



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:59 AM UTC

PDB ID : 5ZX3 / pdb_00005zx3
Title : Mycobacterium tuberculosis RNA polymerase holoenzyme with ECF sigma factor sigma H
Authors : Li, L.; Zhang, Y.
Deposited on : 2018-05-17
Resolution : 2.75 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

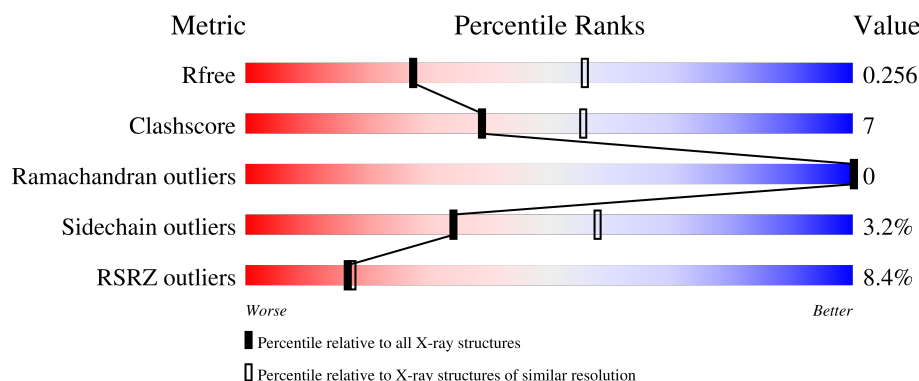
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	368	 3% 51% 8% 40%
1	B	368	 7% 47% 15% 37%
2	C	1174	 11% 78% 15% 6%
3	D	1317	 5% 78% 17% 5%
4	E	110	 5% 55% 13% 31%

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Mol	Chain	Length	Quality of chain
5	F	218	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23311 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	221	Total	C	N	O	S	0	0	0
			1673	1054	288	329	2			
1	B	231	Total	C	N	O	S	0	0	0
			1728	1090	293	342	3			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP P9WGZ1
A	-19	GLY	-	expression tag	UNP P9WGZ1
A	-18	HIS	-	expression tag	UNP P9WGZ1
A	-17	HIS	-	expression tag	UNP P9WGZ1
A	-16	HIS	-	expression tag	UNP P9WGZ1
A	-15	HIS	-	expression tag	UNP P9WGZ1
A	-14	HIS	-	expression tag	UNP P9WGZ1
A	-13	HIS	-	expression tag	UNP P9WGZ1
A	-12	HIS	-	expression tag	UNP P9WGZ1
A	-11	HIS	-	expression tag	UNP P9WGZ1
A	-10	HIS	-	expression tag	UNP P9WGZ1
A	-9	HIS	-	expression tag	UNP P9WGZ1
A	-8	SER	-	expression tag	UNP P9WGZ1
A	-7	SER	-	expression tag	UNP P9WGZ1
A	-6	GLY	-	expression tag	UNP P9WGZ1
A	-5	HIS	-	expression tag	UNP P9WGZ1
A	-4	ILE	-	expression tag	UNP P9WGZ1
A	-3	GLU	-	expression tag	UNP P9WGZ1
A	-2	GLY	-	expression tag	UNP P9WGZ1
A	-1	ARG	-	expression tag	UNP P9WGZ1
A	0	HIS	-	expression tag	UNP P9WGZ1
B	-20	MET	-	expression tag	UNP P9WGZ1
B	-19	GLY	-	expression tag	UNP P9WGZ1
B	-18	HIS	-	expression tag	UNP P9WGZ1
B	-17	HIS	-	expression tag	UNP P9WGZ1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP P9WGZ1
B	-15	HIS	-	expression tag	UNP P9WGZ1
B	-14	HIS	-	expression tag	UNP P9WGZ1
B	-13	HIS	-	expression tag	UNP P9WGZ1
B	-12	HIS	-	expression tag	UNP P9WGZ1
B	-11	HIS	-	expression tag	UNP P9WGZ1
B	-10	HIS	-	expression tag	UNP P9WGZ1
B	-9	HIS	-	expression tag	UNP P9WGZ1
B	-8	SER	-	expression tag	UNP P9WGZ1
B	-7	SER	-	expression tag	UNP P9WGZ1
B	-6	GLY	-	expression tag	UNP P9WGZ1
B	-5	HIS	-	expression tag	UNP P9WGZ1
B	-4	ILE	-	expression tag	UNP P9WGZ1
B	-3	GLU	-	expression tag	UNP P9WGZ1
B	-2	GLY	-	expression tag	UNP P9WGZ1
B	-1	ARG	-	expression tag	UNP P9WGZ1
B	0	HIS	-	expression tag	UNP P9WGZ1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1105	Total	C	N	O	S	0	0	0
			8188	5112	1443	1596	37			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	5	MET	-	expression tag	UNP P9WGY9
C	6	VAL	-	expression tag	UNP P9WGY9

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1257	Total	C	N	O	S	0	0	0
			9742	6100	1762	1840	40			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	expression tag	UNP P9WGY7
D	1	VAL	-	expression tag	UNP P9WGY7

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	76	Total	C	N	O	0	0	0
			596	380	101	115			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	173	Total	C	N	O	S	0	0	0
			1329	837	224	263	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	GLY	-	expression tag	UNP P9WGH9
F	0	ALA	-	expression tag	UNP P9WGH9

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

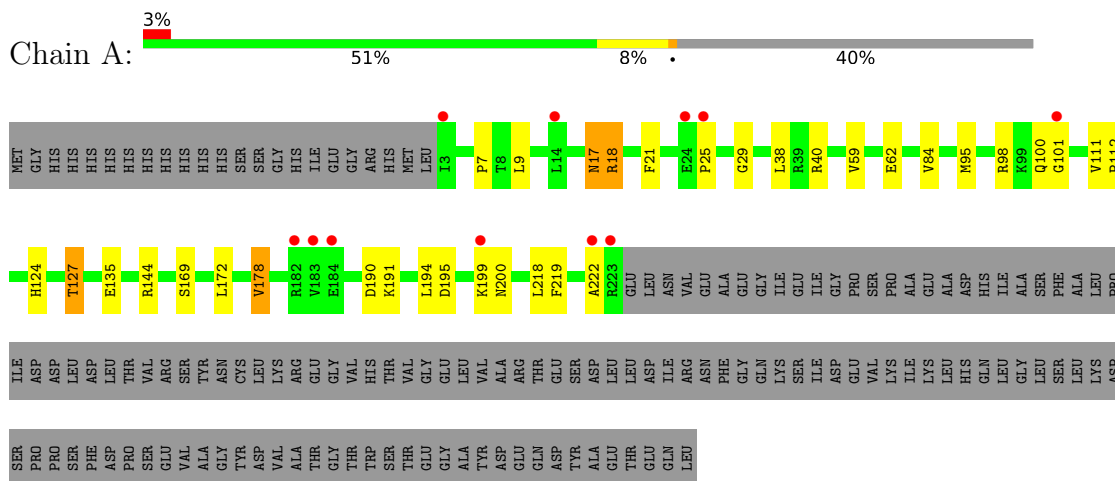
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			1	1		
7	C	29	Total	O	0	0
			29	29		
7	D	22	Total	O	0	0
			22	22		
7	F	1	Total	O	0	0
			1	1		

