



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:12 AM UTC

PDB ID : 5TJG / pdb_00005tjg
Title : Thermus aquaticus delta1.1-sigmaA holoenzyme/downstream-fork promoter complex with an open clamp
Authors : Darst, S.A.; Bae, B.
Deposited on : 2016-10-04
Resolution : 2.60 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:

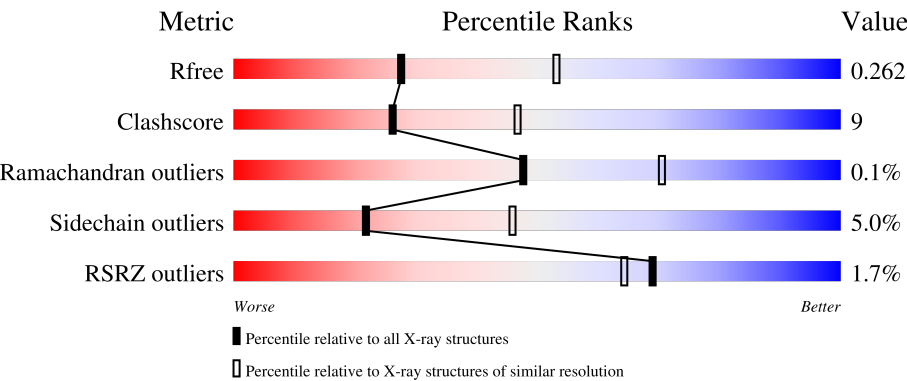
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	52%20%•28%
1	B	314	3% 53%18%•28%
2	C	1119	% 74%24%••
3	D	1524	% 72%23%••
4	E	99	2% 67%21%•10%

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Mol	Chain	Length	Quality of chain
5	F	347	3% 77% 18% . .
6	G	31	19% 13% 68%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 27767 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	227	Total	C	N	O	S	0	0	0
			1777	1134	309	331	3			
1	B	227	Total	C	N	O	S	0	0	0
			1777	1134	309	331	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	ARG	THR	conflict	UNP Q9KWU8
A	18	ARG	ASP	conflict	UNP Q9KWU8
B	14	ARG	THR	conflict	UNP Q9KWU8
B	18	ARG	ASP	conflict	UNP Q9KWU8

- 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
			8739	5531	1553	1632	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1475	Total	C	N	O	S	0	0	0
			11657	7376	2066	2177	38			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	666	ILE	PHE	conflict	UNP Q9KWU6

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			730	464	129	133	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	334	Total	C	N	O	S	0	0	0
			2700	1702	485	509	4			

- Molecule 6 is a DNA chain called DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	10	Total	C	N	O	P	0	0	0
			207	100	41	57	9			

- 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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	18	Total	O	0	0
			18	18		
9	B	10	Total	O	0	0
			10	10		
9	C	48	Total	O	0	0
			48	48		
9	D	77	Total	O	0	0
			77	77		
9	E	7	Total	O	0	0
			7	7		
9	F	14	Total	O	0	0
			14	14		

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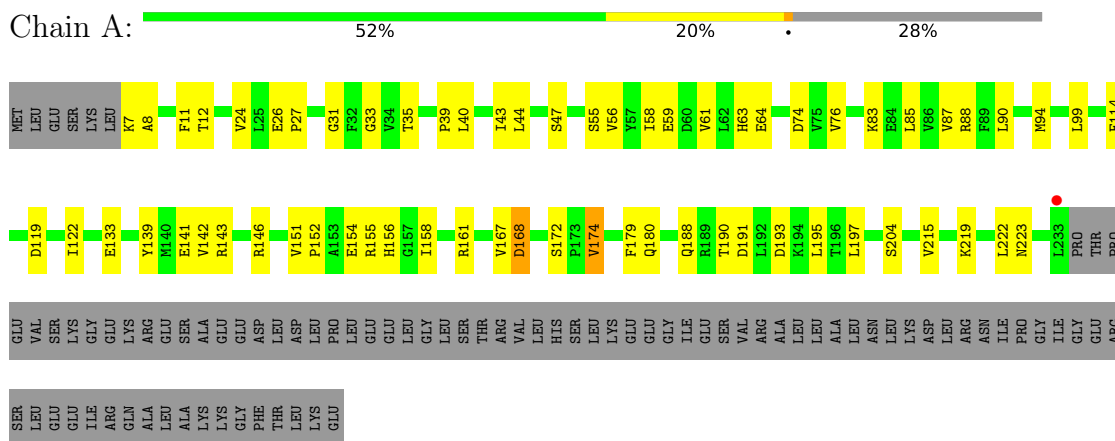
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	G	3	Total	O	0	0
			3	3		

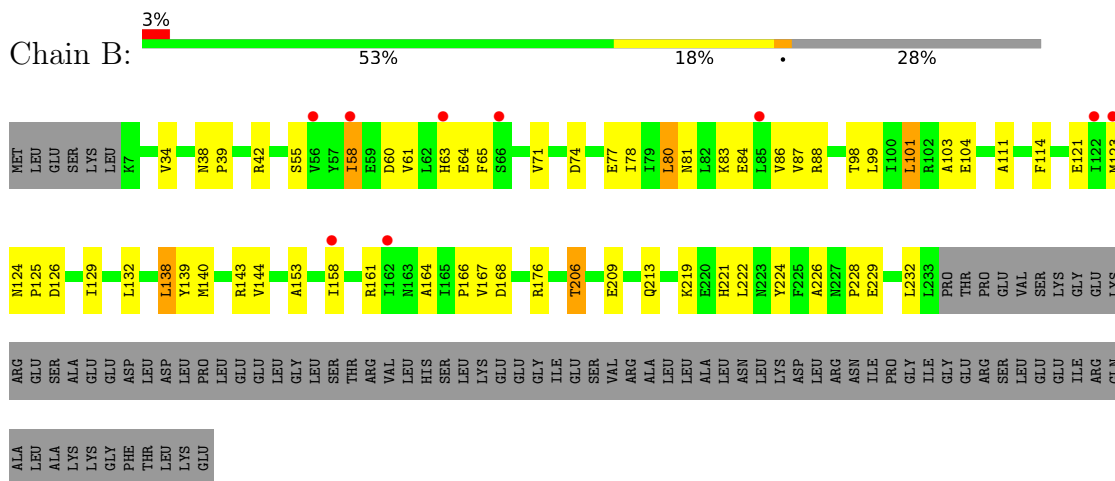
3 Residue-property plots [i](#)

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

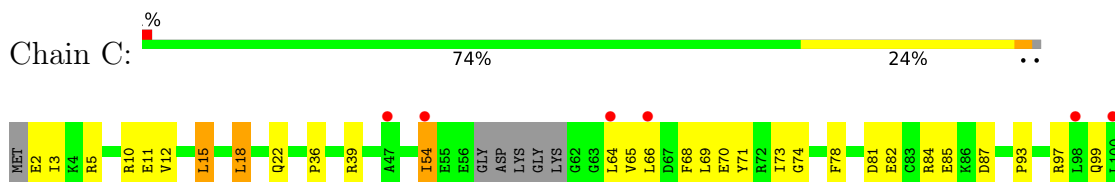
- Molecule 1: DNA-directed RNA polymerase subunit alpha

