



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:25 AM UTC

PDB ID : 3WOD / pdb_00003wod
Title : RNA polymerase-gp39 complex
Authors : Tagami, S.; Sekine, S.; Minakhin, L.; Esyunina, D.; Akasaka, R.; Shirouzu, M.; Kulbachinskiy, A.; Severinov, K.; Yokoyama, S.
Deposited on : 2013-12-26
Resolution : 3.60 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

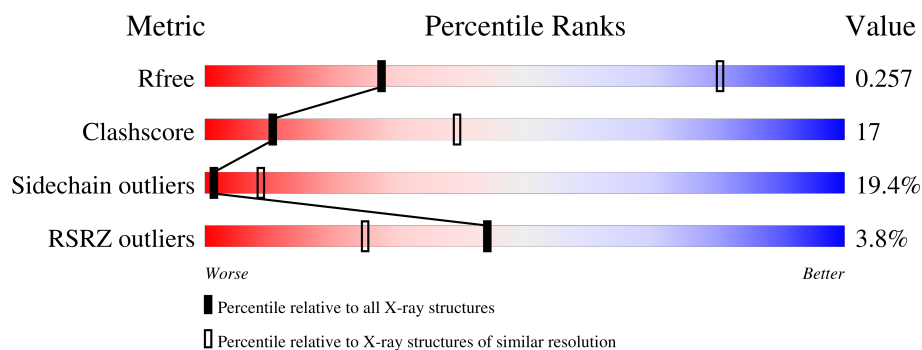
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	315	38% 29% 5% 29%
1	B	315	38% 28% 7% 26%
2	C	1119	3% 49% 37% 8% 6%
3	D	1524	5% 49% 39% 9% .
4	E	99	3% 55% 32% 9% .
5	F	423	5% 39% 21% 5% 34%

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Mol	Chain	Length	Quality of chain
6	G	141	58% 30% • 10%