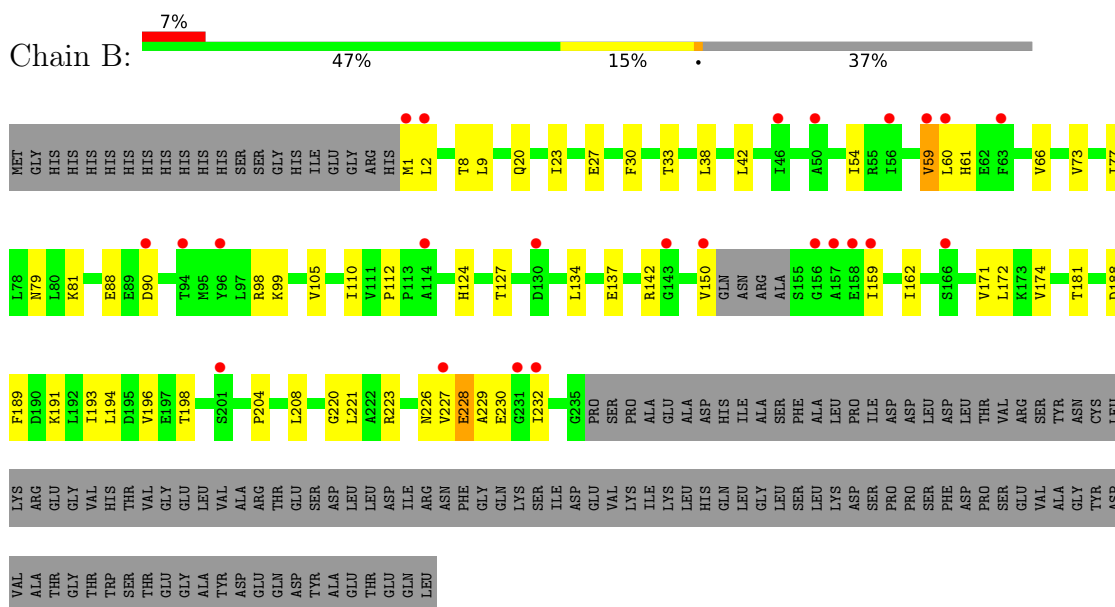
3 Residue-property plots

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.

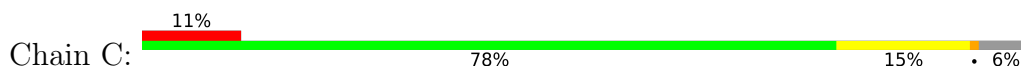
- Molecule 1: DNA-directed RNA polymerase subunit alpha

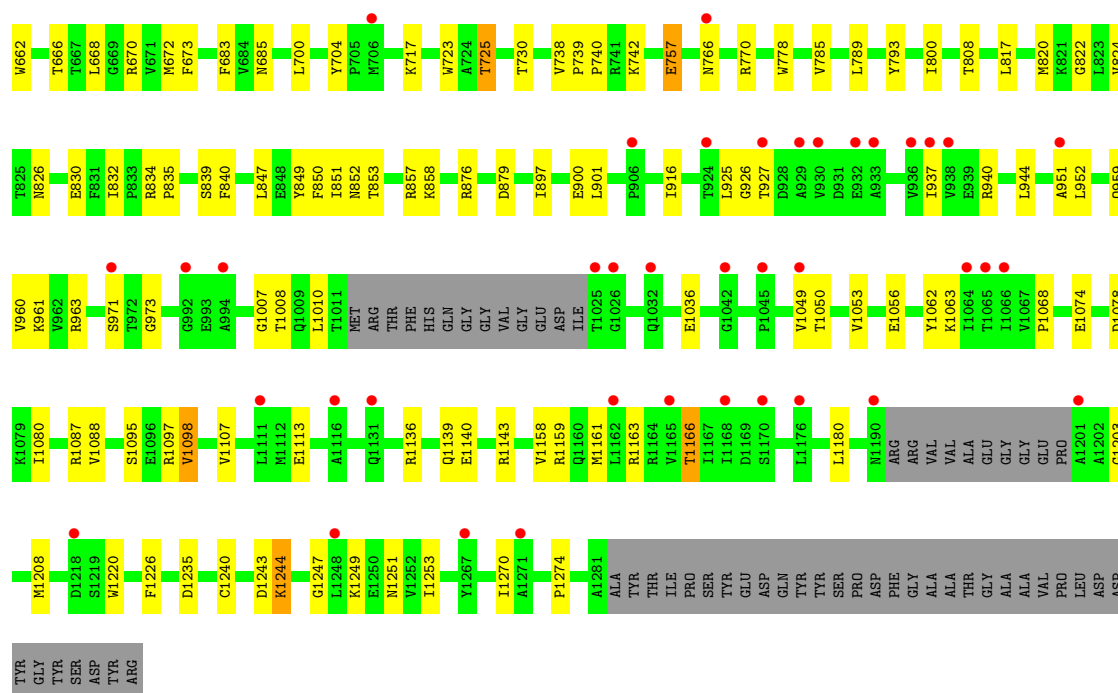


- Molecule 1: DNA-directed RNA polymerase subunit alpha

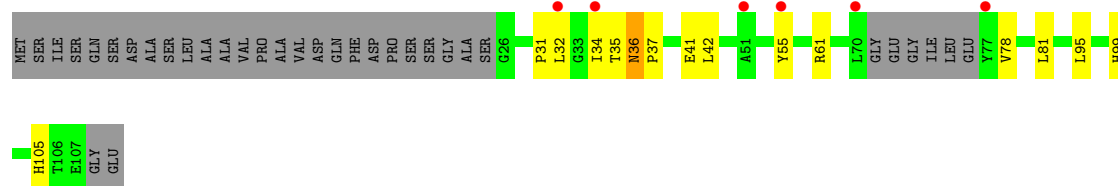


- Molecule 2: DNA-directed RNA polymerase subunit beta

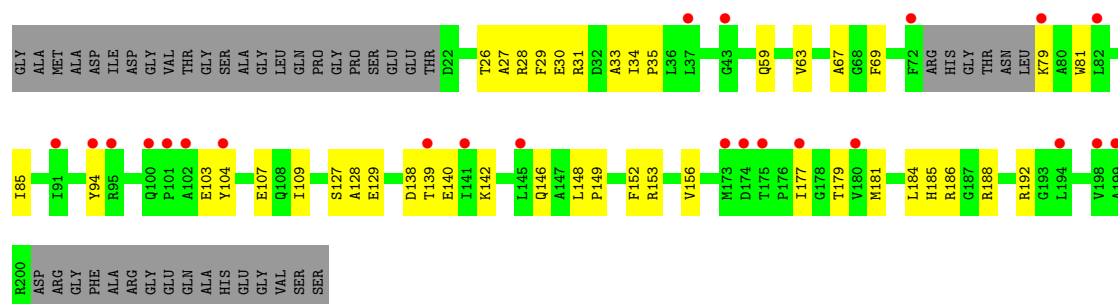




- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: ECF RNA polymerase sigma factor SigH