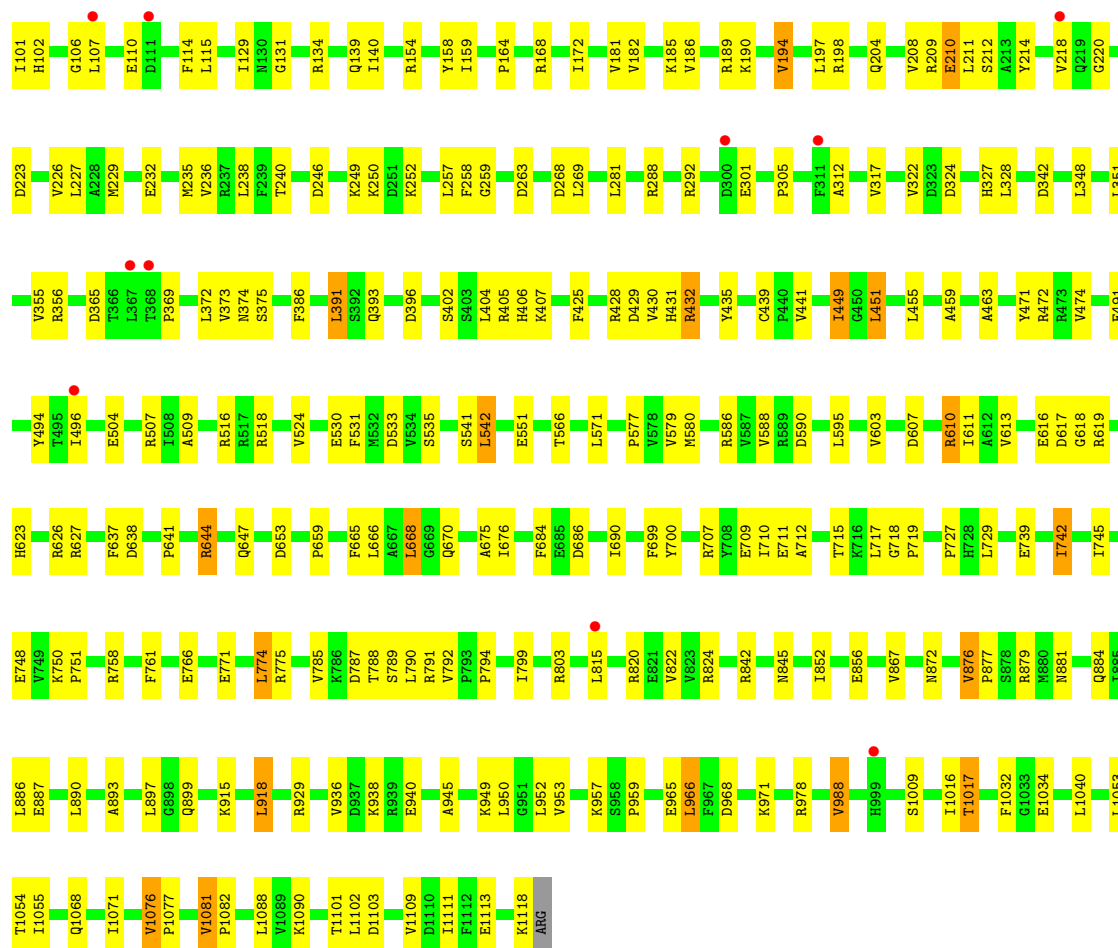


- Molecule 1: DNA-directed RNA polymerase subunit alpha

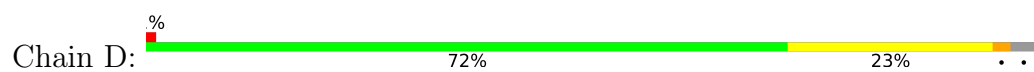


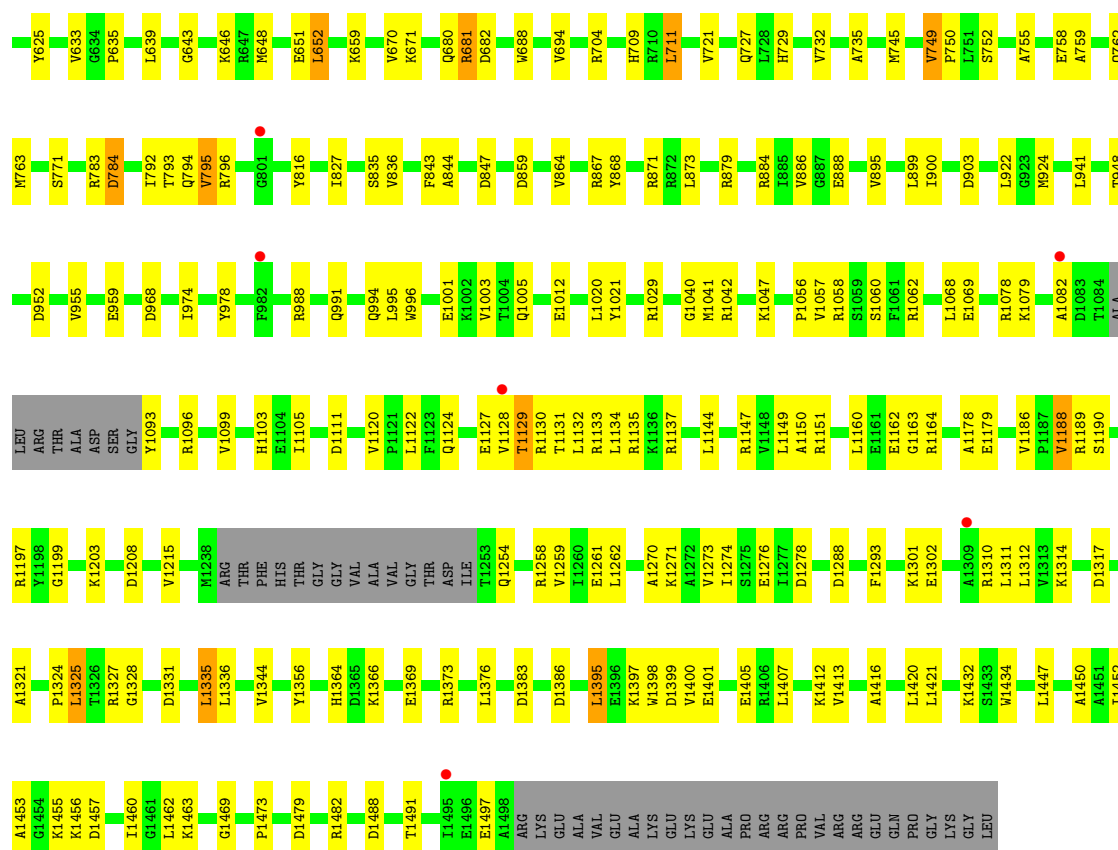
- Molecule 2: DNA-directed RNA polymerase subunit beta



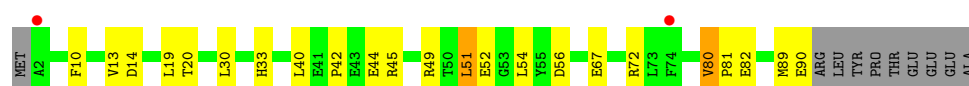


• Molecule 3: DNA-directed RNA polymerase subunit beta'

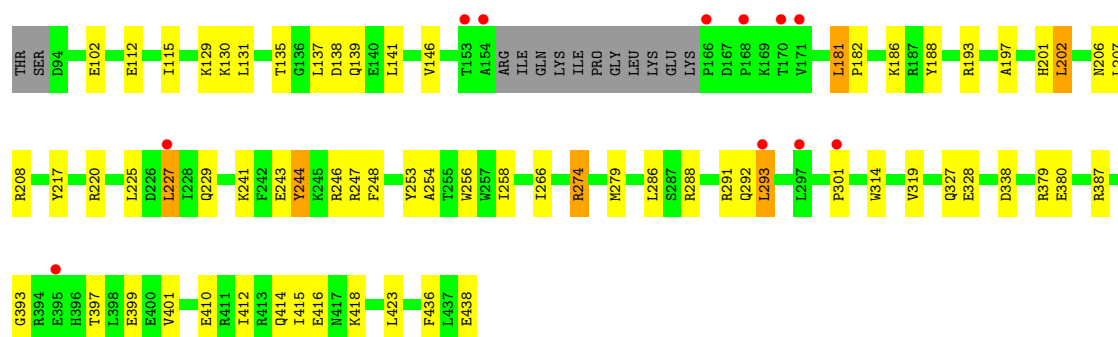
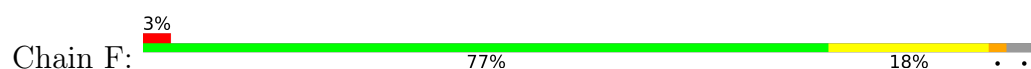




- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: RNA polymerase sigma factor SigA



- Molecule 6: DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*A)-3')



DT	DG	DC	T1	A2	T3	A4	A10	DT	DG	DA	DT	DC	DG	DC	DG	DA	DG	DG	DG	DA	DC	DA	DC	DG	DG
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	104.10Å 111.42Å 143.18Å 104.12° 99.66° 109.43°	Depositor
Resolution (Å)	38.63 – 2.60 38.63 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.4 (38.63-2.60) 84.7 (38.63-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.90 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.10.1-2155-000	Depositor
R, R_{free}	0.224 , 0.262 0.225 , 0.262	Depositor DCC
R_{free} test set	8519 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	27767	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	0.14	0/1811	0.35	0/2462
1	B	0.15	0/1811	0.35	0/2462
2	C	0.12	0/8905	0.35	0/12040
3	D	0.12	0/11857	0.34	0/16021
4	E	0.10	0/743	0.32	0/999
5	F	0.10	0/2740	0.31	0/3683
6	G	0.21	0/233	0.42	0/359
All	All	0.13	0/28100	0.34	0/38026

