



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:32 AM UTC

PDB ID : 4MQ9 / pdb_00004mq9
Title : Crystal structure of Thermus thermophilus RNA polymerase holoenzyme in complex with GE23077
Authors : Ho, M.X.; Arnold, E.; Ebright, R.H.; Zhang, Y.; Tuske, S.
Deposited on : 2013-09-16
Resolution : 3.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

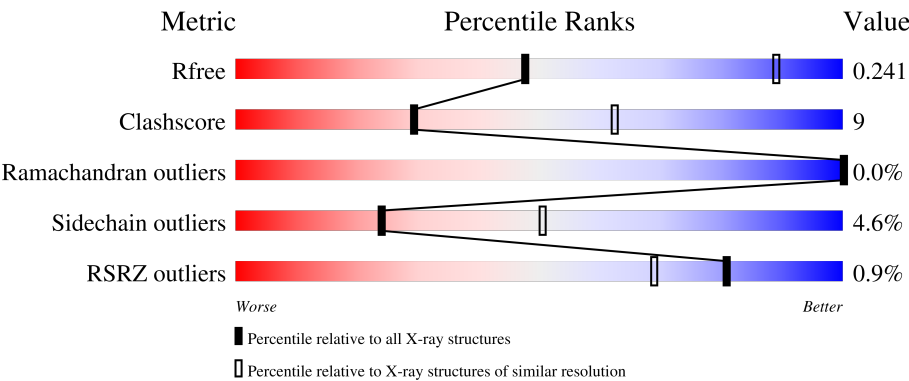
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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

Mol	Chain	Length	Quality of chain
1	A	314	55%15%•28%
1	B	314	% 52%18%•29%
2	C	1119	% 73%24%••
3	D	1524	% 66%22%•10%
4	E	99	% 72%21%•6%

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Mol	Chain	Length	Quality of chain
5	F	443	% 62% 13% 23%
6	I	7	29% 43% 29%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 26552 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	226	Total	C	N	O	S	0	0	0
			1777	1135	309	331	2			
1	B	224	Total	C	N	O	S	0	0	0
			1750	1118	303	327	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1100	Total	C	N	O	S	0	0	0
			8677	5487	1552	1614	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1365	Total	C	N	O	S	0	0	0
			10781	6821	1912	2014	34			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	93	Total	C	N	O	S	0	0	0
			754	481	131	138	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	339	Total	C	N	O	S	0	0	0
			2754	1736	501	513	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 protein called GE23077.

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

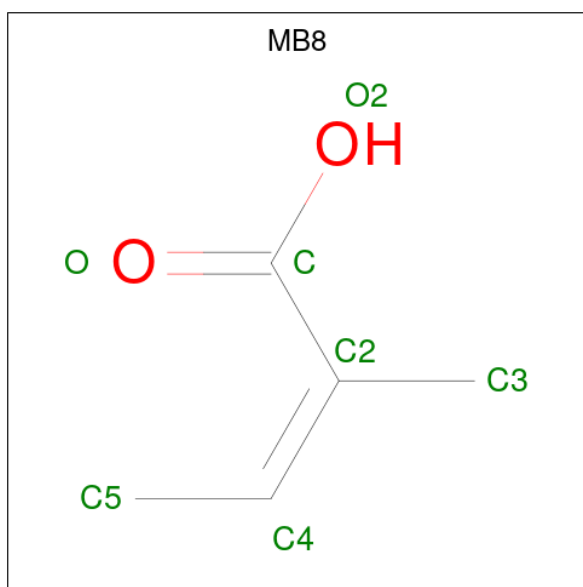
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total	Mg	0	0
			1	1		

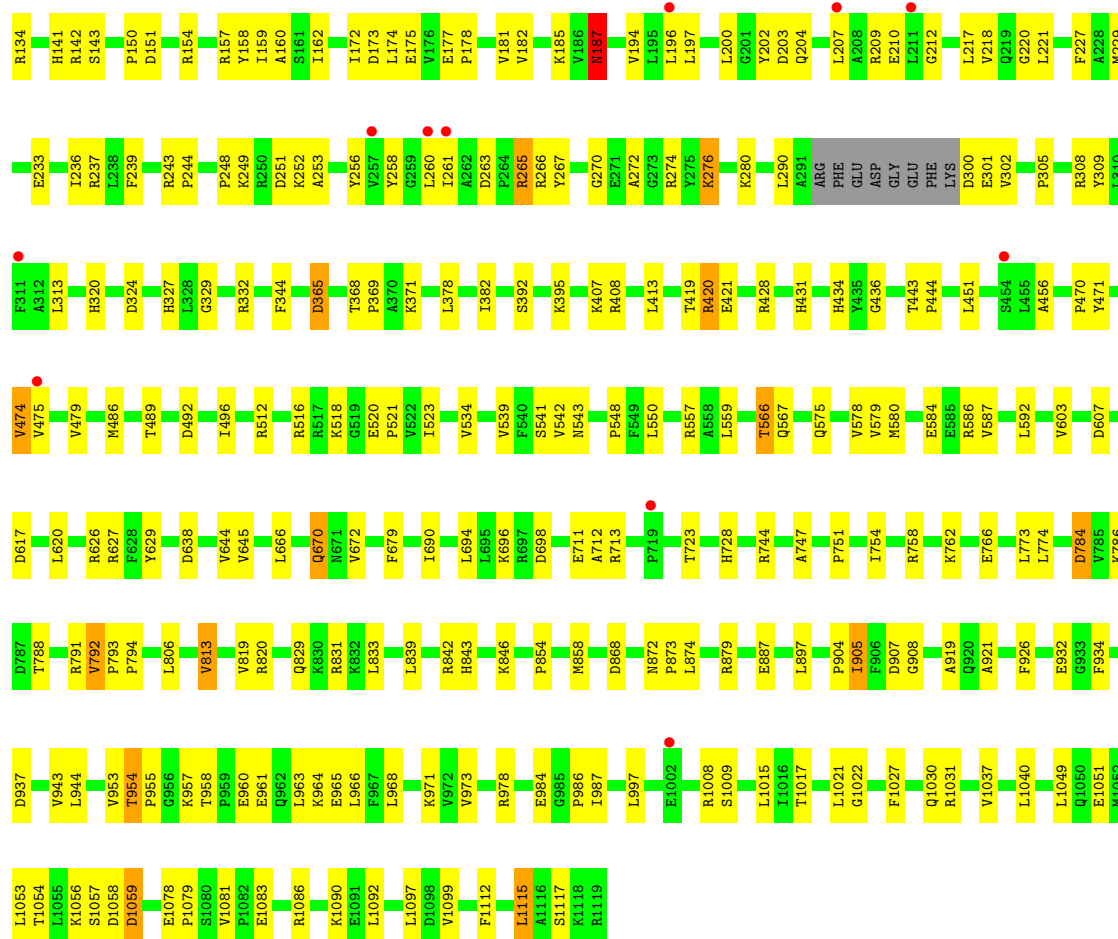
- Molecule 9 is (2Z)-2-methylbut-2-enoic acid (CCD ID: MB8) (formula: C₅H₈O₂).