6	H	141	% 44% 17% • 35%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 28442 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	225	Total	C	N	O	S	0	0	0
			1772	1132	308	330	2			
1	B	232	Total	C	N	O	S	0	0	0
			1814	1158	316	338	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1055	Total	C	N	O	S	0	0	2
			8305	5251	1485	1546	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1488	Total	C	N	O	S	0	0	0
			11752	7450	2069	2197	36			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	61	GLU	VAL	SEE REMARK 999	UNP Q8RQE7
E	92	ILE	LEU	SEE REMARK 999	UNP Q8RQE7
E	95	GLY	VAL	SEE REMARK 999	UNP Q8RQE7

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

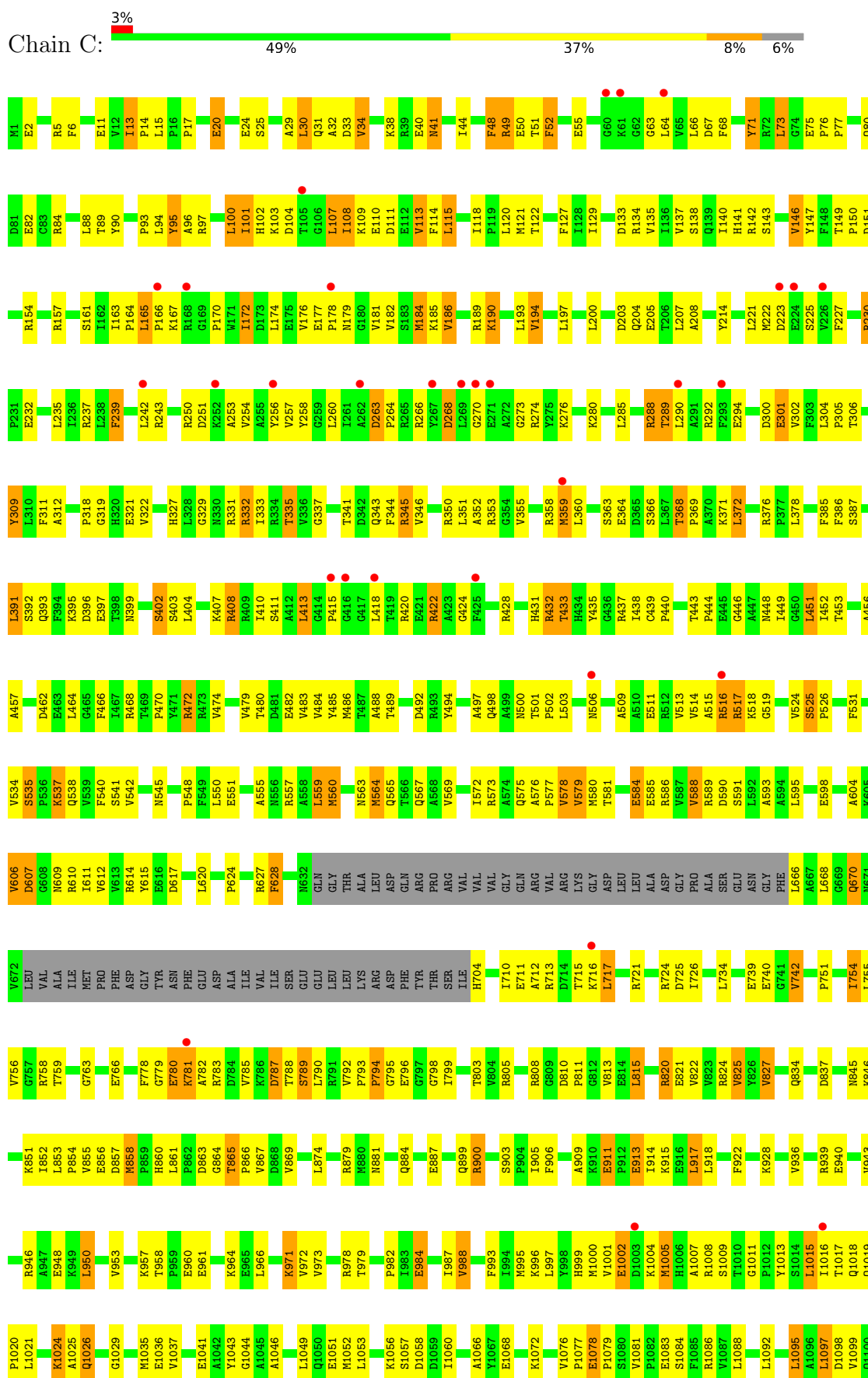
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	278	Total	C	N	O	S	0	0	0
			2242	1421	399	420	2			