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1814	42	0
1	B	1777	0	1814	46	0
2	C	8739	0	8841	170	0
3	D	11657	0	11875	251	0
4	E	730	0	744	15	0
5	F	2700	0	2768	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	207	0	115	3	0
7	D	2	0	0	0	0
8	D	1	0	0	0	0
9	A	18	0	0	1	0
9	B	10	0	0	8	0
9	C	48	0	0	7	0
9	D	77	0	0	20	0
9	E	7	0	0	2	0
9	F	14	0	0	5	0
9	G	3	0	0	0	0
All	All	27767	0	27971	521	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 (521) 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:D:124:GLU:OE2	3:D:587:ARG:NH2	2.06	0.88
3:D:260:GLU:HB3	3:D:271:TYR:HB2	1.57	0.84
3:D:1163:GLY:O	9:D:2102:HOH:O	1.96	0.82
3:D:1124:GLN:HG3	3:D:1135:ARG:HG2	1.61	0.81
3:D:1310:ARG:HG3	3:D:1327:ARG:HG3	1.62	0.81
1:B:58:ILE:HG13	1:B:61:VAL:HB	1.63	0.81
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.64	0.80
1:B:139:TYR:O	9:B:401:HOH:O	2.01	0.79
3:D:73:CYS:HB3	3:D:76:CYS:HB2	1.65	0.78
3:D:771:SER:OG	9:D:2103:HOH:O	2.02	0.78
3:D:680:GLN:HG3	3:D:682:ASP:H	1.48	0.78
5:F:293:LEU:HD11	5:F:301:PRO:HB3	1.65	0.77
3:D:1197:ARG:NH2	3:D:1405:GLU:OE2	2.16	0.76
2:C:65:VAL:HB	2:C:101:ILE:HB	1.68	0.76
2:C:684:PHE:HB3	3:D:633:VAL:HG21	1.68	0.76
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.68	0.76
3:D:376:GLU:OE2	9:D:2104:HOH:O	2.04	0.75
3:D:1164:ARG:O	9:D:2105:HOH:O	2.05	0.75
2:C:929:ARG:NH1	9:C:1205:HOH:O	2.17	0.74
3:D:520:LEU:O	3:D:525:ARG:NH1	2.20	0.74
3:D:1479:ASP:OD1	3:D:1482:ARG:NH2	2.20	0.74
4:E:56:ASP:OD2	9:E:101:HOH:O	2.06	0.73
3:D:473:LEU:HD11	3:D:495:ARG:HH12	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:793:THR:O	3:D:879:ARG:NH1	2.20	0.73
1:B:140:MET:HA	9:B:401:HOH:O	1.87	0.73
2:C:463:ALA:N	9:C:1201:HOH:O	2.03	0.72
4:E:51:LEU:HD22	4:E:52:GLU:HG3	1.70	0.72
5:F:241:LYS:NZ	5:F:253:TYR:OH	2.22	0.72
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.71	0.72
3:D:1386:ASP:HB3	3:D:1412:LYS:HE3	1.70	0.72
5:F:208:ARG:NH2	9:F:504:HOH:O	2.23	0.72
3:D:150:ARG:NH1	9:D:2101:HOH:O	1.91	0.71
1:A:180:GLN:HE22	2:C:929:ARG:HH21	1.37	0.71
2:C:595:LEU:HD21	2:C:623:HIS:HB3	1.70	0.71
3:D:179:VAL:O	3:D:205:TYR:OH	2.08	0.71
5:F:397:THR:OG1	9:F:501:HOH:O	2.08	0.71
2:C:106:GLY:O	9:C:1202:HOH:O	2.10	0.70
3:D:704:ARG:O	9:D:2106:HOH:O	2.09	0.70
5:F:387:ARG:NH1	5:F:416:GLU:OE1	2.25	0.70
1:B:213:GLN:N	9:B:402:HOH:O	2.22	0.70
2:C:449:ILE:HD12	3:D:1082:ALA:HA	1.74	0.70
2:C:516:ARG:HD3	3:D:1068:LEU:HD21	1.74	0.70
3:D:44:LEU:O	3:D:525:ARG:NH2	2.24	0.70
2:C:15:LEU:O	2:C:586:ARG:NH2	2.25	0.70
3:D:104:PHE:HB3	3:D:512:MET:HE2	1.74	0.70
2:C:54:ILE:HG22	2:C:66:LEU:HD11	1.75	0.69
1:B:209:GLU:O	9:B:402:HOH:O	2.11	0.69
3:D:314:PRO:HG2	3:D:317:MET:HB3	1.73	0.69
1:A:55:SER:HB3	1:A:143:ARG:HB3	1.76	0.68
3:D:166:GLN:HB2	3:D:394:LEU:HD11	1.75	0.68
2:C:711:GLU:HG2	2:C:822:VAL:HG12	1.76	0.68
2:C:1103:ASP:OD1	9:C:1203:HOH:O	2.11	0.67
2:C:715:THR:HG22	2:C:717:LEU:H	1.59	0.67
1:B:132:LEU:HD21	1:B:138:LEU:HD12	1.76	0.66
1:B:153:ALA:HB1	1:B:166:PRO:HB2	1.78	0.66
5:F:146:VAL:HG13	5:F:193:ARG:HD3	1.76	0.66
2:C:577:PRO:HG2	2:C:580:MET:HG2	1.76	0.66
3:D:133:ILE:HD11	3:D:460:ALA:HB1	1.77	0.66
3:D:1003:VAL:HG21	3:D:1041:MET:HG2	1.77	0.66
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.76	0.66
2:C:586:ARG:NH1	2:C:590:ASP:OD2	2.29	0.66
3:D:1120:VAL:N	9:D:2107:HOH:O	2.28	0.65
1:A:43:ILE:HG23	1:A:47:SER:HB2	1.77	0.65
3:D:1120:VAL:O	9:D:2107:HOH:O	2.13	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ARG:NH2	1:B:121:GLU:OE1	2.30	0.65
2:C:670:GLN:HE21	2:C:700:TYR:H	1.45	0.65
2:C:425:PHE:HZ	3:D:1079:LYS:HA	1.60	0.65
2:C:787:ASP:OD2	2:C:791:ARG:NH2	2.30	0.64
3:D:209:ARG:N	3:D:389:GLU:O	2.29	0.64
3:D:371:ILE:HG21	5:F:247:ARG:HH12	1.62	0.64
3:D:325:GLU:HB2	3:D:332:HIS:HB3	1.79	0.64
3:D:280:ALA:O	9:D:2109:HOH:O	2.15	0.64
1:B:98:THR:OG1	1:B:143:ARG:NH1	2.31	0.64
3:D:259:VAL:HG23	3:D:270:ILE:HG23	1.81	0.63
3:D:794:GLN:HE21	3:D:795:VAL:H	1.45	0.63
2:C:66:LEU:HD21	2:C:355:VAL:HG11	1.80	0.63
2:C:139:GLN:HB2	2:C:391:LEU:HD21	1.80	0.63
5:F:138:ASP:HB2	5:F:141:LEU:HD13	1.81	0.63
2:C:259:GLY:HA2	2:C:263:ASP:HB2	1.81	0.62
2:C:292:ARG:NE	2:C:301:GLU:OE2	2.33	0.62
3:D:347:VAL:HG23	3:D:351:MET:HB2	1.82	0.61
2:C:1081:VAL:HG21	2:C:1111:ILE:HB	1.82	0.61
2:C:185:LYS:HG2	2:C:190:LYS:HG2	1.81	0.61
2:C:18:LEU:HD23	2:C:404:LEU:HD21	1.81	0.61
2:C:85:GLU:O	2:C:824:ARG:NH2	2.33	0.61
3:D:237:ARG:N	3:D:240:GLU:OE2	2.33	0.61
1:A:133:GLU:OE2	2:C:610:ARG:NH2	2.33	0.61
1:B:87:VAL:HG21	1:B:144:VAL:HG11	1.83	0.61
2:C:235:MET:HG3	2:C:257:LEU:HD12	1.82	0.61
2:C:396:ASP:H	2:C:406:HIS:HD1	1.49	0.61
1:B:34:VAL:HG11	2:C:978:ARG:HB3	1.81	0.61
3:D:60:CYS:N	3:D:76:CYS:SG	2.74	0.61
3:D:209:ARG:HB2	3:D:389:GLU:HB3	1.83	0.60
5:F:380:GLU:OE2	5:F:418:LYS:HE3	2.00	0.60
2:C:54:ILE:HD11	2:C:356:ARG:HH21	1.66	0.60
3:D:1122:LEU:HD23	3:D:1178:ALA:HB2	1.83	0.60
2:C:603:VAL:HA	2:C:613:VAL:HG12	1.82	0.60
3:D:1093:TYR:N	9:D:2122:HOH:O	2.33	0.60
2:C:54:ILE:HG13	2:C:356:ARG:HE	1.65	0.60
2:C:504:GLU:HG3	2:C:509:ALA:HB2	1.83	0.60
3:D:218:LYS:NZ	3:D:338:GLU:OE1	2.34	0.59
2:C:1053:LEU:O	3:D:621:LYS:NZ	2.34	0.59
2:C:18:LEU:HB3	2:C:404:LEU:HD11	1.84	0.59
2:C:699:PHE:O	9:C:1204:HOH:O	2.17	0.59
1:A:11:PHE:HD2	1:B:228:PRO:HA	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:704:ARG:HB2	3:D:745:MET:HG2	1.84	0.59
3:D:388:HIS:O	3:D:390:PRO:HD3	2.02	0.59
3:D:1186:VAL:O	9:D:2107:HOH:O	2.16	0.59
2:C:236:VAL:HG21	2:C:250:LYS:HG2	1.84	0.58
3:D:1258:ARG:NH1	3:D:1261:GLU:OE1	2.36	0.58
2:C:99:GLN:HB3	2:C:110:GLU:HG2	1.85	0.58
3:D:406:ASP:OD1	3:D:407:VAL:N	2.34	0.58
2:C:226:VAL:HA	2:C:229:MET:HE3	1.84	0.58
4:E:42:PRO:HA	4:E:45:ARG:HD2	1.84	0.58
2:C:638:ASP:H	2:C:659:PRO:HG3	1.68	0.58
3:D:1149:LEU:N	9:D:2105:HOH:O	2.24	0.58
1:A:56:VAL:HG22	1:A:142:VAL:HG12	1.85	0.58
2:C:771:GLU:OE2	2:C:775:ARG:NH2	2.37	0.58
1:A:44:LEU:O	1:A:174:VAL:HG11	2.03	0.57
2:C:496:ILE:HG12	2:C:531:PHE:HB2	1.85	0.57
2:C:929:ARG:NH2	2:C:940:GLU:OE2	2.36	0.57
3:D:796:ARG:NH2	3:D:859:ASP:OD2	2.36	0.57
5:F:379:ARG:HD3	5:F:415:ILE:HD13	1.87	0.57