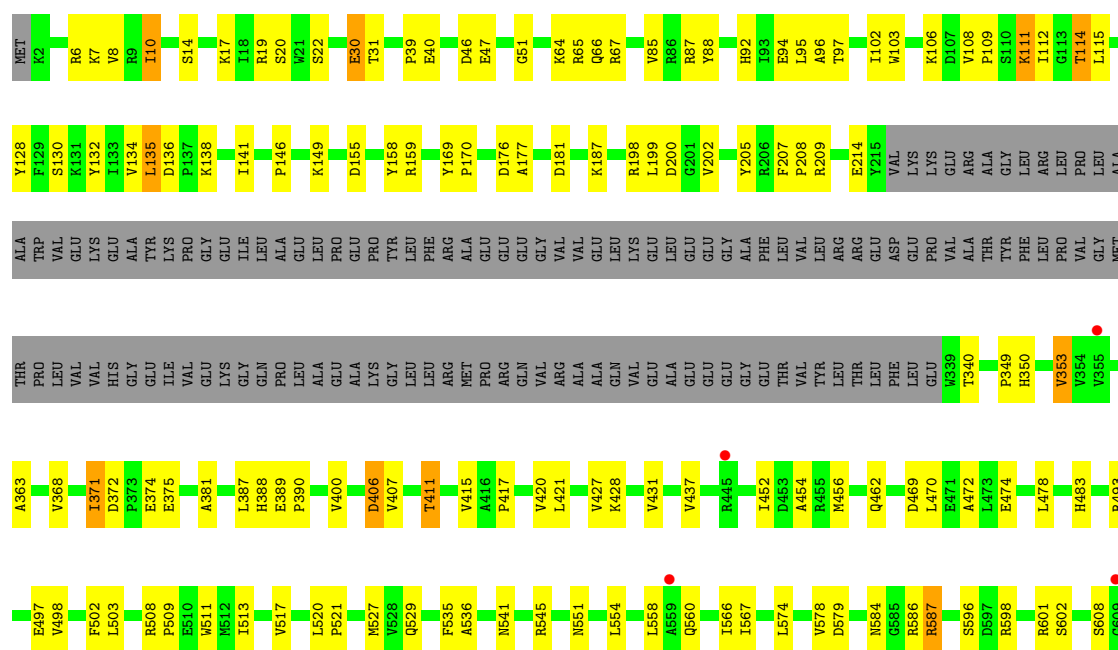
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	I	1	Total	C	O	0	0
			2	1	1		

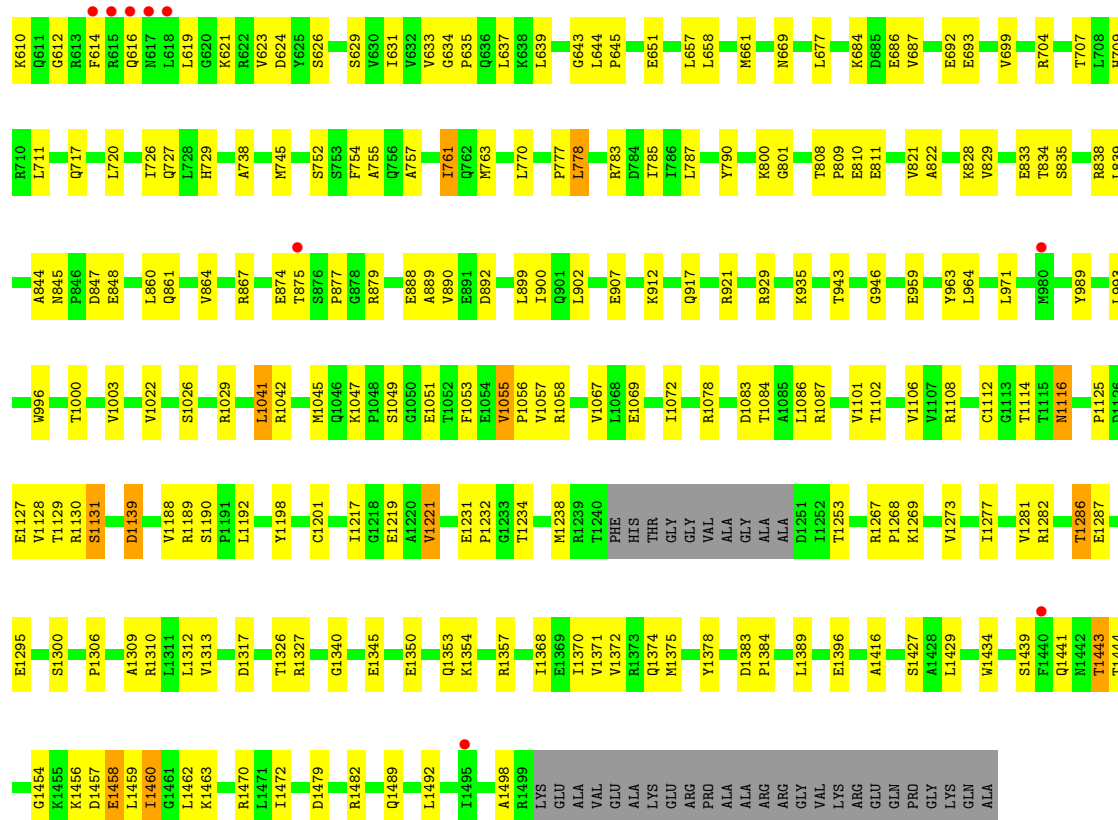
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	4	Total	O	0	0
			4	4		



• Molecule 3: DNA-directed RNA polymerase subunit beta'

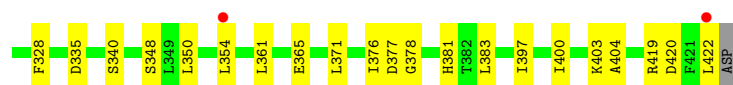
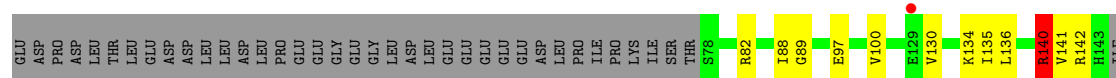
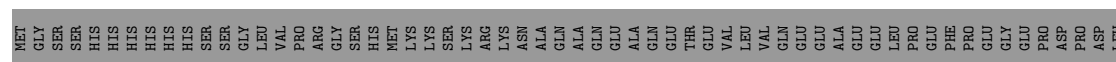




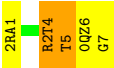
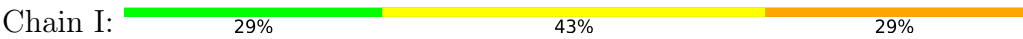
• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: RNA polymerase sigma factor



• Molecule 6: GE23077



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	236.57Å 236.57Å 252.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.97 – 3.35 38.97 – 3.35	Depositor EDS
% Data completeness (in resolution range)	98.9 (38.97-3.35) 98.9 (38.97-3.35)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 3.32Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, R_{free}	0.214 , 0.242 0.215 , 0.241	Depositor DCC
R_{free} test set	2266 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	126.0	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 83.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.032 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26552	wwPDB-VP
Average B, all atoms (Å ²)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% 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: 2RA, R2T, MG, 0QZ, ZN, MB8, 2TL, DSN, DVA, FGL

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	0.32	0/1809	0.84	5/2461 (0.2%)
1	B	0.31	0/1781	0.83	2/2426 (0.1%)
2	C	0.33	0/8841	0.81	9/11956 (0.1%)
3	D	0.34	0/10966	0.80	6/14820 (0.0%)
4	E	0.28	0/768	0.72	0/1035
5	F	0.29	0/2797	0.76	1/3761 (0.0%)
All	All	0.32	0/26962	0.80	23/36459 (0.1%)

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
6	I	0	1

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1058	ASP	N-CA-C	6.93	120.62	111.75
2	C	1078	GLU	CA-C-N	6.91	127.29	119.83
2	C	1078	GLU	C-N-CA	6.91	127.29	119.83
2	C	792	VAL	CA-C-N	6.51	124.42	119.66
2	C	792	VAL	C-N-CA	6.51	124.42	119.66
1	A	186	LEU	N-CA-C	-6.47	105.38	113.28
1	A	172	SER	CA-C-N	6.33	125.95	119.56
1	A	172	SER	C-N-CA	6.33	125.95	119.56
1	B	48	ILE	CA-C-N	6.17	126.08	119.85
1	B	48	ILE	C-N-CA	6.17	126.08	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1340	GLY	CA-C-N	5.73	125.10	118.85
3	D	1340	GLY	C-N-CA	5.73	125.10	118.85
2	C	70	GLU	N-CA-C	5.59	115.49	108.45
3	D	1128	VAL	N-CA-C	-5.55	100.60	109.20
5	F	140	ARG	N-CA-C	-5.53	106.53	113.72
2	C	496	ILE	N-CA-C	5.35	115.28	107.37
2	C	187	ASN	CB-CA-C	-5.33	110.41	116.54
1	A	91	ASN	CA-C-N	5.21	124.87	119.56
1	A	91	ASN	C-N-CA	5.21	124.87	119.56
2	C	1057	SER	N-CA-C	5.19	117.37	109.63
3	D	51	GLY	CA-C-N	5.08	124.84	119.76
3	D	51	GLY	C-N-CA	5.08	124.84	119.76
3	D	1458	GLU	N-CA-C	-5.02	102.27	110.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	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	1777	0	1826	32	0
1	B	1750	0	1794	35	0
2	C	8677	0	8791	170	0
3	D	10781	0	10998	221	0
4	E	754	0	769	17	0
5	F	2754	0	2826	42	0
6	I	50	0	37	2	0
7	D	2	0	0	0	0
8	D	1	0	0	0	0
9	I	2	0	0	0	0
10	D	4	0	0	0	0
All	All	26552	0	27041	463	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 9.