- Molecule 6 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	127	Total	C	N	O	S	0	0	0
			1035	673	175	184	3			
6	H	91	Total	C	N	O	S	0	0	0
			752	495	125	131	1			

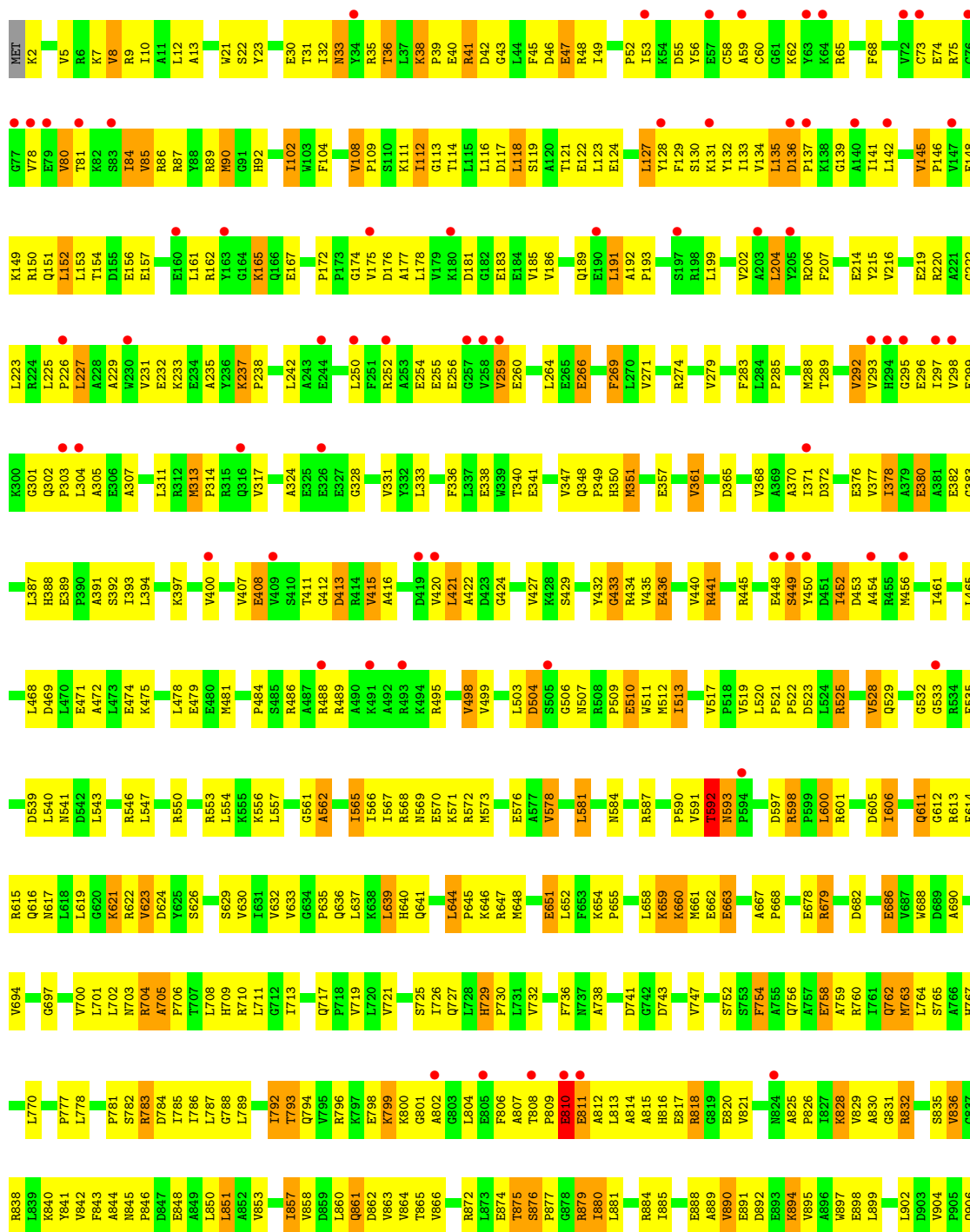
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