3:D:165:LYS:H	3:D:397:LYS:HE3	1.68	0.57
3:D:365:GLU:OE1	9:D:2110:HOH:O	2.17	0.57
5:F:197:ALA:O	5:F:201:HIS:ND1	2.37	0.57
1:A:94:MET:O	1:A:146:ARG:NH1	2.32	0.57
1:A:215:VAL:HG12	1:A:219:LYS:HE2	1.87	0.57
3:D:176:ASP:OD1	3:D:177:ALA:N	2.35	0.57
3:D:570:GLU:HG2	5:F:229:GLN:HE21	1.69	0.57
1:A:141:GLU:OE2	1:A:161:ARG:NH2	2.35	0.57
1:B:77:GLU:O	1:B:81:ASN:ND2	2.38	0.56
2:C:936:VAL:HG21	2:C:959:PRO:HB2	1.87	0.56
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.41	0.56
2:C:198:ARG:HD3	2:C:227:LEU:HA	1.88	0.56
3:D:408:GLU:N	3:D:408:GLU:OE1	2.38	0.56
3:D:648:MET:HG2	3:D:652:LEU:HD22	1.87	0.56
3:D:1127:GLU:HG2	3:D:1312:LEU:HD22	1.87	0.56
2:C:719:PRO:HB3	2:C:820:ARG:HD2	1.87	0.56
2:C:742:ILE:HD11	2:C:803:ARG:HE	1.71	0.56
1:A:156:HIS:HD2	1:A:158:ILE:HG12	1.71	0.56
5:F:328:GLU:OE2	9:F:502:HOH:O	2.18	0.56
2:C:751:PRO:HB3	2:C:794:PRO:HA	1.86	0.55
5:F:399:GLU:OE1	5:F:399:GLU:N	2.37	0.55
3:D:711:LEU:HB3	3:D:735:ALA:HB1	1.88	0.55
1:A:193:ASP:OD1	2:C:938:LYS:NZ	2.30	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:GLU:HA	9:B:403:HOH:O	2.06	0.55
2:C:842:ARG:NH2	2:C:887:GLU:OE1	2.39	0.55
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.88	0.55
1:A:63:HIS:HB2	2:C:799:ILE:HD12	1.89	0.54
2:C:204:GLN:HB2	2:C:227:LEU:HD13	1.89	0.54
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.90	0.54
2:C:78:PHE:HB3	2:C:82:GLU:HG3	1.89	0.54
2:C:617:ASP:OD2	2:C:619:ARG:NH1	2.39	0.54
1:B:58:ILE:HA	9:B:401:HOH:O	2.06	0.54
2:C:428:ARG:HG2	2:C:451:LEU:HD13	1.89	0.54
3:D:625:TYR:HB3	3:D:749:VAL:HG13	1.88	0.54
1:A:154:GLU:OE1	1:A:154:GLU:N	2.40	0.54
3:D:1127:GLU:OE1	3:D:1127:GLU:N	2.37	0.54
5:F:314:TRP:O	9:F:503:HOH:O	2.19	0.54
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.90	0.53
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.89	0.53
3:D:1397:LYS:O	3:D:1401:GLU:HG2	2.07	0.53
2:C:1076:VAL:HG22	3:D:752:SER:HB3	1.90	0.53
3:D:150:ARG:HD2	9:D:2101:HOH:O	2.08	0.53
5:F:254:ALA:O	5:F:258:ILE:HG12	2.09	0.53
2:C:208:VAL:O	2:C:212:SER:OG	2.23	0.53
2:C:644:ARG:HG3	2:C:647:GLN:HB2	1.89	0.53
3:D:847:ASP:OD1	3:D:884:ARG:NH2	2.42	0.53
3:D:1164:ARG:N	9:D:2105:HOH:O	2.41	0.53
2:C:471:TYR:OH	2:C:491:GLU:OE2	2.25	0.53
2:C:709:GLU:HG3	2:C:824:ARG:HG2	1.91	0.53
2:C:750:LYS:HD3	3:D:681:ARG:HH11	1.73	0.53
3:D:224:ARG:NH1	3:D:327:GLU:OE2	2.41	0.52
3:D:1057:VAL:HG12	3:D:1069:GLU:HG2	1.91	0.52
3:D:1144:LEU:HD21	3:D:1186:VAL:HG21	1.91	0.52
3:D:1488:ASP:OD1	3:D:1488:ASP:N	2.39	0.52
1:B:111:ALA:HB3	1:B:124:ASN:O	2.09	0.52
3:D:108:VAL:HG23	3:D:109:PRO:HD3	1.92	0.52
3:D:534:ARG:NH1	5:F:327:GLN:OE1	2.42	0.52
3:D:1197:ARG:HG2	3:D:1398:TRP:CD1	2.44	0.52
2:C:22:GLN:HG3	2:C:407:LYS:HB3	1.92	0.52
3:D:868:TYR:HB3	3:D:873:LEU:HD12	1.91	0.52
2:C:742:ILE:HD11	2:C:803:ARG:NE	2.25	0.52
3:D:133:ILE:HD13	3:D:464:LEU:HD11	1.91	0.52
2:C:68:PHE:HZ	2:C:71:TYR:HD2	1.57	0.52
3:D:44:LEU:HB3	3:D:525:ARG:NH2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1276:GLU:HB2	3:D:1301:LYS:HZ3	1.74	0.52
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.92	0.52
2:C:758:ARG:H	2:C:789:SER:HB3	1.75	0.52
2:C:1016:ILE:HG13	2:C:1017:THR:H	1.74	0.51
3:D:610:LYS:H	3:D:610:LYS:HD2	1.76	0.51
4:E:82:GLU:N	9:E:102:HOH:O	2.18	0.51
3:D:212:ARG:HD2	3:D:342:PRO:HB3	1.93	0.51
3:D:354:ILE:HD11	3:D:369:ALA:HB2	1.92	0.51
3:D:371:ILE:HG21	5:F:247:ARG:NH1	2.25	0.51
3:D:236:TYR:HB2	3:D:319:ALA:HB3	1.92	0.51
2:C:246:ASP:OD1	2:C:246:ASP:N	2.38	0.51
2:C:872:ASN:ND2	3:D:784:ASP:OD1	2.34	0.51
2:C:950:LEU:HD11	2:C:952:LEU:HB2	1.93	0.51
3:D:483:HIS:CD2	3:D:485:SER:H	2.28	0.51
3:D:271:TYR:HA	9:D:2109:HOH:O	2.10	0.51
3:D:758:GLU:HB3	4:E:20:THR:HG21	1.92	0.51
1:B:126:ASP:OD1	1:B:126:ASP:N	2.44	0.51
1:B:103:ALA:O	9:B:403:HOH:O	2.20	0.51
3:D:402:PRO:HA	3:D:443:VAL:HG23	1.93	0.51
2:C:351:LEU:HD11	2:C:373:VAL:HG13	1.93	0.51
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.94	0.50
3:D:270:ILE:HB	3:D:282:TYR:HB2	1.93	0.50
3:D:349:PRO:HB3	5:F:112:GLU:HG2	1.93	0.50
4:E:33:HIS:HE1	4:E:90:GLU:HG3	1.75	0.50
2:C:432:ARG:NH2	2:C:518:ARG:O	2.44	0.50
3:D:1199:GLY:O	3:D:1373:ARG:NH2	2.32	0.50
1:B:80:LEU:HG	3:D:844:ALA:HA	1.94	0.50
3:D:38:LYS:HG2	3:D:39:PRO:HD2	1.93	0.50
3:D:1130:ARG:O	9:D:2111:HOH:O	2.19	0.50
2:C:258:PHE:O	2:C:263:ASP:N	2.45	0.50
2:C:429:ASP:OD1	2:C:430:VAL:N	2.44	0.50
4:E:14:ASP:OD1	4:E:14:ASP:N	2.45	0.50
1:A:74:ASP:OD2	2:C:627:ARG:NH2	2.44	0.50
2:C:430:VAL:HG23	3:D:1078:ARG:HD2	1.94	0.50
3:D:1012:GLU:HG2	3:D:1021:TYR:OH	2.12	0.50
3:D:1328:GLY:N	9:D:2129:HOH:O	2.44	0.50
1:B:101:LEU:N	1:B:140:MET:O	2.28	0.50
3:D:968:ASP:OD1	3:D:1058:ARG:NH2	2.39	0.50
2:C:494:TYR:HB3	2:C:530:GLU:HG3	1.93	0.49
3:D:1103:HIS:CD2	3:D:1463:LYS:H	2.30	0.49
5:F:401:VAL:HG12	5:F:412:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:PHE:CD2	1:B:228:PRO:HA	2.47	0.49
1:B:138:LEU:N	9:B:403:HOH:O	2.45	0.49
3:D:125:GLN:HG2	3:D:130:ASN:HD22	1.77	0.49
3:D:253:ALA:HB2	3:D:304:LEU:HD11	1.94	0.49
3:D:554:LEU:HD12	3:D:574:LEU:HD22	1.93	0.49
3:D:1103:HIS:HD2	3:D:1462:LEU:H	1.58	0.49
2:C:129:ILE:HG12	2:C:386:PHE:HB3	1.94	0.49
3:D:1450:ALA:HA	3:D:1455:LYS:HD2	1.95	0.49
3:D:1462:LEU:HD23	3:D:1473:PRO:HD2	1.94	0.49
2:C:36:PRO:HA	2:C:39:ARG:HD2	1.93	0.49
2:C:281:LEU:HD13	2:C:305:PRO:HB2	1.94	0.49
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.44	0.49
2:C:971:LYS:HA	2:C:988:VAL:HA	1.94	0.49
3:D:1150:ALA:O	3:D:1151:ARG:HD3	2.13	0.49
4:E:13:VAL:HG21	4:E:19:LEU:HB2	1.94	0.49
2:C:402:SER:HA	2:C:566:THR:HG23	1.95	0.48
3:D:136:ASP:OD2	3:D:138:LYS:HE3	2.13	0.48
5:F:288:ARG:O	5:F:291:ARG:HG2	2.13	0.48
1:A:7:LYS:HG2	1:A:188:GLN:NE2	2.28	0.48
1:A:191:ASP:OD1	1:A:191:ASP:N	2.40	0.48
3:D:1147:ARG:HD3	3:D:1188:VAL:CG1	2.40	0.48
2:C:435:TYR:OH	2:C:533:ASP:OD2	2.25	0.48
2:C:551:GLU:H	2:C:551:GLU:CD	2.20	0.48
2:C:504:GLU:N	2:C:507:ARG:O	2.42	0.48
2:C:617:ASP:OD1	2:C:617:ASP:N	2.45	0.48
2:C:676:ILE:O	3:D:948:THR:OG1	2.27	0.48
3:D:407:VAL:O	5:F:186:LYS:NZ	2.34	0.48
1:B:84:GLU:OE2	3:D:867:ARG:NH2	2.44	0.48
2:C:194:VAL:HA	2:C:197:LEU:HB2	1.94	0.48
2:C:666:LEU:HG	2:C:668:LEU:HD13	1.96	0.48