All (463) 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)
1:B:104:GLU:HB2	1:B:137:ARG:HA	1.60	0.82
2:C:102:HIS:HB3	2:C:105:THR:HB	1.65	0.77
3:D:508:ARG:HD3	3:D:509:PRO:HD2	1.66	0.77
3:D:693:GLU:HA	4:E:48:MET:HE1	1.68	0.74
2:C:904:PRO:HB2	2:C:907:ASP:HB3	1.69	0.73
3:D:95:LEU:HD11	3:D:517:VAL:HG23	1.70	0.73
3:D:1087:ARG:NH1	3:D:1234:THR:O	2.22	0.72
2:C:1015:LEU:HA	5:F:335:ASP:HB2	1.72	0.71
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.73	0.71
3:D:1130:ARG:HH22	3:D:1313:VAL:HA	1.57	0.70
2:C:173:ASP:HB2	2:C:185:LYS:HB3	1.75	0.69
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.74	0.68
1:B:22:GLU:HG2	1:B:198:ARG:HG2	1.75	0.68
5:F:136:LEU:HB3	5:F:140:ARG:HD3	1.74	0.68
3:D:889:ALA:O	3:D:929:ARG:NH1	2.27	0.68
2:C:162:ILE:HB	2:C:172:ILE:HB	1.77	0.67
5:F:261:PRO:HG2	5:F:264:MET:HG3	1.76	0.67
3:D:711:LEU:HD22	3:D:778:LEU:HD23	1.76	0.67
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.77	0.66
5:F:397:ILE:HD12	5:F:400:ILE:HD11	1.76	0.66
3:D:19:ARG:NH1	3:D:94:GLU:OE2	2.28	0.66
1:A:215:VAL:HG13	1:B:222:LEU:HD22	1.78	0.66
5:F:135:ILE:HD11	5:F:178:ARG:HB3	1.78	0.65
2:C:428:ARG:HH21	2:C:451:LEU:HD11	1.61	0.65
3:D:1101:VAL:HG23	3:D:1102:THR:HG23	1.78	0.65
2:C:23:VAL:HA	2:C:121:MET:HE1	1.79	0.64
3:D:1219:GLU:HG2	3:D:1221:VAL:HG23	1.80	0.64
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.79	0.64
2:C:53:PRO:O	2:C:265:ARG:NH2	2.29	0.64
3:D:612:GLY:O	3:D:616:GLN:N	2.28	0.64
2:C:229:MET:HE2	2:C:233:GLU:HB3	1.80	0.63
3:D:875:THR:HG21	3:D:902:LEU:HG	1.80	0.63
3:D:657:LEU:HG	3:D:661:MET:HE2	1.79	0.63
1:B:58:ILE:HB	1:B:61:VAL:HB	1.80	0.63
4:E:83:ASP:OD1	4:E:83:ASP:N	2.32	0.63
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.79	0.62
3:D:828:LYS:HG2	3:D:833:GLU:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:LEU:HA	1:B:48:ILE:HD13	1.80	0.62
2:C:1008:ARG:NH1	2:C:1027:PHE:O	2.31	0.62
2:C:22:GLN:HG3	2:C:407:LYS:HB3	1.82	0.62
2:C:711:GLU:O	2:C:758:ARG:NH1	2.31	0.62
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.82	0.62
3:D:349:PRO:HB3	5:F:97:GLU:HG2	1.81	0.61
3:D:1498:ALA:HB1	4:E:84:ARG:HH11	1.63	0.61
2:C:280:LYS:HE3	2:C:309:TYR:HE2	1.66	0.61
2:C:305:PRO:HA	2:C:308:ARG:HG2	1.82	0.61
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.81	0.61
2:C:143:SER:HB3	2:C:332:ARG:HB2	1.82	0.61
1:B:206:THR:HG22	1:B:209:GLU:H	1.66	0.61
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.83	0.60
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.36	0.60
3:D:844:ALA:HB1	3:D:867:ARG:HH21	1.65	0.60
2:C:21:ILE:HD12	2:C:21:ILE:H	1.67	0.60
2:C:1083:GLU:OE2	3:D:87:ARG:NH1	2.35	0.60
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.83	0.59
2:C:263:ASP:OD2	2:C:266:ARG:N	2.20	0.59
1:A:58:ILE:HG12	1:A:140:MET:HG2	1.85	0.58
3:D:7:LYS:HG2	3:D:1458:GLU:HG3	1.85	0.58
1:A:198:ARG:NH2	2:C:932:GLU:OE1	2.36	0.57
5:F:232:ARG:HH11	5:F:232:ARG:HB2	1.69	0.57
2:C:15:LEU:O	2:C:586:ARG:NH2	2.37	0.57
3:D:94:GLU:O	3:D:551:ASN:ND2	2.37	0.57
1:B:216:GLU:OE1	1:B:219:ARG:NH2	2.29	0.57
3:D:363:ALA:HA	3:D:381:ALA:HA	1.87	0.57
5:F:160:ASP:OD1	5:F:178:ARG:NH2	2.37	0.57
3:D:890:VAL:HG23	3:D:892:ASP:H	1.70	0.56
3:D:838:ARG:NH1	3:D:874:GLU:OE1	2.39	0.56
2:C:758:ARG:HH21	2:C:788:THR:HB	1.69	0.56
2:C:1115:LEU:HB3	3:D:85:VAL:HG12	1.88	0.56
2:C:151:ASP:HB2	2:C:159:ILE:HG13	1.88	0.55
3:D:102:ILE:HD11	3:D:587:ARG:HB3	1.87	0.55
3:D:411:THR:HB	3:D:437:VAL:H	1.71	0.55
1:A:83:LYS:NZ	2:C:698:ASP:OD2	2.40	0.55
1:B:220:GLU:O	1:B:223:THR:OG1	2.20	0.55
2:C:958:THR:HG23	2:C:961:GLU:H	1.71	0.55
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.88	0.55
2:C:644:VAL:HG22	2:C:645:VAL:H	1.71	0.55
3:D:536:ALA:HA	5:F:315:VAL:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:512:ARG:HB3	2:C:523:ILE:HD11	1.89	0.55
3:D:558:LEU:HD23	3:D:567:ILE:HD12	1.90	0.54
3:D:899:LEU:HD22	3:D:917:GLN:HB3	1.88	0.54
1:B:176:ARG:NH2	3:D:888:GLU:OE2	2.40	0.54
2:C:141:HIS:ND1	2:C:142:ARG:O	2.41	0.54
2:C:207:LEU:HD23	2:C:221:LEU:HD13	1.88	0.54
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.90	0.54
3:D:208:PRO:HA	3:D:389:GLU:O	2.08	0.54
2:C:203:ASP:OD2	2:C:204:GLN:N	2.41	0.54
3:D:770:LEU:HA	3:D:777:PRO:HA	1.90	0.54
3:D:808:THR:HB	3:D:811:GLU:HG3	1.89	0.53