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	130.57Å 159.79Å 131.44Å 90.00° 118.72° 90.00°	Depositor
Resolution (Å)	41.64 – 2.75 41.64 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.7 (41.64-2.75) 97.7 (41.64-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.218 , 0.258 0.219 , 0.256	Depositor DCC
R_{free} test set	2160 reflections (1.80%)	wwPDB-VP
Wilson B-factor (Å ²)	78.9	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.002 for -h-l,k,h 0.002 for l,k,-h-l 0.014 for h,-k,-h-l 0.014 for -h-l,-k,l 0.011 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23311	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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

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	0.13	0/1699	0.37	0/2313
1	B	0.13	0/1753	0.36	0/2386
2	C	0.15	1/8333 (0.0%)	0.36	0/11331
3	D	0.14	0/9905	0.35	0/13402
4	E	0.13	0/607	0.34	0/826
5	F	0.13	0/1355	0.35	0/1843
All	All	0.14	1/23652 (0.0%)	0.36	0/32101

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	94	SER	C-N	5.05	1.45	1.33

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	1673	0	1707	24	0
1	B	1728	0	1747	35	0
2	C	8188	0	7786	111	0
3	D	9742	0	9715	147	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	596	0	594	13	0
5	F	1329	0	1231	29	0
6	D	2	0	0	0	0
7	A	1	0	0	0	0
7	C	29	0	0	0	0
7	D	22	0	0	0	0
7	F	1	0	0	0	0
All	All	23311	0	22780	314	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 7.