1:A:168:ASP:OD1	1:A:168:ASP:N	2.46	0.48
2:C:718:GLY:HA3	2:C:761:PHE:CD2	2.49	0.48
3:D:215:TYR:HD2	3:D:381:ALA:HB3	1.79	0.48
3:D:991:GLN:HA	3:D:994:GLN:HG2	1.95	0.48
3:D:758:GLU:O	3:D:762:GLN:HG2	2.14	0.48
3:D:1271:LYS:HD2	3:D:1331:ASP:HB2	1.96	0.48
5:F:338:ASP:OD1	5:F:338:ASP:N	2.47	0.48
2:C:73:ILE:HG13	9:C:1218:HOH:O	2.12	0.48
2:C:181:VAL:HA	2:C:220:GLY:O	2.14	0.48
3:D:207:PHE:HB2	3:D:391:ALA:HB3	1.96	0.48
2:C:69:LEU:HB2	2:C:97:ARG:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1278:ASP:OD1	3:D:1321:ALA:N	2.47	0.47
3:D:398:ALA:HB2	3:D:447:VAL:HG12	1.96	0.47
5:F:387:ARG:HD2	5:F:401:VAL:HG21	1.94	0.47
2:C:455:LEU:HG	2:C:459:ALA:HB3	1.95	0.47
1:A:33:GLY:HA2	1:A:195:LEU:HD12	1.97	0.47
3:D:400:VAL:HG12	3:D:443:VAL:HG21	1.97	0.47
1:A:85:LEU:HD11	1:A:122:ILE:HD12	1.97	0.47
2:C:269:LEU:O	2:C:288:ARG:HB3	2.14	0.47
3:D:924:MET:HE1	4:E:10:PHE:CE1	2.50	0.47
5:F:246:ARG:HB3	5:F:248:PHE:CE1	2.49	0.47
3:D:502:PHE:CZ	3:D:1452:ILE:HD12	2.49	0.47
3:D:784:ASP:OD2	3:D:784:ASP:N	2.48	0.47
3:D:568:ARG:NH2	5:F:102:GLU:OE2	2.47	0.47
3:D:759:ALA:HA	3:D:763:MET:HE3	1.96	0.47
3:D:1001:GLU:OE2	3:D:1005:GLN:NE2	2.46	0.47
3:D:1208:ASP:HB2	3:D:1215:VAL:HA	1.97	0.47
3:D:1336:LEU:HD22	3:D:1421:LEU:HB2	1.97	0.47
3:D:28:LYS:HB3	3:D:30:GLU:OE1	2.15	0.47
3:D:97:THR:HG21	3:D:571:LYS:HG2	1.97	0.47
5:F:131:LEU:O	5:F:135:THR:OG1	2.30	0.47
1:B:206:THR:HG22	1:B:209:GLU:HG2	1.96	0.47
2:C:369:PRO:HA	2:C:372:LEU:HB3	1.96	0.47
2:C:1009:SER:HB3	3:D:651:GLU:O	2.15	0.47
3:D:31:THR:OG1	3:D:32:ILE:N	2.48	0.46
3:D:1130:ARG:O	3:D:1131:THR:OG1	2.29	0.46
2:C:11:GLU:HG3	2:C:535:SER:HB2	1.96	0.46
3:D:1399:ASP:OD2	3:D:1432:LYS:HD3	2.16	0.46
5:F:130:LYS:HD2	5:F:188:TYR:CE2	2.51	0.46
1:B:176:ARG:NH1	3:D:888:GLU:OE2	2.30	0.46
3:D:65:ARG:HA	3:D:65:ARG:HD2	1.75	0.46
3:D:1383:ASP:HB3	3:D:1416:ALA:HB3	1.96	0.46
2:C:758:ARG:HH21	2:C:788:THR:HB	1.79	0.46
3:D:260:GLU:HA	3:D:294:GLU:OE1	2.16	0.46
1:A:83:LYS:HE3	1:A:168:ASP:HB2	1.97	0.46
1:B:221:HIS:HA	1:B:224:TYR:CE2	2.51	0.46
3:D:179:VAL:C	3:D:205:TYR:HH	2.24	0.46
3:D:1042:ARG:HB3	3:D:1057:VAL:CG2	2.46	0.46
1:A:215:VAL:HG13	1:B:222:LEU:HB3	1.98	0.46
2:C:1082:PRO:HG2	3:D:1469:GLY:O	2.16	0.46
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.97	0.46
3:D:404:GLU:HG3	3:D:405:ASP:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.16	0.46
3:D:1271:LYS:HB3	3:D:1271:LYS:HE2	1.78	0.46
1:A:11:PHE:CE2	1:B:228:PRO:HB3	2.51	0.46
2:C:102:HIS:NE2	2:C:365:ASP:O	2.48	0.46
2:C:626:ARG:HD2	2:C:637:PHE:CD2	2.50	0.46
2:C:710:ILE:HD12	2:C:790:LEU:HB2	1.99	0.45
3:D:230:TRP:CZ3	3:D:331:VAL:HG21	2.51	0.45
3:D:362:GLN:HA	3:D:382:GLU:HG2	1.98	0.45
1:B:55:SER:HB2	1:B:158:ILE:HG21	1.99	0.45
1:B:123:MET:C	1:B:125:PRO:HD3	2.42	0.45
3:D:162:ARG:O	3:D:449:SER:HB3	2.17	0.45
3:D:843:PHE:CE1	3:D:864:VAL:HG11	2.50	0.45
3:D:74:GLU:OE1	3:D:74:GLU:N	2.49	0.45
2:C:154:ARG:NH2	9:C:1207:HOH:O	2.27	0.45
2:C:876:VAL:H	2:C:877:PRO:HD2	1.81	0.45
2:C:1113:GLU:OE1	2:C:1113:GLU:N	2.44	0.45
3:D:73:CYS:CB	3:D:76:CYS:HB2	2.43	0.45
1:A:58:ILE:HB	1:A:61:VAL:HB	1.98	0.45
2:C:168:ARG:HD2	2:C:268:ASP:HB3	1.98	0.45
3:D:363:ALA:HB2	3:D:381:ALA:HA	1.98	0.45
3:D:220:ARG:HG3	3:D:336:PHE:HD1	1.81	0.45
3:D:1491:THR:HG21	4:E:89:MET:HG3	1.98	0.45
5:F:181:LEU:HG	5:F:182:PRO:HD2	1.99	0.45
3:D:268:HIS:HB2	3:D:284:LEU:HB2	1.99	0.45
3:D:709:HIS:CD2	3:D:711:LEU:HB2	2.52	0.45
3:D:827:ILE:HG12	3:D:835:SER:HA	1.99	0.45
3:D:924:MET:HE1	4:E:10:PHE:HE1	1.80	0.45
5:F:202:LEU:O	5:F:206:ASN:ND2	2.42	0.45
3:D:244:GLU:HG3	3:D:310:LEU:HB3	1.98	0.44
4:E:40:LEU:HG	4:E:67:GLU:HG2	1.99	0.44
2:C:54:ILE:HD12	2:C:54:ILE:HA	1.65	0.44
2:C:1071:ILE:HG23	3:D:670:VAL:HG21	1.99	0.44
3:D:1273:VAL:HG23	3:D:1325:LEU:HB2	1.99	0.44
2:C:611:ILE:HD11	2:C:641:PRO:HB3	1.99	0.44
2:C:748:GLU:HA	2:C:799:ILE:HG22	2.00	0.44
4:E:80:VAL:HG22	4:E:81:PRO:HD2	2.00	0.44
2:C:134:ARG:HD3	2:C:393:GLN:O	2.17	0.44
2:C:712:ALA:O	2:C:820:ARG:N	2.48	0.44
3:D:792:ILE:HG21	3:D:941:LEU:HD13	2.00	0.44
3:D:1276:GLU:HB2	3:D:1301:LYS:NZ	2.32	0.44
6:G:3:DT:H2'	6:G:4:DA:C8	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:5:ARG:HD3	2:C:10:ARG:NH1	2.32	0.44
3:D:570:GLU:HG2	5:F:229:GLN:NE2	2.31	0.44
3:D:1130:ARG:HG2	3:D:1131:THR:HG23	1.99	0.44
1:B:63:HIS:CD2	1:B:64:GLU:H	2.36	0.44
1:B:206:THR:CG2	1:B:209:GLU:H	2.31	0.44
2:C:431:HIS:CE1	2:C:432:ARG:HD3	2.53	0.44
3:D:248:PRO:HG3	3:D:308:LYS:HD3	2.00	0.44
3:D:584:ASN:H	3:D:602:SER:HB3	1.82	0.44
3:D:1293:PHE:CE2	3:D:1302:GLU:HB2	2.53	0.44
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.99	0.44
2:C:223:ASP:OD2	2:C:226:VAL:HG23	2.17	0.44
2:C:428:ARG:O	3:D:1078:ARG:HD3	2.18	0.44
3:D:455:ARG:HB2	3:D:460:ALA:HB2	1.98	0.44
3:D:1127:GLU:C	3:D:1129:THR:H	2.25	0.44
2:C:1034:GLU:OE2	3:D:1096:ARG:NH2	2.34	0.44
5:F:256:TRP:CZ2	6:G:1:DT:H4'	2.52	0.44
1:A:12:THR:HG22	9:A:405:HOH:O	2.18	0.44
1:A:223:ASN:OD1	1:B:219:LYS:NZ	2.43	0.44
2:C:211:LEU:HD12	2:C:214:TYR:HE2	1.82	0.44
3:D:46:ASP:OD2	3:D:48:ARG:HB2	2.17	0.44
5:F:410:GLU:O	5:F:414:GLN:HG2	2.18	0.44
1:B:161:ARG:HB2	1:B:164:ALA:HB2	2.00	0.43
2:C:185:LYS:HA	2:C:189:ARG:O	2.17	0.43
2:C:957:LYS:HD2	2:C:965:GLU:OE2	2.18	0.43
3:D:1335:LEU:HB3	3:D:1344:VAL:HG22	2.00	0.43
2:C:815:LEU:HD21	2:C:822:VAL:HG13	2.00	0.43
3:D:1111:ASP:HB2	3:D:1203:LYS:HE2	1.99	0.43
2:C:449:ILE:CD1	3:D:1082:ALA:HA	2.47	0.43
3:D:1314:LYS:N	3:D:1317:ASP:OD2	2.41	0.43
2:C:774:LEU:HD11	5:F:436:PHE:HB2	1.99	0.43
1:A:26:GLU:HA	1:A:27:PRO:HA	1.77	0.43
2:C:168:ARG:HG3	2:C:268:ASP:H	1.83	0.43
2:C:1101:THR:OG1	2:C:1109:VAL:O	2.36	0.43
3:D:252:ARG:HA	3:D:303:PRO:HA	2.01	0.43
1:A:59:GLU:HB2	1:A:139:TYR:HB2	2.00	0.43
2:C:249:LYS:HB2	2:C:252:LYS:HE2	2.00	0.43
3:D:64:LYS:HG3	5:F:393:GLY:HA3	2.00	0.43
1:B:38:ASN:O	1:B:42:ARG:HG3	2.18	0.43
2:C:745:ILE:HG13	2:C:803:ARG:HD3	2.00	0.43
3:D:45:PHE:O	3:D:86:ARG:NH2	2.52	0.43
3:D:278:VAL:HG11	3:D:281:ARG:HE	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:978:TYR:CG	3:D:988:ARG:HD3	2.53	0.43
3:D:1453:ALA:HB3	3:D:1455:LYS:HG3	2.00	0.43