1:A:128:HIS:CE1	1:A:131:THR:HG23	2.43	0.53
3:D:658:LEU:HA	3:D:661:MET:HE3	1.91	0.53
3:D:39:PRO:HG3	3:D:47:GLU:HG3	1.91	0.53
3:D:634:GLY:HA3	3:D:637:LEU:HD12	1.89	0.53
4:E:37:ASN:HD22	4:E:89:MET:HE1	1.73	0.53
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.90	0.53
4:E:46:PRO:HG3	4:E:66:LYS:HD3	1.90	0.53
3:D:835:SER:HB3	3:D:838:ARG:HB2	1.90	0.53
1:B:51:THR:OG1	1:B:87:VAL:O	2.25	0.53
2:C:32:ALA:HB2	2:C:73:LEU:HD12	1.91	0.53
2:C:987:ILE:HD11	3:D:946:GLY:HA2	1.90	0.53
2:C:270:GLY:O	2:C:274:ARG:N	2.38	0.53
2:C:124:ASP:HA	2:C:592:LEU:HD21	1.90	0.53
2:C:784:ASP:OD1	2:C:784:ASP:N	2.42	0.53
3:D:65:ARG:HG2	5:F:376:ILE:HD12	1.90	0.53
5:F:256:ARG:NH1	5:F:311:ALA:O	2.35	0.53
5:F:130:VAL:HG21	5:F:159:ILE:HG21	1.91	0.52
2:C:365:ASP:OD1	2:C:365:ASP:N	2.41	0.52
2:C:1030:GLN:HB2	3:D:626:SER:HB2	1.92	0.52
3:D:614:PHE:HB3	3:D:1439:SER:HA	1.90	0.52
3:D:709:HIS:HD2	3:D:711:LEU:H	1.56	0.52
5:F:181:GLU:OE2	5:F:184:ARG:NH1	2.35	0.52
2:C:202:TYR:OH	2:C:300:ASP:O	2.25	0.52
2:C:236:ILE:HG23	2:C:248:PRO:HB3	1.91	0.52
4:E:39:VAL:O	4:E:72:ARG:NH1	2.42	0.52
2:C:187:ASN:N	2:C:187:ASN:OD1	2.43	0.52
3:D:907:GLU:HB2	3:D:1026:SER:HA	1.92	0.52
2:C:239:PHE:CZ	2:C:256:TYR:HB3	2.45	0.52
2:C:751:PRO:HB3	2:C:794:PRO:HA	1.91	0.52
3:D:809:PRO:HB3	3:D:839:LEU:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.93	0.51
2:C:550:LEU:HB3	2:C:905:ILE:HG22	1.91	0.51
3:D:181:ASP:CG	3:D:205:TYR:HB3	2.36	0.51
2:C:17:PRO:HB2	2:C:20:GLU:HB2	1.92	0.51
3:D:1310:ARG:HD2	3:D:1327:ARG:HD2	1.92	0.51
3:D:684:LYS:HB3	3:D:687:VAL:HG23	1.92	0.51
2:C:984:GLU:O	3:D:946:GLY:HA3	2.10	0.51
3:D:989:TYR:CZ	3:D:993:LEU:HD11	2.46	0.51
1:A:55:SER:HB3	1:A:143:ARG:HB3	1.92	0.51
1:A:89:PHE:HB2	1:A:146:ARG:HH21	1.74	0.51
2:C:474:VAL:HG12	2:C:479:VAL:HG13	1.93	0.51
4:E:52:GLU:OE1	4:E:52:GLU:N	2.44	0.51
2:C:105:THR:HG22	2:C:107:LEU:HD13	1.93	0.50
2:C:134:ARG:NH2	2:C:392:SER:O	2.44	0.50
2:C:1054:THR:HG21	2:C:1079:PRO:CB	2.41	0.50
3:D:469:ASP:HB3	3:D:472:ALA:HB3	1.91	0.50
3:D:709:HIS:CD2	3:D:711:LEU:HB2	2.45	0.50
3:D:67:ARG:NH2	5:F:377:ASP:OD1	2.31	0.50
3:D:834:THR:HG23	3:D:838:ARG:HD2	1.93	0.50
3:D:1087:ARG:HG2	3:D:1238:MET:HE2	1.92	0.50
2:C:41:ASN:HD21	2:C:49:ARG:HG2	1.77	0.50
2:C:368:THR:H	2:C:371:LYS:HD2	1.77	0.50
5:F:136:LEU:HB3	5:F:140:ARG:CD	2.42	0.50
2:C:944:LEU:HD11	2:C:963:LEU:HG	1.92	0.50
3:D:808:THR:HG22	3:D:810:GLU:H	1.76	0.50
3:D:1084:THR:HG22	3:D:1087:ARG:NH2	2.27	0.50
3:D:1372:VAL:HA	3:D:1375:MET:HE3	1.93	0.50
2:C:197:LEU:HD13	2:C:207:LEU:HD21	1.93	0.50
2:C:261:ILE:HG23	2:C:290:LEU:HB2	1.93	0.50
1:B:74:ASP:N	1:B:74:ASP:OD1	2.40	0.50
2:C:408:ARG:NH2	2:C:456:ALA:O	2.45	0.50
3:D:879:ARG:HD3	3:D:902:LEU:O	2.12	0.50
3:D:1306:PRO:HG2	3:D:1309:ALA:HB2	1.94	0.50
2:C:68:PHE:HA	2:C:98:LEU:HG	1.93	0.50
2:C:872:ASN:OD1	2:C:873:PRO:HD2	2.11	0.50
2:C:897:LEU:HG	2:C:921:ALA:HB2	1.94	0.50
3:D:1057:VAL:HG13	3:D:1069:GLU:CD	2.37	0.50
3:D:1479:ASP:OD2	3:D:1482:ARG:NH2	2.40	0.50
3:D:141:ILE:HA	3:D:146:PRO:HA	1.94	0.49
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.93	0.49
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:239:PHE:HZ	2:C:256:TYR:HB3	1.77	0.49
1:A:186:LEU:HD23	1:A:188:GLN:H	1.77	0.49
2:C:1086:ARG:NH1	3:D:88:TYR:OH	2.40	0.49
3:D:1312:LEU:HD13	3:D:1327:ARG:HG2	1.94	0.49
3:D:30:GLU:OE2	5:F:259:ARG:NH1	2.44	0.49
3:D:138:LYS:HB2	3:D:452:ILE:HA	1.94	0.49
1:A:150:TYR:CD1	2:C:696:LYS:HG2	2.48	0.49
2:C:212:GLY:HA2	2:C:218:VAL:HB	1.95	0.49
2:C:762:LYS:HD3	2:C:786:LYS:HD3	1.93	0.49
2:C:806:LEU:HB3	2:C:813:VAL:HG21	1.94	0.49
3:D:847:ASP:OD1	3:D:847:ASP:N	2.45	0.49
3:D:1459:LEU:HB2	3:D:1470:ARG:HH21	1.77	0.49
4:E:40:LEU:HG	4:E:67:GLU:HG2	1.93	0.49
2:C:879:ARG:HH11	3:D:1029:ARG:HH21	1.60	0.49
3:D:198:ARG:HD2	3:D:199:LEU:HG	1.95	0.49
3:D:1045:MET:HB2	3:D:1072:ILE:HG22	1.95	0.49
3:D:1000:THR:HA	3:D:1041:LEU:HD21	1.95	0.49
3:D:350:HIS:HD2	5:F:100:VAL:HG21	1.77	0.48
3:D:699:VAL:HG12	3:D:717:GLN:HB3	1.94	0.48
3:D:1378:TYR:CE2	3:D:1396:GLU:HG2	2.48	0.48
3:D:574:LEU:O	3:D:578:VAL:HG23	2.13	0.48
3:D:64:LYS:HB2	5:F:378:GLY:HA3	1.95	0.48
3:D:1192:LEU:HD22	3:D:1345:GLU:OE2	2.13	0.48
2:C:954:THR:OG1	2:C:965:GLU:OE2	2.31	0.48
2:C:239:PHE:CZ	2:C:253:ALA:HA	2.48	0.48
2:C:679:PHE:HA	3:D:943:THR:HG23	1.96	0.48