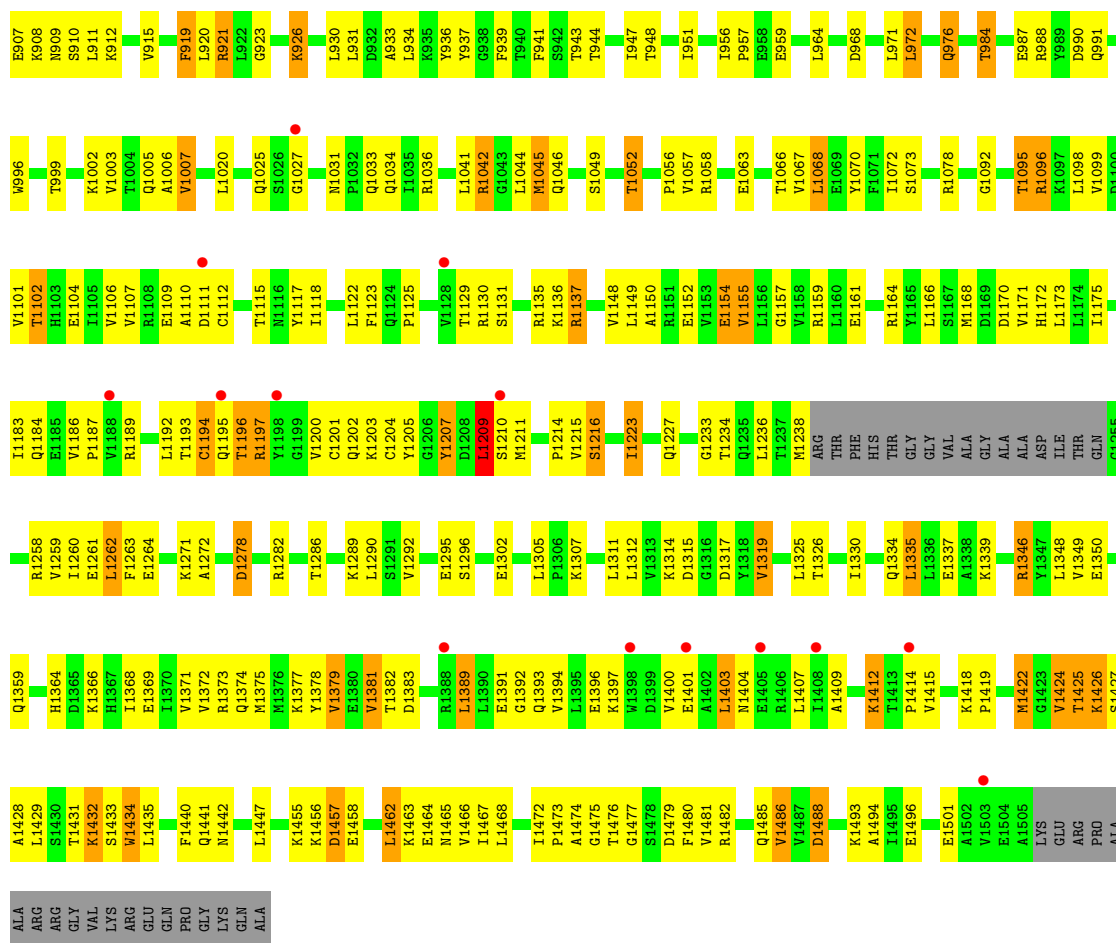
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Zn	0	0
			1	1		