1:A:12:THR:HG23	1:A:24:VAL:HB	2.00	0.43
1:A:40:LEU:HD23	1:A:40:LEU:HA	1.82	0.43
2:C:232:GLU:OE1	2:C:232:GLU:N	2.52	0.43
2:C:953:VAL:HG13	2:C:966:LEU:HD13	2.01	0.43
3:D:483:HIS:CG	3:D:484:PRO:HD2	2.54	0.43
3:D:646:LYS:HB3	3:D:688:TRP:CZ3	2.54	0.43
3:D:671:LYS:HE2	5:F:436:PHE:HA	2.01	0.43
3:D:871:ARG:HD2	3:D:873:LEU:HD21	2.01	0.43
5:F:286:LEU:HD22	5:F:319:VAL:HG23	2.00	0.43
2:C:675:ALA:HB2	2:C:867:VAL:HG11	2.01	0.43
2:C:1016:ILE:HG13	2:C:1017:THR:N	2.34	0.43
3:D:546:ARG:HE	3:D:546:ARG:HB3	1.58	0.43
4:E:44:GLU:OE2	4:E:72:ARG:NH2	2.52	0.43
1:A:88:ARG:HB3	1:A:204:SER:HA	2.01	0.42
2:C:1071:ILE:O	3:D:659:LYS:HD3	2.19	0.42
3:D:1134:LEU:HD11	3:D:1179:GLU:HB3	2.00	0.42
2:C:1113:GLU:O	2:C:1113:GLU:HG2	2.19	0.42
3:D:407:VAL:HG23	3:D:422:ALA:HB2	2.00	0.42
5:F:129:LYS:HA	5:F:139:GLN:OE1	2.19	0.42
1:A:99:LEU:HB3	1:A:114:PHE:CD2	2.54	0.42
2:C:580:MET:HE1	2:C:665:PHE:CD1	2.54	0.42
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.86	0.42
1:B:63:HIS:CE1	1:B:65:PHE:HB2	2.54	0.42
2:C:18:LEU:HG	2:C:542:LEU:HD21	2.01	0.42
2:C:881:ASN:O	2:C:884:GLN:HG2	2.19	0.42
3:D:554:LEU:HG	3:D:570:GLU:HB3	2.01	0.42
3:D:566:ILE:HD11	5:F:207:LEU:HD21	2.00	0.42
3:D:750:PRO:HB2	3:D:755:ALA:HB1	2.01	0.42
3:D:1105:ILE:HG23	3:D:1199:GLY:HA2	2.01	0.42
3:D:30:GLU:OE1	3:D:30:GLU:N	2.53	0.42
3:D:1160:LEU:HD22	3:D:1164:ARG:HH11	1.85	0.42
2:C:893:ALA:HB2	2:C:918:LEU:HD13	2.02	0.42
2:C:966:LEU:HD12	2:C:966:LEU:HA	1.91	0.42
5:F:274:ARG:NH1	9:F:508:HOH:O	2.52	0.42
1:A:99:LEU:HB3	1:A:114:PHE:HD2	1.85	0.42
1:B:86:VAL:HG12	1:B:124:ASN:OD1	2.20	0.42
1:B:153:ALA:HB2	1:B:167:VAL:C	2.44	0.42
2:C:84:ARG:HA	2:C:131:GLY:HA2	2.02	0.42
3:D:186:VAL:HA	3:D:200:ASP:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:994:GLN:HG3	3:D:995:LEU:N	2.35	0.42
2:C:114:PHE:HD2	2:C:115:LEU:N	2.18	0.42
3:D:179:VAL:HG22	3:D:180:LYS:H	1.85	0.42
3:D:729:HIS:O	3:D:732:VAL:HG22	2.19	0.42
3:D:30:GLU:HB3	3:D:40:GLU:HG3	2.02	0.42
3:D:317:MET:SD	3:D:337:LEU:HD22	2.60	0.42
1:B:71:VAL:HG22	1:B:132:LEU:HD22	2.01	0.41
5:F:217:TYR:C	5:F:227:LEU:HD21	2.44	0.41
1:A:152:PRO:HD2	1:A:155:ARG:HD3	2.00	0.41
3:D:361:VAL:HG21	3:D:367:ILE:CD1	2.50	0.41
3:D:886:VAL:HB	3:D:900:ILE:HD11	2.02	0.41
3:D:1099:VAL:O	3:D:1103:HIS:HB3	2.20	0.41
3:D:585:GLY:HA2	3:D:590:PRO:HG3	2.03	0.41
3:D:633:VAL:HG13	3:D:635:PRO:HD3	2.00	0.41
3:D:843:PHE:HE1	3:D:864:VAL:HG11	1.85	0.41
3:D:1407:LEU:HD23	3:D:1413:VAL:O	2.20	0.41
1:A:39:PRO:HG3	1:B:39:PRO:CG	2.47	0.41
2:C:209:ARG:HG3	2:C:210:GLU:N	2.34	0.41
2:C:1071:ILE:HD13	2:C:1071:ILE:HA	1.88	0.41
3:D:9:ARG:HB2	3:D:1456:LYS:HG2	2.03	0.41
3:D:895:VAL:O	3:D:899:LEU:HG	2.21	0.41
3:D:1274:ILE:HG22	3:D:1324:PRO:HA	2.01	0.41
1:B:226:ALA:O	1:B:228:PRO:HD3	2.20	0.41
3:D:370:ALA:O	9:D:2113:HOH:O	2.21	0.41
3:D:1301:LYS:HB3	3:D:1301:LYS:HE3	1.84	0.41
3:D:1434:TRP:NE1	3:D:1457:ASP:HB2	2.36	0.41
5:F:293:LEU:HD21	5:F:301:PRO:HG3	2.03	0.41
1:B:83:LYS:HE3	1:B:168:ASP:HB2	2.03	0.41
5:F:115:ILE:HG23	5:F:244:TYR:HD2	1.86	0.41
2:C:439:CYS:HB2	2:C:541:SER:HB3	2.03	0.41
2:C:616:GLU:C	2:C:618:GLY:H	2.29	0.41
3:D:783:ARG:CZ	3:D:1029:ARG:HD3	2.50	0.41
3:D:1068:LEU:HD23	3:D:1068:LEU:HA	1.88	0.41
3:D:1254:GLN:CB	3:D:1258:ARG:HB2	2.46	0.41
5:F:246:ARG:HB3	5:F:248:PHE:CD1	2.56	0.41
1:A:90:LEU:HD12	1:A:119:ASP:HA	2.03	0.41
2:C:504:GLU:HB2	2:C:507:ARG:HG3	2.03	0.41
2:C:607:ASP:OD1	2:C:610:ARG:HG3	2.21	0.41
2:C:1118:LYS:HG3	3:D:23:TYR:CZ	2.56	0.41
3:D:71:LYS:O	3:D:80:VAL:HG13	2.21	0.41
3:D:625:TYR:HB3	3:D:749:VAL:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1364:HIS:CD2	3:D:1366:LYS:HE2	2.56	0.41
3:D:1420:LEU:HD12	3:D:1420:LEU:HA	1.94	0.41
4:E:49:ARG:HD3	4:E:54:LEU:HD11	2.03	0.41
5:F:243:GLU:HG2	6:G:2:DA:H61	1.85	0.41
1:B:99:LEU:HB3	1:B:114:PHE:CD2	2.56	0.41
2:C:81:ASP:OD1	2:C:81:ASP:N	2.53	0.41
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.53	0.41
2:C:945:ALA:O	2:C:949:LYS:HG2	2.21	0.41
3:D:44:LEU:HB3	3:D:525:ARG:HH21	1.84	0.41
3:D:103:TRP:O	3:D:107:ASP:HB2	2.21	0.41
3:D:1270:ALA:N	9:D:2135:HOH:O	2.54	0.41
1:A:7:LYS:HB3	1:A:8:ALA:H	1.72	0.41
2:C:168:ARG:HD3	2:C:168:ARG:HA	1.93	0.41
2:C:1054:THR:OG1	2:C:1055:ILE:N	2.54	0.41
3:D:212:ARG:HB3	3:D:388:HIS:HD2	1.86	0.41
3:D:903:ASP:OD1	3:D:903:ASP:N	2.46	0.41
3:D:974:ILE:HD13	3:D:991:GLN:HB3	2.03	0.41
2:C:1076:VAL:HA	2:C:1077:PRO:HD3	1.88	0.40
3:D:179:VAL:HG22	3:D:183:GLU:HB3	2.02	0.40
3:D:1259:VAL:HG21	3:D:1356:TYR:HE1	1.85	0.40
3:D:1395:LEU:HD11	3:D:1400:VAL:HB	2.02	0.40
2:C:312:ALA:HB1	2:C:317:VAL:HG11	2.03	0.40
3:D:278:VAL:HG11	3:D:281:ARG:NE	2.35	0.40
3:D:394:LEU:HG	3:D:396:VAL:HG23	2.03	0.40
3:D:816:TYR:CG	3:D:836:VAL:HG11	2.56	0.40
1:A:31:GLY:O	1:A:35:THR:OG1	2.33	0.40
1:B:221:HIS:HA	1:B:224:TYR:CD2	2.56	0.40
2:C:74:GLY:N	2:C:93:PRO:O	2.49	0.40
2:C:374:ASN:OD1	2:C:375:SER:N	2.53	0.40
2:C:690:ILE:HD11	2:C:852:ILE:HG12	2.03	0.40
2:C:918:LEU:HB3	2:C:968:ASP:HA	2.03	0.40
3:D:557:LEU:HD12	3:D:570:GLU:HG3	2.02	0.40
3:D:573:MET:SD	5:F:225:LEU:HB3	2.61	0.40
3:D:952:ASP:OD1	3:D:1062:ARG:NH2	2.54	0.40
3:D:1147:ARG:HH22	3:D:1369:GLU:CD	2.28	0.40
3:D:1189:ARG:HH12	3:D:1203:LYS:HE3	1.87	0.40
1:B:74:ASP:O	1:B:78:ILE:HG12	2.21	0.40
2:C:211:LEU:HD12	2:C:214:TYR:CE2	2.56	0.40
2:C:686:ASP:OD1	2:C:879:ARG:NH1	2.53	0.40
3:D:288:MET:HG2	3:D:305:ALA:HB1	2.04	0.40
3:D:1150:ALA:O	3:D:1162:GLU:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:279:MET:HE2	5:F:279:MET:HB3	1.94	0.40
2:C:2:GLU:HG3	2:C:899:GLN:HB3	2.04	0.40
2:C:1032:PHE:HZ	2:C:1040:LEU:HD22	1.85	0.40
3:D:348:ALA:HB1	3:D:349:PRO:HD2	2.03	0.40
3:D:1047:LYS:HB3	3:D:1047:LYS:HE2	1.90	0.40
5:F:220:ARG:HD2	5:F:266:ILE:HD13	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	225/314 (72%)	218 (97%)	7 (3%)	0	100	100
1	B	225/314 (72%)	210 (93%)	15 (7%)	0	100	100
2	C	1108/1119 (99%)	1065 (96%)	40 (4%)	3 (0%)	36	58
3	D	1469/1524 (96%)	1416 (96%)	51 (4%)	2 (0%)	48	70
4	E	87/99 (88%)	84 (97%)	3 (3%)	0	100	100
5	F	330/347 (95%)	324 (98%)	6 (2%)	0	100	100
All	All	3444/3717 (93%)	3317 (96%)	122 (4%)	5 (0%)	48	70