3:D:1372:VAL:HG22	3:D:1375:MET:HE3	1.96	0.48
1:B:68:ILE:HB	1:B:71:VAL:HB	1.96	0.48
2:C:290:LEU:HD22	2:C:302:VAL:HG11	1.95	0.48
3:D:39:PRO:HB2	3:D:46:ASP:HA	1.96	0.48
3:D:353:VAL:HG12	3:D:368:VAL:HG22	1.96	0.48
2:C:713:ARG:HA	2:C:819:VAL:HA	1.96	0.48
2:C:774:LEU:HD22	5:F:350:LEU:HD11	1.94	0.48
1:A:213:GLN:O	1:A:217:ILE:HG13	2.14	0.47
2:C:1031:ARG:HD3	3:D:619:LEU:HG	1.96	0.47
3:D:474:GLU:O	3:D:478:LEU:HB2	2.14	0.47
2:C:919:ALA:HB2	2:C:968:LEU:HD21	1.95	0.47
3:D:661:MET:HE1	3:D:677:LEU:HD11	1.95	0.47
2:C:971:LYS:HB3	2:C:986:PRO:HB2	1.96	0.47
2:C:1051:GLU:OE1	3:D:752:SER:OG	2.27	0.47
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:560:GLN:O	5:F:184:ARG:NH2	2.38	0.47
3:D:959:GLU:HB3	3:D:963:TYR:CE2	2.50	0.47
3:D:1106:VAL:O	3:D:1108:ARG:HG3	2.14	0.47
3:D:1112:CYS:HB3	3:D:1201:CYS:HB3	1.97	0.47
3:D:1434:TRP:CD1	3:D:1457:ASP:HB2	2.49	0.47
3:D:1460:ILE:H	3:D:1460:ILE:HG13	1.56	0.47
2:C:150:PRO:HB3	2:C:158:TYR:HD1	1.79	0.47
2:C:313:LEU:HG	2:C:320:HIS:HB3	1.96	0.47
2:C:492:ASP:HB3	2:C:518:LYS:HD3	1.96	0.47
2:C:249:LYS:HG3	2:C:251:ASP:OD2	2.14	0.47
3:D:111:LYS:HA	3:D:114:THR:HB	1.96	0.47
3:D:187:LYS:HB2	3:D:200:ASP:HB2	1.97	0.47
3:D:629:SER:HB3	3:D:726:ILE:HG13	1.96	0.47
3:D:639:LEU:HA	3:D:729:HIS:CD2	2.50	0.47
3:D:684:LYS:HG3	3:D:686:GLU:H	1.80	0.47
3:D:709:HIS:ND1	3:D:1231:GLU:HG3	2.30	0.47
3:D:801:GLY:HA2	3:D:821:VAL:HG13	1.95	0.47
2:C:100:LEU:HB2	2:C:369:PRO:HG3	1.96	0.47
2:C:754:ILE:HG13	2:C:791:ARG:HG2	1.97	0.47
2:C:833:LEU:HD21	2:C:839:LEU:HD11	1.97	0.47
4:E:47:LYS:NZ	4:E:56:ASP:OD1	2.47	0.47
5:F:228:GLU:HG3	5:F:231:ARG:HH21	1.79	0.47
1:A:14:ARG:HG2	1:B:231:ALA:HB3	1.97	0.47
1:A:211:LEU:O	1:A:215:VAL:HG23	2.15	0.47
1:B:24:VAL:HG22	1:B:196:THR:HG23	1.96	0.47
3:D:114:THR:HG21	3:D:498:VAL:HG21	1.96	0.47
5:F:89:GLY:HA2	5:F:193:ARG:HH21	1.80	0.47
2:C:516:ARG:HA	2:C:520:GLU:O	2.14	0.46
1:A:63:HIS:O	1:A:66:SER:OG	2.30	0.46
4:E:46:PRO:HD2	4:E:63:TRP:CZ2	2.50	0.46
3:D:374:GLU:HG3	3:D:375:GLU:H	1.81	0.46
3:D:1429:LEU:HD21	3:D:1441:GLN:NE2	2.30	0.46
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.50	0.46
3:D:860:LEU:HA	3:D:877:PRO:HB2	1.97	0.46
1:A:209:GLU:O	1:A:213:GLN:HG2	2.16	0.46
2:C:567:GLN:HB2	2:C:997:LEU:HD22	1.98	0.46
2:C:690:ILE:HB	2:C:694:LEU:HD12	1.97	0.46
2:C:1054:THR:HG21	2:C:1079:PRO:HB2	1.98	0.46
2:C:258:TYR:O	2:C:263:ASP:N	2.48	0.46
2:C:672:VAL:HB	2:C:868:ASP:HB2	1.98	0.46
3:D:155:ASP:O	3:D:159:ARG:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1198:TYR:OH	3:D:1396:GLU:OE1	2.23	0.46
1:B:64:GLU:HG2	1:B:76:VAL:HG22	1.97	0.46
2:C:943:VAL:HG11	2:C:973:VAL:HG22	1.98	0.46
3:D:900:ILE:HD13	3:D:902:LEU:HD13	1.98	0.46
3:D:964:LEU:HD21	3:D:1058:ARG:HD2	1.98	0.46
3:D:1368:ILE:HD12	3:D:1368:ILE:H	1.80	0.46
5:F:208:SER:HB3	5:F:211:ASP:OD2	2.15	0.46
5:F:371:LEU:O	5:F:381:HIS:ND1	2.44	0.46
2:C:1090:LYS:HE2	2:C:1112:PHE:CZ	2.51	0.46
3:D:65:ARG:HG3	3:D:67:ARG:H	1.81	0.45
3:D:1353:GLN:O	3:D:1357:ARG:HG3	2.16	0.45
2:C:926:PHE:HE2	2:C:960:GLU:HG2	1.81	0.45
3:D:128:TYR:OH	3:D:579:ASP:OD2	2.33	0.45
3:D:350:HIS:CD2	5:F:100:VAL:HG21	2.51	0.45
2:C:267:TYR:CE2	2:C:290:LEU:HG	2.52	0.45
2:C:344:PHE:HD2	2:C:382:ILE:HD11	1.81	0.45
1:B:153:ALA:HB1	1:B:166:PRO:HB2	1.99	0.45
2:C:773:LEU:HD11	5:F:354:LEU:HD22	1.99	0.45
2:C:744:ARG:HG3	2:C:747:ALA:HB2	1.99	0.45
3:D:529:GLN:HB3	3:D:535:PHE:CE2	2.52	0.45
3:D:1383:ASP:HB3	3:D:1416:ALA:HB3	1.99	0.45
3:D:584:ASN:HB2	3:D:602:SER:HB3	1.99	0.45
2:C:124:ASP:HB3	2:C:592:LEU:HD11	1.97	0.45
2:C:157:ARG:HA	2:C:157:ARG:HD3	1.66	0.45
3:D:669:ASN:HD21	5:F:420:ASP:CG	2.24	0.45
3:D:1217:ILE:HD12	3:D:1217:ILE:H	1.82	0.45
2:C:954:THR:HA	2:C:955:PRO:HD3	1.87	0.45
2:C:1056:LYS:HA	3:D:624:ASP:HB2	1.98	0.45
3:D:10:ILE:O	3:D:1454:GLY:HA2	2.16	0.45
3:D:417:PRO:HG3	3:D:431:VAL:HA	1.99	0.45
3:D:1139:ASP:N	3:D:1139:ASP:OD1	2.49	0.45
2:C:548:PRO:O	2:C:843:HIS:HE1	2.00	0.45
2:C:728:HIS:ND1	5:F:422:LEU:HG	2.32	0.45
3:D:1498:ALA:O	4:E:84:ARG:NH1	2.50	0.45
4:E:13:VAL:HG21	4:E:19:LEU:HB2	1.98	0.45
2:C:905:ILE:C	2:C:907:ASP:H	2.25	0.45
3:D:134:VAL:HG12	3:D:454:ALA:HB2	1.99	0.45
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.98	0.45
1:A:115:LEU:HA	1:A:116:PRO:HD3	1.81	0.44
2:C:541:SER:OG	2:C:542:VAL:N	2.50	0.44
