207	LEU	4.7
5	F	422	LEU	3.8
5	F	146	GLY	3.8
2	C	766	GLU	3.8
5	F	149	GLU	3.8
5	F	373	LYS	3.7
3	D	345	TYR	3.6
3	D	1491	THR	3.5
3	D	203	ALA	3.4
4	E	89	MET	3.4
3	D	174	GLY	3.3
3	D	211	VAL	3.2
3	D	322	VAL	3.2
3	D	1287	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
3	D	445	ARG	2.9
2	C	777	ILE	2.9
2	C	221	LEU	2.9
1	A	232	ALA	2.9
2	C	251	ASP	2.8
3	D	1499	ARG	2.8
3	D	974	ILE	2.8
4	E	93	TYR	2.8
2	C	311	PHE	2.8
3	D	360	ARG	2.8
5	F	399	GLN	2.7
3	D	1495	ILE	2.7
5	F	386	VAL	2.7
5	F	381	HIS	2.7
2	C	159	ILE	2.7
3	D	1292	VAL	2.6
3	D	213	VAL	2.6
2	C	64	LEU	2.6
3	D	1297	GLU	2.5
5	F	369	LEU	2.5
4	E	95	VAL	2.5
3	D	323	GLU	2.5
3	D	1130	ARG	2.4
3	D	367	ILE	2.4
2	C	176	VAL	2.4
3	D	409	VAL	2.4
2	C	260	LEU	2.4
3	D	406	ASP	2.4
2	C	296	GLY	2.3
3	D	324	ALA	2.3
2	C	179	ASN	2.3
3	D	350	HIS	2.3
3	D	353	VAL	2.3
3	D	378	ILE	2.3
4	E	79	LEU	2.3
2	C	226	VAL	2.2
3	D	269	PHE	2.2
3	D	368	VAL	2.2
5	F	396	ARG	2.2
5	F	395	GLU	2.2
3	D	379	ALA	2.1
2	C	741	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
5	F	380	GLU	2.1
2	C	779	GLY	2.1
1	A	4	SER	2.1
2	C	158	TYR	2.1
2	C	188	LYS	2.1
3	D	241	ILE	2.1
2	C	219	GLN	2.0
3	D	212	ARG	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
8	2RA	I	1	6/7	0.87	0.20	40,41,50,55	0
8	FGL	I	7	7/8	0.90	0.20	31,36,41,44	0
8	R2T	I	4	11/12	0.94	0.16	25,32,34,34	0
8	DSN	I	2	6/7	0.95	0.16	33,43,50,50	0
8	DVA	I	3	7/8	0.98	0.16	22,25,33,36	0
8	0QZ	I	6	6/7	0.98	0.24	27,29,29,29	0
8	2TL	I	5	7/8	0.99	0.17	27,28,33,37	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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
10	MG	D	2005	1/1	0.83	0.14	37,37,37,37	0
11	MB8	I	101	2/7	0.88	0.56	54,54,54,59	0
10	MG	F	2001	1/1	0.93	0.18	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	MG	D	2003	1/1	0.97	0.21	26,26,26,26	0
9	ZN	D	2002	1/1	0.98	0.10	82,82,82,82	0
10	MG	D	2004	1/1	0.98	0.40	11,11,11,11	0
9	ZN	D	2001	1/1	1.00	0.21	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.