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	1128	VAL
3	D	109	PRO
2	C	876	VAL
2	C	164	PRO
2	C	727	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/270 (72%)	186 (96%)	8 (4%)	27	54
1	B	194/270 (72%)	185 (95%)	9 (5%)	24	49
2	C	931/936 (100%)	873 (94%)	58 (6%)	16	36
3	D	1244/1281 (97%)	1186 (95%)	58 (5%)	23	48
4	E	79/88 (90%)	76 (96%)	3 (4%)	29	56
5	F	287/299 (96%)	277 (96%)	10 (4%)	32	59
All	All	2929/3144 (93%)	2783 (95%)	146 (5%)	22	46

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	VAL
1	A	151	VAL
1	A	167	VAL
1	A	168	ASP
1	A	172	SER
1	A	174	VAL
1	A	190	THR
1	A	222	LEU
1	B	58	ILE
1	B	60	ASP
1	B	80	LEU
1	B	101	LEU
1	B	129	ILE
1	B	138	LEU
1	B	206	THR
1	B	229	GLU
1	B	232	LEU
2	C	3	ILE
2	C	15	LEU
2	C	18	LEU
2	C	54	ILE
2	C	64	LEU

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Mol	Chain	Res	Type
2	C	70	GLU
2	C	107	LEU
2	C	140	ILE
2	C	158	TYR
2	C	159	ILE
2	C	182	VAL
2	C	194	VAL
2	C	210	GLU
2	C	218	VAL
2	C	238	LEU
2	C	240	THR
2	C	322	VAL
2	C	328	LEU
2	C	342	ASP
2	C	348	LEU
2	C	391	LEU
2	C	405	ARG
2	C	432	ARG
2	C	441	VAL
2	C	449	ILE
2	C	451	LEU
2	C	474	VAL
2	C	524	VAL
2	C	542	LEU
2	C	571	LEU
2	C	579	VAL
2	C	588	VAL
2	C	610	ARG
2	C	644	ARG
2	C	653	ASP
2	C	668	LEU
2	C	707	ARG
2	C	729	LEU
2	C	739	GLU
2	C	742	ILE
2	C	766	GLU
2	C	774	LEU
2	C	785	VAL
2	C	792	VAL
2	C	845	ASN
2	C	856	GLU
2	C	886	LEU