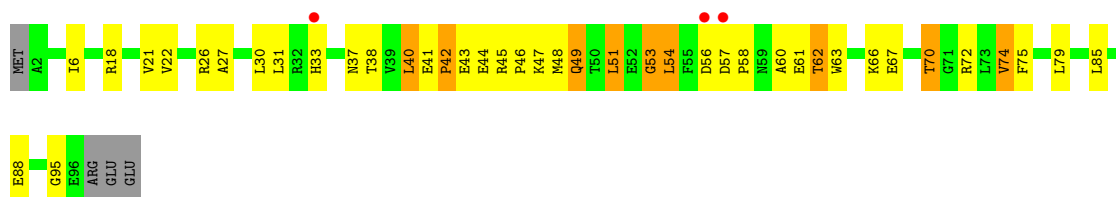


● Molecule 3: DNA-directed RNA polymerase subunit beta'

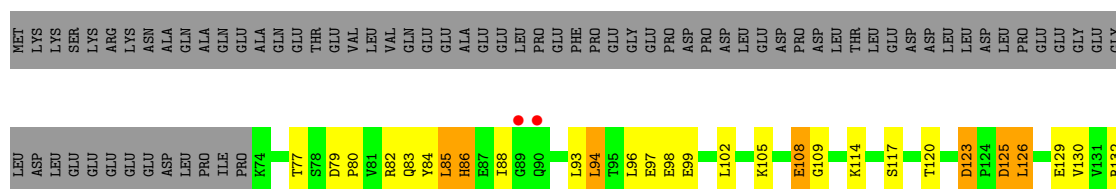


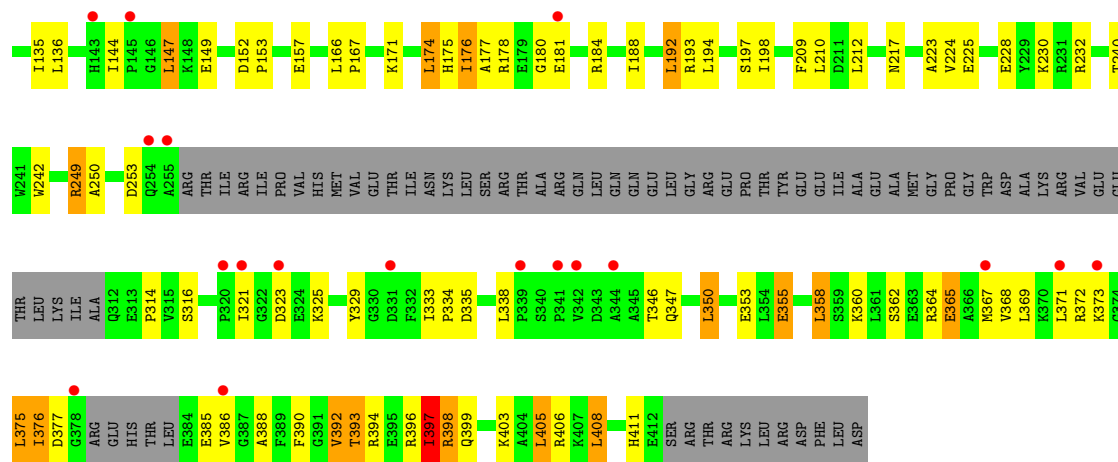


• Molecule 4: DNA-directed RNA polymerase subunit omega

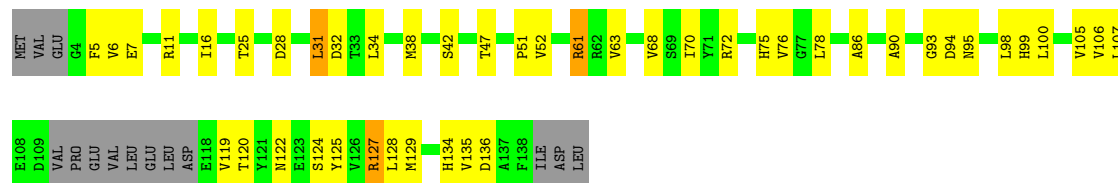


• Molecule 5: RNA polymerase sigma factor

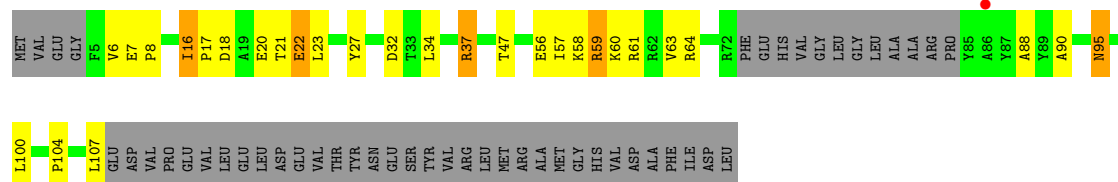
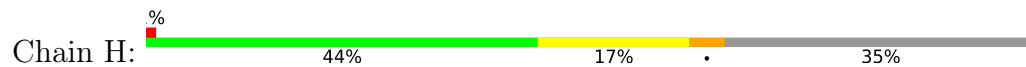




• Molecule 6: Putative uncharacterized protein



• Molecule 6: Putative uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	294.44Å 294.44Å 223.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.88 – 3.60 19.88 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.88-3.60) 98.9 (19.88-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.22	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 3.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.250 , 0.279 (Not available) , 0.257	Depositor DCC
R_{free} test set	6487 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	64.5	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 31.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.16$	Xtriage
Estimated twinning fraction	0.166 for -h,-k,l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	28442	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% 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: 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	0.46	0/1804	0.98	4/2454 (0.2%)
1	B	0.43	0/1846	0.95	1/2511 (0.0%)
2	C	0.43	0/8476	0.96	20/11461 (0.2%)
3	D	0.44	0/11958	0.97	36/16166 (0.2%)
4	E	0.40	0/783	1.07	5/1054 (0.5%)
5	F	0.46	0/2276	0.92	1/3058 (0.0%)
6	G	0.35	0/1065	0.82	3/1449 (0.2%)
6	H	0.34	0/775	0.81	2/1057 (0.2%)
All	All	0.44	0/28983	0.96	72/39210 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	2
3	D	0	3
4	E	0	3
5	F	0	1
All	All	0	9

There are no bond length outliers.