All (314) 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:527:LEU:HD21	3:D:581:MET:HE1	1.61	0.83
3:D:581:MET:HE3	3:D:717:LYS:HA	1.62	0.80
2:C:1046:THR:HG22	5:F:127:SER:HB2	1.62	0.79
3:D:155:MET:HE1	3:D:219:LEU:HB3	1.65	0.78
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.63	0.78
3:D:739:PRO:HG2	3:D:742:LYS:HB2	1.66	0.77
3:D:190:LYS:HD2	3:D:192:ASP:HB3	1.66	0.77
2:C:1024:THR:H	3:D:730:THR:HG21	1.49	0.76
2:C:388:GLN:HG2	2:C:430:PHE:HB2	1.69	0.74
1:A:95:MET:HE3	1:A:112:PRO:HB3	1.73	0.71
2:C:612:GLN:HG2	2:C:1031:MET:HE1	1.72	0.70
3:D:1274:PRO:HG3	4:E:78:VAL:HG11	1.73	0.70
2:C:782:ALA:O	2:C:791:ARG:NH2	2.25	0.70
5:F:26:THR:O	5:F:29:PHE:HB3	1.92	0.70
3:D:1274:PRO:HB3	4:E:81:LEU:HD11	1.74	0.69
3:D:824:VAL:HG11	3:D:852:ASN:HA	1.77	0.67
1:B:98:ARG:HA	1:B:134:LEU:O	1.94	0.67
3:D:834:ARG:HD3	3:D:835:PRO:HD2	1.77	0.67
2:C:758:ASP:HB3	2:C:868:LEU:HD23	1.77	0.66
2:C:611:MET:HE1	2:C:892:LYS:HG2	1.77	0.66
3:D:360:LEU:HD21	5:F:67:ALA:HB2	1.78	0.66
3:D:879:ASP:OD2	3:D:1249:LYS:NZ	2.29	0.65
1:A:9:LEU:HD11	1:A:21:PHE:HB3	1.78	0.65
3:D:417:LEU:HD22	3:D:1253:ILE:HG23	1.79	0.64
3:D:573:PRO:HG2	3:D:576:MET:HE2	1.80	0.64
1:B:90:ASP:OD2	1:B:142:ARG:NH1	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:458:LEU:HD21	2:C:496:LEU:HD13	1.81	0.63
4:E:36:ASN:CG	4:E:37:PRO:HD3	2.24	0.63
2:C:93:LEU:HD22	2:C:393:MET:HB3	1.80	0.63
2:C:792:ILE:HG13	2:C:850:ILE:HD12	1.79	0.63
2:C:207:SER:HB3	2:C:309:ALA:HB2	1.81	0.62
3:D:1166:THR:O	3:D:1203:GLY:HA2	1.99	0.62
3:D:971:SER:O	3:D:1163:ARG:NH2	2.33	0.62
2:C:1067:ARG:HH12	3:D:415:GLN:HA	1.65	0.61
3:D:876:ARG:NH1	3:D:1036:GLU:OE1	2.33	0.61
2:C:124:ASP:OD1	2:C:851:ARG:NH1	2.33	0.61
3:D:1062:TYR:N	3:D:1080:ILE:O	2.33	0.61
3:D:47:PHE:O	3:D:88:ARG:NH2	2.34	0.61
5:F:28:ARG:O	5:F:31:ARG:HG3	2.01	0.61
3:D:357:LEU:HD21	5:F:63:VAL:HG22	1.82	0.61
1:A:40:ARG:HG3	2:C:902:GLU:HG3	1.83	0.61
2:C:315:LYS:NZ	2:C:375:ASN:OD1	2.34	0.61
2:C:474:ASP:HA	3:D:857:ARG:HG2	1.82	0.61
3:D:326:PRO:HG2	5:F:109:ILE:HD12	1.81	0.61
3:D:456:VAL:O	3:D:460:LEU:HB2	2.01	0.61
3:D:1247:GLY:O	3:D:1251:ASN:ND2	2.34	0.61
2:C:635:ALA:HB2	2:C:713:MET:HG2	1.83	0.61
2:C:453:ARG:NH1	2:C:500:LEU:O	2.33	0.60
3:D:113:ARG:NH2	3:D:1235:ASP:OD1	2.34	0.60
3:D:599:TYR:HA	3:D:610:GLY:HA3	1.83	0.60
2:C:1043:ALA:HB2	3:D:447:MET:HG2	1.84	0.60
4:E:31:PRO:HB3	4:E:35:THR:HG23	1.84	0.60
2:C:684:ALA:HA	2:C:706:PRO:HG3	1.84	0.60
1:A:7:PRO:HA	1:A:25:PRO:HG2	1.84	0.60
1:B:1:MET:HE2	1:B:2:LEU:HG	1.83	0.59
1:B:226:ASN:OD1	1:B:227:VAL:N	2.36	0.59
2:C:1052:ILE:HG12	3:D:326:PRO:HG3	1.83	0.59
3:D:565:ILE:HG23	3:D:575:ALA:HB3	1.84	0.58
2:C:921:GLY:O	2:C:925:ARG:HG2	2.03	0.58
3:D:1158:VAL:HA	3:D:1161:MET:HE3	1.84	0.58
1:A:222:ALA:HA	1:B:9:LEU:HD22	1.85	0.58
3:D:45:GLY:H	3:D:48:CYS:HB2	1.69	0.57
1:A:17:ASN:OD1	1:A:17:ASN:N	2.37	0.57
2:C:62:GLU:OE2	2:C:69:ARG:NH2	2.38	0.57
2:C:1087:GLU:HG3	2:C:1091:ILE:HD11	1.86	0.57
3:D:345:ARG:NH2	5:F:103:GLU:OE1	2.37	0.57
2:C:741:LEU:HA	2:C:746:VAL:HG13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:307:ASN:HD21	3:D:1240:CYS:HB2	1.70	0.56
3:D:1139:GLN:HG3	3:D:1143:ARG:HD2	1.86	0.56
2:C:723:ILE:O	3:D:730:THR:HG23	2.05	0.56
1:A:172:LEU:HD13	1:A:199:LYS:HG2	1.87	0.55
3:D:826:ASN:N	3:D:830:GLU:O	2.32	0.55
4:E:36:ASN:OD1	4:E:36:ASN:N	2.37	0.55
5:F:31:ARG:O	5:F:35:PRO:HD2	2.06	0.55
3:D:739:PRO:HD3	3:D:789:LEU:HD13	1.89	0.55
3:D:973:GLY:O	3:D:1159:ARG:NH2	2.40	0.55
2:C:549:ASP:OD1	2:C:550:ALA:N	2.40	0.55
3:D:577:PRO:HB3	3:D:581:MET:HE2	1.89	0.55
1:A:124:HIS:HE1	1:A:127:THR:HG22	1.72	0.54
1:A:222:ALA:HB1	1:B:208:LEU:HG	1.88	0.54
2:C:255:SER:O	2:C:259:ARG:CB	2.55	0.54
3:D:400:LYS:HG3	5:F:107:GLU:HG3	1.90	0.54
2:C:1109:GLY:HA3	3:D:458:LYS:HE3	1.90	0.54
2:C:474:ASP:OD1	2:C:474:ASP:N	2.41	0.54
3:D:412:ARG:HA	3:D:416:ASN:HB2	1.90	0.54
1:A:169:SER:O	1:A:199:LYS:NZ	2.41	0.53
4:E:32:LEU:O	4:E:35:THR:HG22	2.09	0.53
1:B:99:LYS:HD3	1:B:105:VAL:HG22	1.91	0.53
2:C:557:PRO:HB2	2:C:558:ARG:HD3	1.91	0.53
3:D:876:ARG:HG2	3:D:1226:PHE:HZ	1.74	0.53
2:C:1112:ILE:O	4:E:61:ARG:NH2	2.42	0.53
3:D:1270:ILE:HD13	4:E:55:TYR:HE1	1.74	0.53
2:C:1076:MET:HE1	3:D:497:LEU:HD13	1.91	0.52
5:F:181:MET:HE3	5:F:185:HIS:HE1	1.74	0.52
2:C:1045:SER:HB3	3:D:450:GLU:O	2.09	0.52
3:D:447:MET:HE1	3:D:543:VAL:HG21	1.91	0.52
3:D:487:LEU:O	3:D:491:ILE:HG12	2.08	0.52
1:B:77:ILE:HG22	1:B:81:LYS:HE2	1.90	0.52
3:D:491:ILE:HG23	3:D:514:PRO:HG2	1.90	0.52
2:C:486:ILE:HD11	3:D:849:TYR:HE1	1.74	0.52
3:D:384:ASN:HB2	3:D:401:SER:HB3	1.92	0.52
2:C:619:VAL:HG12	2:C:750:ILE:HG13	1.92	0.51
1:A:29:GLY:N	1:A:190:ASP:OD2	2.42	0.51
1:B:124:HIS:HE1	1:B:127:THR:HG23	1.75	0.51
1:B:191:LYS:HE2	1:B:193:ILE:HD11	1.92	0.51
2:C:288:THR:HB	2:C:291:SER:HB3	1.91	0.51
1:B:228:GLU:HG3	1:B:229:ALA:N	2.25	0.51
2:C:442:GLN:HE21	2:C:679:ASN:H	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:ILE:HA	1:B:137:GLU:O	2.10	0.50