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Mol	Chain	Res	Type
2	C	890	LEU
2	C	897	LEU
2	C	918	LEU
2	C	966	LEU
2	C	988	VAL
2	C	1017	THR
2	C	1068	GLN
2	C	1076	VAL
2	C	1081	VAL
2	C	1088	LEU
2	C	1102	LEU
3	D	5	VAL
3	D	80	VAL
3	D	87	ARG
3	D	108	VAL
3	D	133	ILE
3	D	142	LEU
3	D	153	LEU
3	D	154	THR
3	D	185	VAL
3	D	227	LEU
3	D	240	GLU
3	D	259	VAL
3	D	261	LEU
3	D	279	VAL
3	D	289	THR
3	D	313	LEU
3	D	323	GLU
3	D	335	LEU
3	D	347	VAL
3	D	361	VAL
3	D	372	ASP
3	D	389	GLU
3	D	405	ASP
3	D	435	VAL
3	D	525	ARG
3	D	540	LEU
3	D	546	ARG
3	D	554	LEU
3	D	591	VAL
3	D	639	LEU
3	D	652	LEU

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Mol	Chain	Res	Type
3	D	681	ARG
3	D	694	VAL
3	D	711	LEU
3	D	721	VAL
3	D	749	VAL
3	D	784	ASP
3	D	795	VAL
3	D	922	LEU
3	D	955	VAL
3	D	959	GLU
3	D	1020	LEU
3	D	1129	THR
3	D	1132	LEU
3	D	1133	ARG
3	D	1137	ARG
3	D	1188	VAL
3	D	1190	SER
3	D	1262	LEU
3	D	1288	ASP
3	D	1311	LEU
3	D	1325	LEU
3	D	1335	LEU
3	D	1376	LEU
3	D	1395	LEU
3	D	1447	LEU
3	D	1460	ILE
3	D	1497	GLU
4	E	30	LEU
4	E	51	LEU
4	E	80	VAL
5	F	137	LEU
5	F	181	LEU
5	F	202	LEU
5	F	227	LEU
5	F	244	TYR
5	F	274	ARG
5	F	292	GLN
5	F	293	LEU
5	F	423	LEU
5	F	438	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	156	HIS
1	A	180	GLN
1	A	213	GLN
1	B	63	HIS
1	B	124	ASN
1	B	212	ASN
2	C	99	GLN
2	C	390	GLN
2	C	575	GLN
2	C	670	GLN
2	C	860	HIS
2	C	991	GLN
2	C	1050	GLN
3	D	130	ASN
3	D	388	HIS
3	D	483	HIS
3	D	680	GLN
3	D	768	ASN
3	D	794	GLN
3	D	917	GLN
3	D	961	GLN
3	D	1103	HIS
3	D	1323	GLN
3	D	1333	HIS
3	D	1364	HIS
3	D	1367	HIS
4	E	33	HIS
5	F	98	GLN
5	F	200	GLN
5	F	284	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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	227/314 (72%)	0.11	1 (0%) 88 86	49, 70, 108, 133	0
1	B	227/314 (72%)	0.48	9 (3%) 42 37	60, 94, 142, 176	0
2	C	1112/1119 (99%)	0.16	16 (1%) 73 69	35, 77, 136, 170	0
3	D	1475/1524 (96%)	0.13	19 (1%) 75 71	36, 75, 136, 163	0
4	E	89/99 (89%)	0.13	2 (2%) 62 57	56, 85, 141, 147	0
5	F	334/347 (96%)	0.25	11 (3%) 49 43	49, 97, 145, 166	0
6	G	10/31 (32%)	0.11	0 100 100	100, 109, 139, 151	0
All	All	3474/3748 (92%)	0.17	58 (1%) 69 64	35, 80, 137, 176	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1495	ILE	3.6
2	C	311	PHE	3.3
3	D	431	ILE	3.2
3	D	324	ALA	3.1
2	C	100	LEU	3.1
2	C	66	LEU	3.0
2	C	54	ILE	3.0
1	B	123	MET	2.9
3	D	205	TYR	2.9
5	F	153	THR	2.9
1	B	66	SER	2.8
1	B	56	VAL	2.7
3	D	1128	VAL	2.7
3	D	206	ARG	2.7
3	D	370	ALA	2.6
3	D	236	TYR	2.6
2	C	98	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	58	ILE	2.5
5	F	170	THR	2.5
2	C	999	HIS	2.5
5	F	166	PRO	2.5
1	A	233	LEU	2.4
2	C	368	THR	2.4
3	D	440	VAL	2.4
3	D	982	PHE	2.4
3	D	1309	ALA	2.4
4	E	74	PHE	2.3
1	B	85	LEU	2.3
1	B	158	ILE	2.3
2	C	496	ILE	2.3
5	F	171	VAL	2.3
1	B	63	HIS	2.3
1	B	162	ILE	2.3
5	F	168	PRO	2.3
3	D	282	TYR	2.2
3	D	432	TYR	2.2
2	C	367	LEU	2.2
1	B	122	ILE	2.2
4	E	2	ALA	2.2
2	C	111	ASP	2.2
2	C	64	LEU	2.2
3	D	265	ALA	2.2
5	F	301	PRO	2.2
5	F	154	ALA	2.1
2	C	218	VAL	2.1
2	C	300	ASP	2.1
3	D	400	VAL	2.1
3	D	1082	ALA	2.1
5	F	227	LEU	2.1
3	D	191	LEU	2.1
5	F	395	GLU	2.1
2	C	107	LEU	2.1
5	F	297	LEU	2.1
2	C	47	ALA	2.0
2	C	815	LEU	2.0
3	D	801	GLY	2.0
3	D	322	VAL	2.0
5	F	293	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	MG	D	2003	1/1	0.89	0.08	74,74,74,74	0
7	ZN	D	2002	1/1	0.93	0.18	216,216,216,216	0
7	ZN	D	2001	1/1	0.99	0.11	110,110,110,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.