3:D:567:ILE:HG13	5:F:140:ARG:NH2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:428:ARG:O	3:D:1078:ARG:NH1	2.50	0.44
2:C:431:HIS:H	2:C:434:HIS:CE1	2.36	0.44
2:C:944:LEU:HD21	2:C:963:LEU:HD23	1.98	0.44
3:D:1049:SER:OG	3:D:1051:GLU:HG2	2.17	0.44
2:C:712:ALA:O	2:C:820:ARG:N	2.51	0.44
2:C:1009:SER:HB3	3:D:651:GLU:O	2.18	0.44
3:D:8:VAL:HG12	3:D:1434:TRP:HZ2	1.82	0.44
3:D:1130:ARG:NH2	3:D:1317:ASP:OD2	2.50	0.44
3:D:132:TYR:CE2	3:D:456:MET:HE3	2.52	0.44
3:D:790:TYR:CD2	3:D:1022:VAL:HG13	2.53	0.44
4:E:46:PRO:HD2	4:E:63:TRP:CE2	2.52	0.44
1:A:57:TYR:CD1	1:A:161:ARG:HD3	2.53	0.44
2:C:251:ASP:OD2	2:C:251:ASP:N	2.51	0.44
3:D:108:VAL:HB	3:D:109:PRO:HD3	1.98	0.44
3:D:135:LEU:O	3:D:149:LYS:NZ	2.41	0.44
3:D:785:ILE:HD13	3:D:935:LYS:HA	2.00	0.44
3:D:1372:VAL:HA	3:D:1375:MET:HG3	1.99	0.44
1:A:222:LEU:HD22	1:B:215:VAL:HG13	1.98	0.44
2:C:874:LEU:HD11	3:D:787:LEU:HD22	1.98	0.44
3:D:631:ILE:HG22	3:D:726:ILE:HB	1.98	0.44
3:D:1253:THR:HG23	3:D:1269:LYS:HG3	1.98	0.44
3:D:1489:GLN:HG2	3:D:1492:LEU:HD13	1.99	0.44
1:A:42:ARG:NH2	1:B:34:VAL:HB	2.33	0.44
1:B:13:VAL:HG22	1:B:23:PHE:HD1	1.83	0.44
2:C:470:PRO:HB2	2:C:534:VAL:HG21	1.99	0.44
2:C:521:PRO:HB2	3:D:1055:VAL:HG11	2.00	0.44
3:D:861:GLN:OE1	3:D:861:GLN:N	2.48	0.44
4:E:57:ASP:HA	4:E:58:PRO:HD3	1.90	0.44
5:F:318:GLU:HA	5:F:328:PHE:HB3	2.00	0.44
1:A:196:THR:HG21	2:C:934:PHE:HE1	1.83	0.44
3:D:1463:LYS:HE3	3:D:1463:LYS:HB2	1.88	0.44
1:B:110:LYS:HD3	1:B:126:ASP:HA	2.00	0.43
2:C:626:ARG:HD3	2:C:629:TYR:CD2	2.53	0.43
2:C:846:LYS:NZ	6:I:4:R2T:HG2	2.33	0.43
3:D:693:GLU:HG2	4:E:48:MET:HE1	1.99	0.43
3:D:1459:LEU:HD12	3:D:1470:ARG:HH21	1.83	0.43
2:C:575:GLN:HG3	2:C:670:GLN:NE2	2.32	0.43
3:D:1286:THR:HG22	3:D:1287:GLU:H	1.82	0.43
3:D:1462:LEU:HD22	3:D:1472:ILE:HB	2.00	0.43
2:C:587:VAL:HG11	2:C:666:LEU:HD22	2.01	0.43
3:D:22:SER:HB3	3:D:92:HIS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:864:VAL:HG22	3:D:877:PRO:HD3	2.01	0.43
1:A:218:LEU:HD23	1:B:222:LEU:HD21	2.00	0.43
1:B:30:ARG:NH2	2:C:854:PRO:HB3	2.34	0.43
3:D:1114:THR:OG1	3:D:1116:ASN:OD1	2.31	0.43
3:D:1231:GLU:HB3	3:D:1232:PRO:HD3	2.01	0.43
3:D:1370:ILE:O	3:D:1374:GLN:HG2	2.18	0.43
3:D:1384:PRO:HB3	3:D:1389:LEU:O	2.19	0.43
1:B:91:ASN:HA	1:B:92:PRO:HD3	1.88	0.43
1:B:99:LEU:HD23	1:B:114:PHE:HB3	2.00	0.43
1:B:226:SER:O	1:B:228:PRO:HD3	2.19	0.43
2:C:557:ARG:CZ	2:C:879:ARG:HD2	2.48	0.43
2:C:1054:THR:O	2:C:1059:ASP:HB3	2.19	0.43
1:B:43:ILE:HG23	1:B:47:SER:HB2	2.01	0.43
2:C:792:VAL:HA	2:C:793:PRO:HD3	1.90	0.43
3:D:17:LYS:O	3:D:20:SER:OG	2.34	0.43
3:D:899:LEU:HD21	3:D:921:ARG:HG3	2.00	0.43
1:B:91:ASN:HB3	1:B:94:LEU:HG	2.01	0.43
2:C:177:GLU:HB3	2:C:178:PRO:HD2	2.00	0.43
2:C:627:ARG:NH1	2:C:638:ASP:OD2	2.52	0.43
2:C:1053:LEU:O	3:D:621:LYS:NZ	2.52	0.43
3:D:176:ASP:OD1	3:D:177:ALA:N	2.51	0.43
3:D:209:ARG:HH12	3:D:349:PRO:HD3	1.83	0.43
3:D:1281:VAL:HG21	3:D:1313:VAL:HG21	1.99	0.43
1:A:72:LYS:HA	2:C:607:ASP:HA	2.01	0.43
1:B:138:LEU:HD21	1:B:140:MET:HE3	2.00	0.43
2:C:35:PRO:HA	2:C:36:PRO:HD3	1.88	0.43
3:D:67:ARG:HD3	5:F:376:ILE:HD11	2.00	0.43
3:D:115:LEU:HD23	3:D:115:LEU:HA	1.81	0.43
3:D:1086:LEU:HD22	3:D:1238:MET:HE3	2.01	0.43
2:C:70:GLU:HG2	2:C:97:ARG:HB2	2.00	0.43
1:A:174:VAL:HA	1:A:201:THR:HG22	2.01	0.42
3:D:757:ALA:O	3:D:761:ILE:HG12	2.18	0.42
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.83	0.42
3:D:65:ARG:HD3	3:D:66:GLN:H	1.84	0.42
3:D:207:PHE:O	3:D:390:PRO:HA	2.18	0.42
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.54	0.42
3:D:1350:GLU:O	3:D:1354:LYS:HG3	2.20	0.42
5:F:223:ALA:HB2	5:F:242:TRP:HB2	2.01	0.42
2:C:209:ARG:HG3	2:C:210:GLU:H	1.83	0.42
2:C:1021:LEU:HD12	2:C:1022:GLY:H	1.84	0.42
5:F:152:ASP:OD1	5:F:152:ASP:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:633:VAL:HG22	3:D:635:PRO:HD3	2.01	0.42
3:D:761:ILE:HG12	3:D:761:ILE:H	1.73	0.42
1:A:99:LEU:HD23	1:A:114:PHE:CG	2.54	0.42
1:B:213:GLN:O	1:B:217:ILE:HG13	2.19	0.42
2:C:124:ASP:OD2	2:C:395:LYS:NZ	2.45	0.42
2:C:329:GLY:HA3	2:C:489:THR:HG23	2.01	0.42
2:C:829:GLN:NE2	2:C:831:ARG:HH21	2.17	0.42
3:D:601:ARG:HH11	3:D:610:LYS:HD2	1.85	0.42
3:D:1116:ASN:OD1	3:D:1116:ASN:N	2.52	0.42
1:B:34:VAL:HG11	2:C:978:ARG:HB3	2.02	0.42
2:C:122:THR:OG1	2:C:124:ASP:OD1	2.33	0.42
3:D:95:LEU:HA	3:D:551:ASN:HD21	1.84	0.42