2:C:1046:THR:HG21	5:F:129:GLU:H	1.76	0.50
2:C:1091:ILE:HD12	2:C:1102:VAL:HG21	1.93	0.50
3:D:98:ALA:HB3	3:D:354:LEU:HD23	1.94	0.50
5:F:27:ALA:O	5:F:30:GLU:HB2	2.12	0.50
2:C:792:ILE:HD12	2:C:792:ILE:H	1.76	0.50
3:D:56:ARG:NH1	3:D:59:GLU:OE2	2.44	0.50
3:D:778:TRP:CD2	3:D:835:PRO:HG3	2.47	0.50
3:D:1049:VAL:HA	3:D:1107:VAL:HG22	1.93	0.50
1:B:66:VAL:HG23	1:B:73:VAL:HG22	1.94	0.50
2:C:115:VAL:HG11	2:C:129:TYR:CE1	2.47	0.50
2:C:926:MET:HE2	3:D:840:PHE:HB2	1.92	0.50
3:D:1270:ILE:HD13	4:E:55:TYR:CE1	2.47	0.50
2:C:473:ARG:O	3:D:857:ARG:NH1	2.44	0.50
3:D:1244:LYS:NZ	3:D:1244:LYS:H	2.09	0.50
2:C:717:LYS:HG3	2:C:746:VAL:HG23	1.94	0.50
3:D:482:GLN:OE1	3:D:482:GLN:N	2.41	0.50
3:D:103:HIS:HB3	3:D:106:TYR:HD2	1.77	0.49
4:E:42:LEU:HD13	4:E:95:LEU:HD22	1.93	0.49
2:C:403:ARG:NH1	2:C:416:THR:O	2.46	0.49
2:C:715:LEU:HB2	2:C:1031:MET:HE2	1.93	0.49
3:D:666:THR:HG21	3:D:683:PHE:CE1	2.48	0.49
2:C:1136:GLU:OE1	3:D:11:ARG:NH2	2.40	0.49
3:D:271:ASP:OD1	3:D:303:GLN:NE2	2.40	0.49
3:D:670:ARG:NH1	3:D:685:ASN:OD1	2.39	0.49
2:C:183:PRO:HB2	2:C:312:GLY:HA3	1.95	0.48
3:D:1136:ARG:O	3:D:1140:GLU:HG2	2.12	0.48
2:C:967:GLN:HG3	2:C:968:PRO:HD2	1.95	0.48
3:D:138:SER:OG	3:D:253:THR:OG1	2.27	0.48
2:C:355:MET:N	2:C:363:VAL:O	2.46	0.48
3:D:820:MET:HE2	3:D:822:GLY:HA2	1.94	0.48
3:D:901:LEU:HD11	3:D:952:LEU:HD13	1.95	0.48
2:C:1053:THR:HG23	2:C:1055:GLN:H	1.78	0.48
1:A:40:ARG:HH11	2:C:1014:ARG:HA	1.79	0.48
5:F:152:PHE:HE2	5:F:186:ARG:HB2	1.78	0.48
2:C:77:ARG:HH11	2:C:505:ARG:HH12	1.61	0.48
2:C:464:SER:HB2	2:C:467:ARG:HG3	1.95	0.48
3:D:116:TYR:O	3:D:295:ARG:NH1	2.47	0.48
3:D:925:LEU:HB3	3:D:940:ARG:HA	1.95	0.48
5:F:138:ASP:C	5:F:140:GLU:H	2.22	0.48
3:D:599:TYR:OH	3:D:608:GLU:OE2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LEU:HD13	1:A:194:LEU:HD22	1.96	0.47
2:C:558:ARG:H	2:C:558:ARG:HH11	1.62	0.47
3:D:668:LEU:HG	3:D:672:MET:HE2	1.96	0.47
2:C:926:MET:HE3	2:C:926:MET:HA	1.96	0.47
2:C:473:ARG:HB3	2:C:495:GLY:HA3	1.97	0.47
2:C:113:ASP:HB3	2:C:132:PRO:HD2	1.96	0.47
5:F:149:PRO:HG2	5:F:152:PHE:CD1	2.50	0.47
2:C:771:ARG:NH1	2:C:784:LEU:O	2.48	0.47
1:A:124:HIS:CE1	1:A:127:THR:HG22	2.48	0.47
1:B:30:PHE:HA	1:B:33:THR:OG1	2.15	0.47
3:D:700:LEU:O	3:D:704:TYR:HB2	2.15	0.47
2:C:727:GLU:H	3:D:725:THR:CG2	2.27	0.47
3:D:144:ARG:NH2	3:D:229:LEU:O	2.44	0.47
2:C:311:VAL:HG13	2:C:509:PHE:HB3	1.97	0.46
1:B:181:THR:O	1:B:189:PHE:HB2	2.15	0.46
2:C:408:ASP:O	2:C:412:ILE:HG23	2.16	0.46
2:C:507:ASN:HB2	2:C:511:PHE:O	2.15	0.46
2:C:338:VAL:O	2:C:342:ILE:HG12	2.15	0.46
3:D:409:LYS:O	3:D:415:GLN:HG3	2.15	0.46
3:D:876:ARG:HG2	3:D:1226:PHE:CZ	2.51	0.46
1:B:223:ARG:HH12	1:B:227:VAL:HA	1.81	0.46
1:B:8:THR:O	1:B:23:ILE:HA	2.16	0.46
2:C:1126:LYS:HE3	3:D:92:MET:HE2	1.98	0.46
1:A:18:ARG:NH1	1:A:195:ASP:OD2	2.49	0.46
2:C:446:LEU:HB2	2:C:713:MET:HE2	1.98	0.46
3:D:595:ASP:HB3	3:D:631:ALA:HB2	1.98	0.46
2:C:1079:TYR:CD2	3:D:559:MET:HG2	2.51	0.46
3:D:1095:SER:OG	3:D:1097:ARG:NH2	2.49	0.46
1:A:219:PHE:HE1	1:B:38:LEU:HG	1.80	0.45
2:C:473:ARG:HD3	2:C:494:ILE:O	2.17	0.45
2:C:803:VAL:HG11	2:C:869:VAL:HG11	1.98	0.45
1:A:100:GLN:HG3	1:A:101:GLY:N	2.32	0.45
3:D:1068:PRO:HD3	3:D:1074:GLU:HA	1.98	0.45
3:D:102:THR:HG22	3:D:313:VAL:HG22	1.99	0.45
1:B:124:HIS:CE1	1:B:127:THR:HG23	2.52	0.45
2:C:623:ALA:HB2	2:C:709:ASP:HB3	1.98	0.45
2:C:926:MET:HE1	3:D:817:LEU:HD13	1.99	0.45
3:D:32:GLU:HB3	3:D:42:GLU:HG3	1.97	0.45
2:C:352:GLN:O	2:C:365:VAL:HB	2.17	0.45
2:C:441:ASP:HA	2:C:680:HIS:NE2	2.32	0.45
3:D:466:ALA:HB2	3:D:475:MET:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:556:GLU:OE1	2:C:558:ARG:NH1	2.41	0.45
3:D:445:LYS:NZ	3:D:518:GLU:OE2	2.48	0.45
3:D:515:MET:HB3	3:D:515:MET:HE2	1.67	0.45
3:D:1078:ASP:OD1	3:D:1078:ASP:N	2.48	0.45
4:E:41:GLU:OE1	4:E:99:HIS:NE2	2.45	0.45
2:C:38:ARG:HG2	2:C:973:SER:HB2	1.98	0.45
3:D:116:TYR:HB3	3:D:298:VAL:HG11	1.99	0.45
3:D:413:PHE:HA	3:D:417:LEU:HD12	1.98	0.45
2:C:759:ALA:HB2	2:C:769:ILE:HG13	1.99	0.45
2:C:848:ILE:HD13	2:C:874:ALA:HB2	1.99	0.45
3:D:3:ASP:OD1	3:D:3:ASP:N	2.48	0.45
3:D:250:GLU:CD	3:D:250:GLU:H	2.25	0.44
3:D:143:MET:HG2	3:D:251:TYR:CE2	2.52	0.44
5:F:29:PHE:O	5:F:30:GLU:C	2.60	0.44
5:F:188:ARG:O	5:F:192:ARG:HG3	2.17	0.44
1:A:7:PRO:HB2	1:B:221:LEU:HD11	2.00	0.44
2:C:77:ARG:NH1	2:C:505:ARG:HH12	2.15	0.44
3:D:757:GLU:OE1	3:D:770:ARG:NH1	2.44	0.44
2:C:896:GLY:HA2	3:D:431:VAL:HB	2.00	0.44
5:F:29:PHE:HB2	5:F:69:PHE:CE2	2.52	0.44
2:C:1103:TYR:CE2	3:D:454:PRO:HG3	2.52	0.44
3:D:766:ASN:O	3:D:770:ARG:N	2.44	0.44
1:A:40:ARG:NH1	2:C:1014:ARG:HA	2.32	0.44
2:C:140:ILE:HG13	2:C:147:ILE:HG12	1.99	0.44
3:D:585:LEU:HD13	3:D:673:PHE:HE1	1.82	0.44
3:D:1166:THR:O	3:D:1203:GLY:CA	2.65	0.44
3:D:26:GLY:HA3	3:D:51:ILE:HG22	2.00	0.44
3:D:292:ALA:O	3:D:296:LEU:HB2	2.18	0.44
3:D:527:LEU:HD22	3:D:575:ALA:O	2.18	0.44
1:B:59:VAL:HG11	1:B:66:VAL:HG22	2.00	0.43
1:B:79:ASN:HB3	3:D:636:ARG:HH12	1.83	0.43