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	237	LYS	CA-C-N	-9.89	110.73	120.52
3	D	237	LYS	C-N-CA	-9.89	110.73	120.52
3	D	136	ASP	CA-C-N	-9.48	107.99	119.84
3	D	136	ASP	C-N-CA	-9.48	107.99	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	ILE	CA-C-N	9.20	129.77	119.93
1	A	68	ILE	C-N-CA	9.20	129.77	119.93
3	D	433	GLY	N-CA-C	8.82	123.23	110.80
3	D	108	VAL	CA-C-N	-8.70	109.48	120.79
3	D	108	VAL	C-N-CA	-8.70	109.48	120.79
3	D	1209	LEU	N-CA-C	-7.90	100.34	110.53
4	E	57	ASP	CA-C-N	-7.58	110.37	119.84
4	E	57	ASP	C-N-CA	-7.58	110.37	119.84
2	C	230	ARG	CA-C-N	7.53	129.25	119.84
2	C	230	ARG	C-N-CA	7.53	129.25	119.84
3	D	644	LEU	CA-C-N	7.51	127.97	119.93
3	D	644	LEU	C-N-CA	7.51	127.97	119.93
3	D	292	VAL	N-CA-C	7.04	117.55	110.23
3	D	517	VAL	CA-C-N	-6.92	112.84	119.76
3	D	517	VAL	C-N-CA	-6.92	112.84	119.76
2	C	795	GLY	N-CA-C	-6.87	96.90	113.18
1	B	140	MET	N-CA-C	6.82	119.54	108.76
2	C	858	MET	CA-C-N	6.80	128.35	119.84
2	C	858	MET	C-N-CA	6.80	128.35	119.84
3	D	1383	ASP	CA-C-N	6.63	126.61	119.78
3	D	1383	ASP	C-N-CA	6.63	126.61	119.78
2	C	559	LEU	N-CA-C	-6.60	104.17	111.36
3	D	528	VAL	N-CA-C	6.50	116.98	107.75
3	D	857	ILE	N-CA-C	-6.50	105.41	111.45
2	C	517	ARG	N-CA-C	-6.40	99.20	109.96
1	A	8	ALA	CA-C-N	6.38	126.76	119.93
1	A	8	ALA	C-N-CA	6.38	126.76	119.93
2	C	913	GLU	N-CA-C	-6.35	104.28	111.14
4	E	57	ASP	N-CA-C	6.34	123.82	109.81
5	F	397	ILE	N-CA-C	-6.24	104.56	110.42
3	D	80	VAL	N-CA-C	6.16	117.46	108.53
2	C	591	SER	N-CA-C	-6.02	102.02	110.50
6	G	7	GLU	CA-C-N	-6.00	113.50	119.56
6	G	7	GLU	C-N-CA	-6.00	113.50	119.56
2	C	34	VAL	CA-C-N	5.96	126.52	120.38
2	C	34	VAL	C-N-CA	5.96	126.52	120.38
3	D	851	LEU	N-CA-C	-5.88	104.78	111.07
3	D	1418	LYS	CA-C-N	5.71	126.97	119.84
3	D	1418	LYS	C-N-CA	5.71	126.97	119.84
4	E	62	THR	N-CA-C	-5.66	105.03	111.14
3	D	811	GLU	N-CA-C	-5.61	106.27	113.01
3	D	38	LYS	CA-C-N	5.59	126.83	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	38	LYS	C-N-CA	5.59	126.83	119.84
3	D	1393	GLN	N-CA-C	5.55	117.24	108.96
2	C	263	ASP	CA-C-N	-5.49	112.98	119.84
2	C	263	ASP	C-N-CA	-5.49	112.98	119.84
3	D	799	LYS	N-CA-C	5.45	116.84	109.11
2	C	451	LEU	N-CA-C	-5.34	105.57	112.68
3	D	592	THR	N-CA-C	-5.34	102.97	110.50
2	C	1011	GLY	CA-C-N	5.31	126.06	120.11
2	C	1011	GLY	C-N-CA	5.31	126.06	120.11
3	D	923	GLY	N-CA-C	5.29	117.43	112.08
3	D	810	GLU	N-CA-C	-5.29	106.67	113.23
4	E	95	GLY	N-CA-C	-5.27	108.07	114.92
6	G	6	VAL	N-CA-C	5.24	117.60	111.05
3	D	729	HIS	CA-C-N	5.24	125.55	119.47
3	D	729	HIS	C-N-CA	5.24	125.55	119.47
6	H	16	ILE	CA-C-N	5.22	126.37	119.84
6	H	16	ILE	C-N-CA	5.22	126.37	119.84
3	D	705	ALA	CA-C-N	-5.21	113.33	119.84
3	D	705	ALA	C-N-CA	-5.21	113.33	119.84
2	C	494	TYR	N-CA-C	5.20	117.76	109.81
3	D	448	GLU	N-CA-C	5.19	117.16	108.23
2	C	999	HIS	N-CA-C	5.11	117.79	110.68
3	D	449	SER	N-CA-C	5.03	116.07	108.07
3	D	562	ALA	N-CA-C	5.02	117.78	108.94
2	C	268	ASP	N-CA-C	5.00	116.80	109.24
2	C	887	GLU	N-CA-C	-5.00	105.72	111.07

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	260	LEU	Peptide
2	C	794	PRO	Peptide
3	D	1196	THR	Peptide
3	D	1207	TYR	Peptide
3	D	561	GLY	Peptide
4	E	40	LEU	Peptide
4	E	49	GLN	Peptide
4	E	53	GLY	Peptide
5	F	376	ILE	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	1772	0	1821	63	0
1	B	1814	0	1868	77	0
2	C	8305	0	8425	307	0
3	D	11752	0	11990	467	0
4	E	769	0	775	29	0
5	F	2242	0	2305	63	0
6	G	1035	0	1013	22	0
6	H	752	0	748	20	0
7	D	1	0	0	0	0
All	All	28442	0	28945	977	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 17.