5:F:292:ALA:HB2	5:F:301:ALA:HA	2.01	0.42
3:D:964:LEU:HD11	3:D:1058:ARG:HD2	2.00	0.42
1:A:85:LEU:HD22	1:A:87:VAL:HG23	2.02	0.42
2:C:272:ALA:O	2:C:276:LYS:HG2	2.19	0.42
2:C:344:PHE:CD2	2:C:378:LEU:HD11	2.55	0.42
2:C:420:ARG:H	2:C:420:ARG:HG2	1.54	0.42
3:D:106:LYS:O	3:D:586:ARG:NH1	2.52	0.42
3:D:1047:LYS:HG2	3:D:1053:PHE:CD1	2.55	0.42
4:E:45:ARG:HA	4:E:46:PRO:HD3	1.93	0.42
1:B:8:ALA:HA	1:B:9:PRO:HD3	1.84	0.42
2:C:444:PRO:HB3	6:I:1:2RA:HA	2.02	0.42
2:C:580:MET:HB3	2:C:584:GLU:CD	2.45	0.42
3:D:30:GLU:HB3	3:D:40:GLU:HG3	2.01	0.42
3:D:1083:ASP:O	3:D:1087:ARG:HG3	2.20	0.42
3:D:1273:VAL:H	3:D:1326:THR:HG1	1.66	0.42
1:A:83:LYS:HE2	1:A:168:ASP:HB2	2.02	0.41
2:C:436:GLY:H	2:C:539:VAL:HG23	1.85	0.41
2:C:578:VAL:HG23	2:C:579:VAL:HG23	2.01	0.41
2:C:966:LEU:HD22	2:C:986:PRO:HG3	2.01	0.41
3:D:637:LEU:O	3:D:935:LYS:NZ	2.53	0.41
3:D:1047:LYS:HD2	3:D:1051:GLU:HG3	2.02	0.41
1:B:86:VAL:HB	1:B:123:MET:HB2	2.01	0.41
2:C:243:ARG:HA	2:C:244:PRO:HD3	1.78	0.41
2:C:1097:LEU:HD11	3:D:103:TRP:CZ3	2.55	0.41
3:D:371:ILE:HG13	3:D:372:ASP:H	1.85	0.41
3:D:692:GLU:HG2	3:D:720:LEU:HD12	2.01	0.41
3:D:704:ARG:HB2	3:D:745:MET:HE2	2.01	0.41
3:D:31:THR:HB	3:D:527:MET:HE3	2.02	0.41
3:D:205:TYR:H	3:D:205:TYR:HD2	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:566:ILE:HD11	5:F:192:LEU:HD21	2.02	0.41
3:D:1125:PRO:HA	3:D:1131:SER:O	2.21	0.41
5:F:258:ILE:H	5:F:258:ILE:HG13	1.52	0.41
1:B:105:GLY:O	1:B:107:LYS:N	2.53	0.41
2:C:966:LEU:HD13	2:C:986:PRO:HB3	2.01	0.41
2:C:1040:LEU:HD23	2:C:1040:LEU:HA	1.93	0.41
3:D:169:TYR:HA	3:D:170:PRO:HD3	1.87	0.41
3:D:1443:THR:H	3:D:1443:THR:HG23	1.55	0.41
2:C:543:ASN:ND2	2:C:566:THR:HG22	2.35	0.41
2:C:1056:LYS:HB3	3:D:623:VAL:HG13	2.02	0.41
3:D:541:ASN:O	3:D:545:ARG:HG3	2.21	0.41
3:D:596:SER:OG	3:D:598:ARG:HG2	2.21	0.41
3:D:1267:ARG:HA	3:D:1268:PRO:HD3	1.84	0.41
3:D:214:GLU:HB3	3:D:340:THR:HB	2.01	0.41
3:D:1084:THR:HG22	3:D:1087:ARG:HH21	1.86	0.41
1:A:206:THR:HG22	1:A:208:LEU:H	1.86	0.41
1:B:70:GLY:HA3	1:B:136:GLY:HA2	2.03	0.41
2:C:954:THR:OG1	2:C:957:LYS:HD3	2.21	0.41
3:D:845:ASN:HB2	3:D:848:GLU:HB2	2.01	0.41
2:C:159:ILE:HG12	2:C:175:GLU:HG3	2.03	0.41
2:C:258:TYR:CD1	2:C:263:ASP:HB2	2.56	0.41
2:C:953:VAL:HG12	2:C:965:GLU:HB2	2.02	0.41
3:D:462:GLN:HB2	3:D:513:ILE:HG21	2.03	0.41
3:D:763:MET:HE2	3:D:763:MET:HB3	1.82	0.41
3:D:845:ASN:HB3	3:D:847:ASP:OD1	2.21	0.41
3:D:1282:ARG:NH2	3:D:1295:GLU:OE2	2.37	0.41
2:C:520:GLU:HA	2:C:521:PRO:HD3	1.86	0.41
3:D:6:ARG:HB2	3:D:6:ARG:HH11	1.86	0.41
3:D:470:LEU:HB3	3:D:503:LEU:HD23	2.03	0.41
3:D:493:ARG:O	3:D:497:GLU:HG3	2.21	0.41
4:E:35:PHE:HE2	4:E:63:TRP:CG	2.39	0.41
5:F:207:LEU:HD23	5:F:207:LEU:HA	1.86	0.41
1:A:111:ALA:HB3	1:A:125:PRO:HA	2.02	0.40
2:C:471:TYR:CD2	2:C:486:MET:HE2	2.56	0.40
2:C:943:VAL:HG21	2:C:973:VAL:HG13	2.03	0.40
3:D:428:LYS:HE2	3:D:428:LYS:HB3	1.88	0.40
3:D:1295:GLU:HG2	3:D:1300:SER:OG	2.22	0.40
1:A:183:ASP:OD1	1:A:183:ASP:N	2.54	0.40
2:C:842:ARG:HH21	2:C:887:GLU:CD	2.29	0.40
2:C:964:LYS:O	2:C:968:LEU:HG	2.22	0.40
3:D:527:MET:HE2	3:D:527:MET:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:704:ARG:HD2	3:D:738:ALA:HB2	2.04	0.40
3:D:752:SER:HB2	3:D:755:ALA:H	1.85	0.40
3:D:1102:THR:HG21	3:D:1371:VAL:HG22	2.03	0.40
5:F:209:PHE:HA	5:F:212:LEU:HD12	2.03	0.40
2:C:1097:LEU:HD13	3:D:10:ILE:HD11	2.03	0.40
3:D:478:LEU:HD12	3:D:478:LEU:HA	1.90	0.40
5:F:134:LYS:HD3	5:F:134:LYS:HA	1.78	0.40
1:A:97:VAL:HG12	1:A:99:LEU:HD12	2.03	0.40
2:C:249:LYS:O	2:C:252:LYS:N	2.54	0.40
3:D:132:TYR:CD2	3:D:456:MET:HE3	2.56	0.40
2:C:2:GLU:OE1	2:C:2:GLU:N	2.54	0.40
2:C:154:ARG:NH1	2:C:177:GLU:HA	2.36	0.40
2:C:181:VAL:HA	2:C:220:GLY:O	2.22	0.40
2:C:229:MET:HE1	2:C:237:ARG:HE	1.85	0.40
3:D:608:SER:HA	3:D:612:GLY:HA3	2.04	0.40
5:F:383:LEU:HD22	5:F:397:ILE:HG23	2.03	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	224/314 (71%)	223 (100%)	1 (0%)	0	100	100
1	B	220/314 (70%)	217 (99%)	3 (1%)	0	100	100
2	C	1094/1119 (98%)	1059 (97%)	35 (3%)	0	100	100
3	D	1359/1524 (89%)	1317 (97%)	41 (3%)	1 (0%)	48	76
4	E	91/99 (92%)	90 (99%)	1 (1%)	0	100	100
5	F	335/443 (76%)	328 (98%)	7 (2%)	0	100	100
All	All	3323/3813 (87%)	3234 (97%)	88 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	406	ASP