3:D:1087:ARG:HA	3:D:1113:GLU:HG2	2.00	0.43
3:D:793:TYR:HB3	3:D:800:ILE:HG13	2.00	0.43
1:B:230:GLU:O	1:B:232:ILE:HG13	2.18	0.43
2:C:148:LYS:HZ2	2:C:149:SER:N	2.16	0.43
3:D:500:ARG:NH1	3:D:539:ASP:OD2	2.51	0.43
2:C:163:LYS:HE3	2:C:639:GLY:O	2.18	0.43
3:D:900:GLU:OE2	3:D:959:GLN:NE2	2.40	0.43
3:D:925:LEU:HD13	3:D:944:LEU:HD21	2.00	0.43
3:D:1180:LEU:HD13	3:D:1208:MET:HE2	1.98	0.43
2:C:189:GLU:HA	2:C:200:HIS:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:927:THR:HG23	3:D:961:LYS:HD3	2.01	0.43
4:E:55:TYR:CZ	4:E:105:HIS:HB2	2.53	0.43
2:C:764:LEU:HB2	2:C:808:PRO:HB2	1.99	0.43
5:F:153:ARG:HA	5:F:156:VAL:HG22	2.00	0.43
2:C:157:PHE:HE1	2:C:389:ILE:HD11	1.83	0.43
2:C:1131:LEU:HD13	3:D:105:TRP:CH2	2.53	0.43
3:D:850:PHE:O	3:D:853:THR:OG1	2.34	0.43
2:C:188:ASP:HA	2:C:367:THR:HG23	1.99	0.43
2:C:516:TYR:HB3	2:C:578:TYR:HB3	2.01	0.43
2:C:705:GLY:N	2:C:708:THR:OG1	2.52	0.43
3:D:1007:GLY:HA2	3:D:1010:LEU:HD13	2.01	0.43
3:D:325:ARG:HD2	3:D:341:ASN:OD1	2.19	0.43
3:D:579:LEU:HD23	3:D:808:THR:HB	2.00	0.43
3:D:1088:VAL:HG22	3:D:1098:VAL:HG22	2.01	0.43
1:B:171:VAL:HA	1:B:198:THR:HA	2.00	0.42
3:D:817:LEU:O	3:D:839:SER:HB2	2.19	0.42
5:F:29:PHE:O	5:F:33:ALA:N	2.46	0.42
5:F:81:TRP:CZ2	5:F:85:ILE:HD11	2.53	0.42
1:A:178:VAL:HA	1:A:191:LYS:O	2.19	0.42
1:B:20:GLN:HA	1:B:194:LEU:O	2.20	0.42
2:C:515:PRO:HG2	2:C:581:VAL:HG21	2.01	0.42
2:C:1094:ASP:OD1	2:C:1094:ASP:N	2.52	0.42
2:C:344:TYR:CZ	2:C:365:VAL:HA	2.55	0.42
2:C:545:ASN:O	2:C:545:ASN:ND2	2.53	0.42
2:C:828:LYS:HG2	2:C:830:ARG:H	1.84	0.42
1:B:188:ASP:OD1	1:B:188:ASP:N	2.43	0.42
1:B:220:GLY:HA2	1:B:223:ARG:HB3	2.01	0.42
2:C:47:PRO:HG3	2:C:517:ARG:HD2	2.02	0.42
3:D:329:GLN:HB3	3:D:335:PHE:CE2	2.55	0.42
3:D:1056:GLU:HB2	3:D:1063:LYS:HB3	2.01	0.42
3:D:203:ARG:HG3	3:D:206:ARG:HH12	1.85	0.42
3:D:1220:TRP:CD1	3:D:1243:ASP:HB2	2.53	0.42
1:B:42:LEU:HD21	1:B:208:LEU:HA	2.02	0.42
3:D:832:ILE:HD12	3:D:851:ILE:HG23	2.01	0.42
3:D:580:ASP:OD1	3:D:580:ASP:N	2.51	0.42
5:F:184:LEU:HA	5:F:184:LEU:HD23	1.82	0.42
2:C:811:GLU:O	2:C:819:ARG:NH1	2.53	0.41
3:D:785:VAL:HG21	3:D:820:MET:SD	2.60	0.41
5:F:59:GLN:O	5:F:63:VAL:HG23	2.20	0.41
2:C:92:GLU:OE2	2:C:390:ARG:NH2	2.53	0.41
1:A:144:ARG:HH12	1:B:2:LEU:HB2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:VAL:HG13	1:B:196:VAL:HG12	2.02	0.41
2:C:938:TRP:HB2	2:C:1026:GLY:HA2	2.02	0.41
2:C:1099:ARG:HD3	5:F:128:ALA:HB2	2.03	0.41
3:D:339:ASP:HB3	3:D:399:LEU:HB3	2.02	0.41
3:D:937:ILE:HD11	3:D:951:ALA:HB1	2.02	0.41
3:D:739:PRO:HA	3:D:740:PRO:HD3	1.89	0.41
5:F:177:ILE:H	5:F:177:ILE:HG13	1.71	0.41
2:C:254:PHE:CG	2:C:255:SER:N	2.88	0.41
2:C:751:HIS:CD2	2:C:877:ARG:HD2	2.56	0.41
3:D:717:LYS:HE2	3:D:717:LYS:HB3	1.96	0.41
3:D:847:LEU:HD23	3:D:847:LEU:HA	1.87	0.41
3:D:926:GLY:HA2	3:D:963:ARG:HG3	2.03	0.41
2:C:1103:TYR:OH	5:F:129:GLU:OE2	2.38	0.41
3:D:288:LYS:HA	3:D:291:ARG:HD2	2.02	0.41
3:D:642:PRO:HG3	3:D:662:TRP:CE2	2.55	0.41
3:D:26:GLY:HA3	3:D:51:ILE:CG2	2.51	0.41
5:F:28:ARG:O	5:F:29:PHE:C	2.62	0.41
3:D:87:VAL:HA	3:D:90:GLU:HG2	2.03	0.41
1:A:144:ARG:NH2	1:B:27:GLU:OE2	2.54	0.41
1:B:110:ILE:O	1:B:112:PRO:HD3	2.21	0.41
2:C:642:VAL:HB	2:C:703:ALA:HB3	2.03	0.41
1:A:218:LEU:HD23	1:A:218:LEU:HA	1.94	0.40
2:C:93:LEU:HD11	2:C:397:GLU:HB2	2.02	0.40
3:D:27:GLU:HB2	3:D:94:HIS:CE1	2.56	0.40
5:F:142:LYS:HE2	5:F:146:GLN:NE2	2.37	0.40
1:A:98:ARG:HG3	1:A:135:GLU:HG3	2.03	0.40
3:D:556:ARG:NE	4:E:34:ILE:HG23	2.37	0.40
3:D:588:LEU:HD13	3:D:723:TRP:CE2	2.55	0.40
1:B:61:HIS:NE2	1:B:159:ILE:HD13	2.36	0.40
2:C:904:MET:HE3	2:C:913:VAL:HG23	2.04	0.40
3:D:459:ARG:HA	3:D:459:ARG:HD2	1.90	0.40
3:D:497:LEU:O	3:D:543:VAL:HA	2.21	0.40
3:D:1050:THR:OG1	3:D:1107:VAL:HG23	2.21	0.40
1:B:223:ARG:HH22	1:B:227:VAL:HG13	1.85	0.40
2:C:185:VAL:HG22	2:C:204:VAL:HG22	2.03	0.40
2:C:713:MET:HB3	2:C:713:MET:HE3	1.85	0.40
3:D:34:ILE:HG22	3:D:41:PRO:HA	2.03	0.40
3:D:288:LYS:HE2	3:D:288:LYS:HB3	1.85	0.40
3:D:527:LEU:HA	3:D:527:LEU:HD23	1.89	0.40
3:D:666:THR:HG22	3:D:685:ASN:OD1	2.22	0.40
5:F:138:ASP:O	5:F:139:THR:OG1	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:VAL:HG23	1:B:204:PRO:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	219/368 (60%)	213 (97%)	6 (3%)	0	100	100
1	B	227/368 (62%)	216 (95%)	11 (5%)	0	100	100
2	C	1097/1174 (93%)	1070 (98%)	27 (2%)	0	100	100
3	D	1251/1317 (95%)	1231 (98%)	20 (2%)	0	100	100
4	E	72/110 (66%)	71 (99%)	1 (1%)	0	100	100
5	F	169/218 (78%)	162 (96%)	7 (4%)	0	100	100
All	All	3035/3555 (85%)	2963 (98%)	72 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	188/315 (60%)	179 (95%)	9 (5%)	23	44
1	B	191/315 (61%)	184 (96%)	7 (4%)	30	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	830/995 (83%)	804 (97%)	26 (3%)	35	59
3	D	1020/1096 (93%)	992 (97%)	28 (3%)	39	62
4	E	64/90 (71%)	63 (98%)	1 (2%)	55	73
5	F	128/175 (73%)	122 (95%)	6 (5%)	23	45
All	All	2421/2986 (81%)	2344 (97%)	77 (3%)	34	58