All (977) 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:820:GLU:HG3	3:D:836:VAL:HG21	1.51	0.92
2:C:164:PRO:HA	2:C:266:ARG:HH22	1.36	0.90
4:E:54:LEU:HA	4:E:58:PRO:HD2	1.57	0.85
2:C:63:GLY:HA3	2:C:103:LYS:HG2	1.58	0.83
3:D:133:ILE:HG21	3:D:454:ALA:HB1	1.60	0.83
1:A:27:PRO:HG3	1:A:186:LEU:HD13	1.60	0.82
3:D:225:LEU:HD13	3:D:231:VAL:HG23	1.63	0.81
3:D:678:GLU:HG3	3:D:679:ARG:HD3	1.64	0.79
3:D:295:GLY:HA2	3:D:302:GLN:HB3	1.65	0.79
1:B:18:ARG:NH1	1:B:203:GLY:O	2.16	0.79
3:D:116:LEU:O	3:D:118:LEU:N	2.14	0.79
1:A:18:ARG:HH22	1:A:88:ARG:HH21	1.31	0.78
1:A:18:ARG:HH12	1:A:88:ARG:HE	1.32	0.78
3:D:697:GLY:O	3:D:760:ARG:NH1	2.18	0.77
3:D:252:ARG:HA	3:D:301:GLY:HA3	1.67	0.77
2:C:716:LYS:HG3	3:D:533:GLY:HA3	1.68	0.76
2:C:289:THR:HG22	2:C:290:LEU:HD23	1.67	0.76
3:D:181:ASP:O	3:D:183:GLU:N	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1488:ASP:OD1	3:D:1488:ASP:N	2.20	0.75
3:D:711:LEU:HD12	3:D:778:LEU:HD23	1.68	0.75
2:C:874:LEU:HD13	3:D:783:ARG:HB2	1.68	0.74
3:D:591:VAL:HG13	3:D:597:ASP:HA	1.69	0.74
3:D:1045:MET:HG2	3:D:1073:SER:HA	1.67	0.74
1:A:88:ARG:HB2	1:A:123:MET:HE2	1.70	0.73
1:B:22:GLU:HG2	1:B:198:ARG:HG2	1.69	0.73
2:C:576:ALA:O	2:C:900:ARG:NH2	2.21	0.73
3:D:815:ALA:O	3:D:818:ARG:HG3	1.89	0.72
5:F:109:GLY:HA2	5:F:177:ALA:HA	1.71	0.72
5:F:385:GLU:HA	5:F:388:ALA:HB2	1.71	0.72
2:C:1078:GLU:HG3	2:C:1079:PRO:HD3	1.71	0.72
3:D:1155:VAL:O	3:D:1157:GLY:N	2.22	0.72
6:H:20:GLU:HA	6:H:61:ARG:HD2	1.71	0.72
3:D:520:LEU:O	3:D:525:ARG:NH1	2.23	0.71
2:C:34:VAL:HB	2:C:38:LYS:HG3	1.71	0.71
2:C:555:ALA:HB2	3:D:1070:TYR:HE1	1.56	0.71
5:F:85:LEU:HD22	5:F:193:ARG:HD3	1.71	0.71
1:A:94:LEU:O	1:A:146:ARG:NH1	2.23	0.71
3:D:617:ASN:ND2	3:D:1466:VAL:O	2.23	0.71
5:F:403:LYS:HA	5:F:406:ARG:HD2	1.72	0.71
3:D:640:HIS:HB3	3:D:641:GLN:HG3	1.71	0.70
3:D:543:LEU:HD13	3:D:581:LEU:HA	1.73	0.70
2:C:1083:GLU:OE1	3:D:87:ARG:NH1	2.24	0.70
1:B:34:VAL:HG11	2:C:978:ARG:HB2	1.73	0.70
2:C:1099:VAL:HG12	3:D:10:ILE:HG12	1.73	0.70
3:D:1209:LEU:HD13	3:D:1215:VAL:HA	1.72	0.70
2:C:464:LEU:O	2:C:466:PHE:N	2.25	0.70
1:A:160:ASP:OD1	1:A:160:ASP:N	2.26	0.69
6:G:90:ALA:HB2	6:G:100:LEU:HD23	1.74	0.69
6:H:90:ALA:HB2	6:H:100:LEU:HD23	1.74	0.69
1:A:41:ARG:NH1	1:A:177:VAL:O	2.25	0.69
3:D:1098:LEU:O	3:D:1102:THR:OG1	2.10	0.69
1:B:77:GLU:HB2	3:D:872:ARG:HH21	1.57	0.69
3:D:1194:CYS:SG	3:D:1195:GLN:N	2.65	0.69
2:C:573:ARG:O	2:C:670:GLN:NE2	2.26	0.69
3:D:810:GLU:O	3:D:813:LEU:HG	1.92	0.69
3:D:119:SER:H	3:D:123:LEU:HD12	1.57	0.69
3:D:1476:THR:HG23	4:E:21:VAL:HG22	1.75	0.69
6:G:124:SER:HA	6:G:127:ARG:HG3	1.74	0.69