5.3.2 Protein sidechains [i](#)

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	197/272 (72%)	187 (95%)	10 (5%)	21	48
1	B	193/272 (71%)	186 (96%)	7 (4%)	31	56
2	C	926/941 (98%)	886 (96%)	40 (4%)	26	52
3	D	1155/1279 (90%)	1102 (95%)	53 (5%)	24	50
4	E	82/88 (93%)	80 (98%)	2 (2%)	43	62
5	F	295/388 (76%)	277 (94%)	18 (6%)	17	44
All	All	2848/3240 (88%)	2718 (95%)	130 (5%)	24	50

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	66	SER
1	A	67	THR
1	A	85	LEU
1	A	86	VAL
1	A	131	THR
1	A	162	ILE
1	A	170	VAL
1	A	186	LEU
1	A	206	THR
1	B	12	THR
1	B	73	GLU
1	B	74	ASP
1	B	104	GLU
1	B	107	LYS
1	B	204	SER

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Mol	Chain	Res	Type
1	B	206	THR
2	C	42	VAL
2	C	69	LEU
2	C	120	LEU
2	C	182	VAL
2	C	187	ASN
2	C	194	VAL
2	C	196	LEU
2	C	200	LEU
2	C	217	LEU
2	C	227	PHE
2	C	260	LEU
2	C	265	ARG
2	C	276	LYS
2	C	301	GLU
2	C	365	ASP
2	C	419	THR
2	C	420	ARG
2	C	421	GLU
2	C	443	THR
2	C	474	VAL
2	C	475	VAL
2	C	559	LEU
2	C	566	THR
2	C	603	VAL
2	C	617	ASP
2	C	620	LEU
2	C	670	GLN
2	C	723	THR
2	C	766	GLU
2	C	784	ASP
2	C	813	VAL
2	C	858	MET
2	C	905	ILE
2	C	937	ASP
2	C	954	THR
2	C	1017	THR
2	C	1059	ASP
2	C	1081	VAL
2	C	1115	LEU
2	C	1117	SER
3	D	10	ILE

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Mol	Chain	Res	Type
3	D	30	GLU
3	D	97	THR
3	D	111	LYS
3	D	112	ILE
3	D	114	THR
3	D	130	SER
3	D	135	LEU
3	D	136	ASP
3	D	202	VAL
3	D	353	VAL
3	D	371	ILE
3	D	387	LEU
3	D	388	HIS
3	D	400	VAL
3	D	406	ASP
3	D	407	VAL
3	D	411	THR
3	D	415	VAL
3	D	420	VAL
3	D	421	LEU
3	D	427	VAL
3	D	483	HIS
3	D	502	PHE
3	D	587	ARG
3	D	707	THR
3	D	754	PHE
3	D	761	ILE
3	D	778	LEU
3	D	783	ARG
3	D	829	VAL
3	D	912	LYS
3	D	971	LEU
3	D	1003	VAL
3	D	1041	LEU
3	D	1055	VAL
3	D	1067	VAL
3	D	1116	ASN
3	D	1127	GLU
3	D	1129	THR
3	D	1131	SER
3	D	1139	ASP
3	D	1188	VAL

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Mol	Chain	Res	Type
3	D	1189	ARG
3	D	1190	SER
3	D	1221	VAL
3	D	1277	ILE
3	D	1286	THR
3	D	1427	SER
3	D	1443	THR
3	D	1444	THR
3	D	1456	LYS
3	D	1460	ILE
4	E	50	THR
4	E	83	ASP
5	F	82	ARG
5	F	88	ILE
5	F	140	ARG
5	F	141	VAL
5	F	142	ARG
5	F	156	VAL
5	F	229	TYR
5	F	231	ARG
5	F	232	ARG
5	F	258	ILE
5	F	264	MET
5	F	271	LEU
5	F	315	VAL
5	F	318	GLU
5	F	340	SER
5	F	348	SER
5	F	361	LEU
5	F	419	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	95	GLN
1	A	128	HIS
1	A	212	ASN
1	A	227	ASN
2	C	204	GLN
2	C	500	ASN
2	C	567	GLN

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Mol	Chain	Res	Type
2	C	632	ASN
2	C	999	HIS
2	C	1019	GLN
2	C	1026	GLN
3	D	617	ASN
3	D	709	HIS
3	D	816	HIS
3	D	1374	GLN
3	D	1441	GLN
3	D	1442	ASN
5	F	83	GLN
5	F	170	HIS
5	F	217	ASN

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	$\# Z > 2$
6	0QZ	I	6	6	4,5,6	1.66	1 (25%)	2,5,7	0.78	0
6	R2T	I	4	6	8,10,11	1.95	2 (25%)	6,13,15	0.83	0
6	FGL	I	7	6	5,6,7	1.47	1 (20%)	1,7,9	1.83	0
6	2TL	I	5	6	5,6,7	1.20	1 (20%)	5,7,9	0.99	0
6	2RA	I	1	6,9	4,5,6	0.54	0	1,5,7	0.26	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
6	0QZ	I	6	6	-	2/3/4/6	-
6	R2T	I	4	6	-	7/13/14/16	-
6	FGL	I	7	6	-	3/4/6/8	-
6	2TL	I	5	6	-	1/5/6/8	-
6	2RA	I	1	6,9	-	0/2/4/6	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	4	R2T	CD-NE2	4.55	1.43	1.32
6	I	6	0QZ	OB-CA	-3.20	1.38	1.43
6	I	7	FGL	OG2-CB	2.14	1.28	1.22
6	I	5	2TL	OG1-CB	-2.14	1.37	1.43
6	I	4	R2T	OB1-CB	-2.11	1.37	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	I	4	R2T	CA-CB-CG-CD
6	I	4	R2T	CA-CB-CG-OG1
6	I	4	R2T	OB1-CB-CG-CD
6	I	4	R2T	OB1-CB-CG-OG1
6	I	4	R2T	OE1-CD-CG-OG1
6	I	4	R2T	NE2-CD-CG-OG1
6	I	5	2TL	O-C-CA-CB
6	I	6	0QZ	N-C1-CA-C
6	I	6	0QZ	N-C1-CA-OB
6	I	7	FGL	C-CA-CB-OG2
6	I	7	FGL	C-CA-CB-OG1
6	I	7	FGL	N-CA-CB-OG2
6	I	4	R2T	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	4	R2T	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	1	2RA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 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	$\# Z > 2$
9	MB8	I	101	6	0,1,6	-	-	-		

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	226/314 (71%)	-0.31	0 100 100	84, 110, 169, 198	0
1	B	224/314 (71%)	0.08	3 (1%) 75 61	97, 165, 233, 259	0
2	C	1100/1119 (98%)	-0.05	11 (1%) 79 66	67, 135, 240, 281	0
3	D	1365/1524 (89%)	-0.23	13 (0%) 79 66	68, 114, 213, 249	0
4	E	93/99 (93%)	-0.17	1 (1%) 78 65	96, 142, 212, 216	0
5	F	339/443 (76%)	-0.11	3 (0%) 81 69	89, 153, 249, 267	0
6	I	0/7	-	-	-	-
All	All	3347/3820 (87%)	-0.14	31 (0%) 81 69	67, 129, 230, 281	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	422	LEU	4.8
2	C	211	LEU	4.4
5	F	129	GLU	3.3
3	D	616	GLN	3.1
2	C	454	SER	2.8
3	D	617	ASN	2.7
2	C	196	LEU	2.6
2	C	260	LEU	2.6
3	D	614	PHE	2.5
3	D	1440	PHE	2.5
3	D	875	THR	2.4
3	D	559	ALA	2.4
2	C	261	ILE	2.4
4	E	2	ALA	2.4
3	D	618	LEU	2.4
2	C	207	LEU	2.4
2	C	719	PRO	2.4
3	D	615	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	1495	ILE	2.3
1	B	103	ALA	2.3
3	D	609	GLY	2.2
3	D	980	MET	2.2
1	B	150	TYR	2.2
2	C	257	VAL	2.2
1	B	117	VAL	2.2
3	D	355	VAL	2.1
5	F	354	LEU	2.1
3	D	445	ARG	2.1
2	C	311	PHE	2.1
2	C	1002	GLU	2.1
2	C	475	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	2RA	I	1	6/7	0.92	0.09	85,96,99,111	0
6	DSN	I	2	6/7	0.93	0.08	80,85,93,97	0
6	R2T	I	4	11/12	0.93	0.07	77,87,94,97	0
6	DVA	I	3	7/8	0.97	0.14	81,85,91,93	0
6	FGL	I	7	7/8	0.97	0.06	82,93,106,108	0
6	2TL	I	5	7/8	0.97	0.09	78,84,91,93	0
6	0QZ	I	6	6/7	0.98	0.05	75,79,86,87	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
9	MB8	I	101	2/7	0.90	0.19	102,102,102,107	0
7	ZN	D	1601	1/1	0.98	0.03	159,159,159,159	0
8	MG	D	1603	1/1	1.00	0.02	75,75,75,75	0
7	ZN	D	1602	1/1	1.00	0.04	105,105,105,105	0

6.5 Other polymers [i](#)

There are no such residues in this entry.