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	18	ARG
1	A	59	VAL
1	A	62	GLU
1	A	84	VAL
1	A	111	VAL
1	A	127	THR
1	A	178	VAL
1	A	200	ASN
1	B	59	VAL
1	B	60	LEU
1	B	88	GLU
1	B	150	VAL
1	B	162	ILE
1	B	172	LEU
1	B	228	GLU
2	C	144	THR
2	C	146	GLU
2	C	148	LYS
2	C	211	TRP
2	C	232	GLN
2	C	290	GLU
2	C	320	LEU
2	C	336	GLU
2	C	342	ILE
2	C	465	ARG
2	C	540	VAL
2	C	541	VAL
2	C	558	ARG
2	C	571	VAL
2	C	641	VAL
2	C	660	VAL

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Mol	Chain	Res	Type
2	C	746	VAL
2	C	776	ILE
2	C	787	ARG
2	C	817	GLU
2	C	821	LEU
2	C	869	VAL
2	C	892	LYS
2	C	945	LYS
2	C	992	THR
2	C	1107	VAL
3	D	73	ILE
3	D	82	VAL
3	D	88	ARG
3	D	110	VAL
3	D	126	GLU
3	D	139	VAL
3	D	144	ARG
3	D	199	ASP
3	D	298	VAL
3	D	304	GLN
3	D	427	ARG
3	D	447	MET
3	D	451	LEU
3	D	517	VAL
3	D	580	ASP
3	D	590	THR
3	D	725	THR
3	D	738	VAL
3	D	757	GLU
3	D	858	LYS
3	D	897	ILE
3	D	916	ILE
3	D	960	VAL
3	D	1008	THR
3	D	1053	VAL
3	D	1098	VAL
3	D	1166	THR
3	D	1244	LYS
4	E	36	ASN
5	F	34	ILE
5	F	79	LYS
5	F	94	TYR

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Mol	Chain	Res	Type
5	F	104	TYR
5	F	148	LEU
5	F	179	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	5	GLN
2	C	29	ASN
2	C	232	GLN
2	C	435	GLN
2	C	442	GLN
2	C	545	ASN
2	C	612	GLN
2	C	1129	GLN
3	D	262	GLN
3	D	499	ASN
3	D	759	GLN
3	D	761	GLN
3	D	1109	GLN
3	D	1251	ASN
4	E	64	ASN
5	F	50	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 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	221/368 (60%)	0.33	11 (4%) 34 34	57, 75, 117, 149	0
1	B	231/368 (62%)	0.82	24 (10%) 11 11	65, 100, 138, 153	0
2	C	1105/1174 (94%)	0.57	127 (11%) 9 8	49, 74, 172, 200	0
3	D	1257/1317 (95%)	0.53	66 (5%) 32 31	50, 83, 139, 164	0
4	E	76/110 (69%)	0.96	6 (7%) 18 19	79, 98, 121, 127	0
5	F	173/218 (79%)	0.98	23 (13%) 7 6	56, 119, 141, 151	0
All	All	3063/3555 (86%)	0.59	257 (8%) 17 17	49, 83, 149, 200	0

All (257) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	337	ASP	6.5
2	C	341	THR	5.4
3	D	1201	ALA	5.0
2	C	308	LEU	5.0
3	D	933	ALA	4.8
3	D	1025	THR	4.8
2	C	322	LEU	4.6
1	B	1	MET	4.6
1	B	2	LEU	4.6
3	D	281	ILE	4.6
3	D	280	VAL	4.2
5	F	91	ILE	4.2
2	C	356	THR	4.1
2	C	559	VAL	4.1
3	D	929	ALA	4.1
2	C	257	ILE	4.1
2	C	238	LEU	4.1
2	C	296	LEU	4.1
2	C	1163	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	3	ILE	4.1
3	D	1049	VAL	4.0
2	C	540	VAL	3.9
2	C	570	TYR	3.9
2	C	411	ALA	3.9
2	C	292	ALA	3.9
3	D	1026	GLY	3.9
3	D	4	VAL	3.9
2	C	342	ILE	3.8
3	D	418	LEU	3.7
2	C	346	VAL	3.7
3	D	286	GLY	3.7
2	C	254	PHE	3.7
3	D	1168	ILE	3.6
2	C	568	VAL	3.6
2	C	560	LEU	3.6
2	C	566	GLY	3.5
2	C	288	THR	3.5
3	D	287	GLN	3.5
3	D	994	ALA	3.5
3	D	1111	LEU	3.5
3	D	277	LEU	3.4
2	C	202	VAL	3.4
5	F	180	VAL	3.4
5	F	177	ILE	3.4
1	B	96	TYR	3.4
2	C	543	GLN	3.4
3	D	285	LYS	3.4
1	B	150	VAL	3.4
2	C	274	LEU	3.4
4	E	77	TYR	3.3
2	C	234	VAL	3.3
2	C	311	VAL	3.3
2	C	212	LEU	3.3
2	C	200	HIS	3.3
2	C	300	PHE	3.3
1	B	130	ASP	3.3
2	C	320	LEU	3.2
5	F	194	LEU	3.2
2	C	287	PRO	3.2
3	D	932	GLU	3.2
1	A	223	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	571	VAL	3.1
1	B	227	VAL	3.1
2	C	236	VAL	3.1
5	F	198	VAL	3.1
3	D	1267	TYR	3.1
2	C	541	VAL	3.1
2	C	278	TYR	3.0
2	C	297	GLU	3.0
2	C	275	LEU	3.0
3	D	1190	ASN	3.0
2	C	235	THR	3.0
4	E	55	TYR	3.0
3	D	937	ILE	3.0
2	C	562	ARG	2.9
2	C	201	SER	2.9
3	D	416	ASN	2.9
2	C	316	VAL	2.9
2	C	345	LEU	2.9
2	C	181	ARG	2.9
2	C	507	ASN	2.9
3	D	927	THR	2.9
3	D	1248	LEU	2.8
4	E	32	LEU	2.8
2	C	575	GLU	2.8
3	D	414	ARG	2.8
2	C	260	SER	2.8
5	F	104	TYR	2.8
5	F	72	PHE	2.8
1	B	157	ALA	2.8
2	C	565	ALA	2.8
2	C	291	SER	2.8
1	B	94	THR	2.8
2	C	270	THR	2.8
5	F	101	PRO	2.7
1	B	59	VAL	2.7
5	F	43	GLY	2.7
2	C	1149	GLU	2.7
1	A	25	PRO	2.7
2	C	147	ILE	2.7
2	C	299	LEU	2.7
1	A	182	ARG	2.7
3	D	1116	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
5	F	100	GLN	2.7
2	C	237	LEU	2.7
1	A	24	GLU	2.7
4	E	51	ALA	2.7
2	C	1145	ILE	2.6
2	C	563	ARG	2.6
2	C	349	HIS	2.6
3	D	282	ARG	2.6
1	B	231	GLY	2.6
2	C	284	GLY	2.6
1	B	63	PHE	2.6
2	C	829	ALA	2.6
3	D	936	VAL	2.6
2	C	286	PRO	2.6
3	D	906	PRO	2.6
3	D	1045	PRO	2.6
2	C	355	MET	2.6
5	F	141	ILE	2.6
3	D	650	LEU	2.6
1	A	184	GLU	2.6
2	C	283	PRO	2.6
2	C	340	ALA	2.6
2	C	211	TRP	2.6
3	D	1032	GLN	2.6
2	C	289	LYS	2.6
2	C	204	VAL	2.6
2	C	519	VAL	2.6
3	D	971	SER	2.5
3	D	1065	THR	2.5
2	C	512	ILE	2.5
3	D	293	LEU	2.5
2	C	576	VAL	2.5
2	C	309	ALA	2.5
5	F	102	ALA	2.5
2	C	207	SER	2.5
2	C	310	ARG	2.5
3	D	1176	LEU	2.5
3	D	5	ASN	2.5
3	D	283	ASN	2.5
2	C	265	ASP	2.5
3	D	409	LYS	2.5
5	F	145	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	459	GLY	2.5
2	C	99	PHE	2.5
2	C	258	MET	2.5
2	C	317	ASN	2.5
2	C	412	ILE	2.5
3	D	412	ARG	2.5
2	C	321	GLY	2.5
3	D	992	GLY	2.5
3	D	6	PHE	2.5
1	B	56	ILE	2.4
1	A	199	LYS	2.4
1	B	159	ILE	2.4
2	C	539	HIS	2.4
2	C	573	SER	2.4
2	C	205	ILE	2.4
2	C	226	ILE	2.4
2	C	294	THR	2.4
3	D	1131	GLN	2.4
1	A	183	VAL	2.4
2	C	561	VAL	2.4
2	C	578	TYR	2.4
4	E	70	LEU	2.4
2	C	569	GLU	2.4
2	C	521	ASP	2.4
2	C	551	ASP	2.4
1	B	156	GLY	2.4
2	C	185	VAL	2.4
2	C	338	VAL	2.4
2	C	365	VAL	2.4
1	A	101	GLY	2.3
2	C	339	VAL	2.3
3	D	1271	ALA	2.3
2	C	188	ASP	2.3
2	C	255	SER	2.3
1	A	222	ALA	2.3
2	C	130	ALA	2.3
2	C	199	LEU	2.3
2	C	276	ASP	2.3
5	F	174	ASP	2.3
1	B	60	LEU	2.3
2	C	532	THR	2.3
5	F	37	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
5	F	82	LEU	2.3
2	C	65	ILE	2.2
3	D	924	THR	2.2
2	C	305	ARG	2.2
3	D	278	ARG	2.2
2	C	577	ASP	2.2
3	D	1170	SER	2.2
2	C	458	LEU	2.2
2	C	470	LEU	2.2
3	D	2	LEU	2.2
4	E	34	ILE	2.2
5	F	199	ALA	2.2
2	C	306	TYR	2.2
5	F	95	ARG	2.2
3	D	296	LEU	2.2
3	D	1162	LEU	2.2
3	D	930	VAL	2.2
3	D	938	VAL	2.2
3	D	1066	ILE	2.2
2	C	542	ALA	2.2
2	C	1146	GLU	2.2
1	B	90	ASP	2.2
2	C	1162	LEU	2.2
5	F	173	MET	2.2
2	C	554	PHE	2.2
2	C	843	GLU	2.2
5	F	94	TYR	2.2
2	C	417	LEU	2.2
3	D	951	ALA	2.1
2	C	233	PRO	2.1
1	B	201	SER	2.1
2	C	1158	ALA	2.1
3	D	272	ALA	2.1
2	C	343	GLU	2.1
5	F	79	LYS	2.1
3	D	706	MET	2.1
2	C	186	TYR	2.1
3	D	1042	GLY	2.1
3	D	1165	VAL	2.1
1	B	158	GLU	2.1
2	C	261	THR	2.1
5	F	139	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	1051	MET	2.1
1	B	143	GLY	2.1
3	D	652	GLY	2.1
3	D	1218	ASP	2.1
1	B	114	ALA	2.1
2	C	1160	ALA	2.1
2	C	198	THR	2.1
3	D	415	GLN	2.1
1	B	46	ILE	2.1
2	C	1117	ILE	2.1
2	C	79	ASP	2.0
2	C	214	PHE	2.1
2	C	149	SER	2.0
2	C	468	ALA	2.0
1	A	14	LEU	2.0
3	D	410	GLN	2.0
3	D	417	LEU	2.0
1	B	232	ILE	2.0
2	C	347	ARG	2.0
1	B	50	ALA	2.0
1	B	166	SER	2.0
2	C	464	SER	2.0
2	C	82	PRO	2.0
5	F	175	THR	2.0
2	C	370	ILE	2.0
3	D	51	ILE	2.0
3	D	766	ASN	2.0
3	D	1064	ILE	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
6	ZN	D	2001	1/1	0.99	0.04	89,89,89,89	0
6	ZN	D	2002	1/1	0.99	0.04	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.