3:D:127:LEU:HD11	3:D:461:ILE:HD11	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:432:ARG:HG3	2:C:519:GLY:HA2	1.73	0.68
3:D:119:SER:O	3:D:121:THR:N	2.23	0.68
2:C:607:ASP:HB3	2:C:609:ASN:H	1.57	0.68
2:C:41:ASN:ND2	2:C:268:ASP:OD1	2.26	0.68
3:D:422:ALA:HB3	3:D:427:VAL:HB	1.75	0.68
2:C:391:LEU:HD13	2:C:415:PRO:HD3	1.75	0.67
3:D:504:ASP:C	3:D:506:GLY:H	2.02	0.67
2:C:31:GLN:NE2	2:C:40:GLU:O	2.28	0.66
3:D:615:ARG:HH22	3:D:1441:GLN:HA	1.60	0.66
3:D:153:LEU:HB2	3:D:157:GLU:HG3	1.76	0.66
1:B:96:THR:OG1	1:B:97:VAL:N	2.29	0.66
3:D:906:GLN:HB3	3:D:911:LEU:HD11	1.77	0.66
2:C:939:ARG:HD2	2:C:982:PRO:HD3	1.78	0.66
3:D:226:PRO:HB2	3:D:229:ALA:HB3	1.78	0.66
5:F:123:ASP:H	5:F:126:LEU:HD23	1.61	0.66
1:A:31:GLY:O	1:B:42:ARG:NH2	2.29	0.65
2:C:30:LEU:O	2:C:32:ALA:N	2.29	0.65
3:D:591:VAL:HG12	3:D:592:THR:O	1.96	0.65
3:D:679:ARG:NE	3:D:682:ASP:OD2	2.27	0.65
3:D:288:MET:HG3	3:D:305:ALA:HB1	1.77	0.65
3:D:1379:VAL:HG12	3:D:1419:PRO:HA	1.78	0.65
1:A:24:VAL:HG22	1:A:196:THR:HB	1.78	0.65
2:C:565:GLN:HG2	2:C:995:MET:HE1	1.78	0.65
2:C:164:PRO:CA	2:C:266:ARG:HH22	2.10	0.65
3:D:540:LEU:HD11	3:D:606:ILE:HD11	1.77	0.65
2:C:327:HIS:HD2	2:C:329:GLY:H	1.44	0.65
3:D:407:VAL:HG22	3:D:408:GLU:H	1.61	0.65
3:D:139:GLY:HA3	3:D:452:ILE:HD12	1.78	0.65
2:C:948:GLU:HB3	2:C:953:VAL:HG23	1.79	0.64
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.78	0.64
1:B:100:LEU:HB2	1:B:115:LEU:HD11	1.80	0.64
4:E:41:GLU:HA	4:E:45:ARG:HG3	1.79	0.64
6:G:34:LEU:HD23	6:G:129:MET:HE2	1.79	0.64
3:D:1101:VAL:HG21	3:D:1424:VAL:HG13	1.79	0.64
3:D:368:VAL:HB	3:D:377:VAL:HB	1.78	0.63
3:D:23:TYR:O	3:D:49:ILE:HG23	1.99	0.63
2:C:550:LEU:HD23	2:C:905:ILE:HD11	1.79	0.63
3:D:216:VAL:HG22	3:D:340:THR:HG22	1.81	0.63
3:D:238:PRO:HA	3:D:313:MET:HG2	1.80	0.63
3:D:145:VAL:HG22	3:D:146:PRO:HD2	1.79	0.63
3:D:1400:VAL:HG12	3:D:1401:GLU:HG2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:408:LEU:O	6:G:122:ASN:ND2	2.31	0.62
2:C:274:ARG:HG3	2:C:285:LEU:HB3	1.82	0.62
3:D:1290:LEU:HB2	3:D:1305:LEU:HB2	1.81	0.62
1:B:77:GLU:O	1:B:81:ASN:ND2	2.32	0.62
2:C:304:LEU:HB3	2:C:305:PRO:HD3	1.82	0.62
2:C:97:ARG:HH21	2:C:109:LYS:HD2	1.65	0.62
5:F:364:ARG:O	5:F:368:VAL:HG23	1.99	0.62
3:D:10:ILE:HG13	3:D:1434:TRP:CZ2	2.35	0.62
2:C:905:ILE:HG23	2:C:906:PHE:H	1.65	0.61
3:D:789:LEU:O	3:D:793:THR:OG1	2.15	0.61
3:D:1150:ALA:HB3	3:D:1187:PRO:HB2	1.81	0.61
3:D:124:GLU:OE2	3:D:124:GLU:N	2.28	0.61
3:D:407:VAL:HG11	5:F:171:LYS:HD3	1.82	0.61
6:H:21:THR:HG22	6:H:22:GLU:H	1.65	0.61
1:A:42:ARG:NH1	2:C:857:ASP:HB3	2.15	0.61
3:D:58:CYS:SG	3:D:59:ALA:N	2.74	0.61
2:C:100:LEU:HD21	2:C:368:THR:HA	1.83	0.61
3:D:1378:TYR:HE2	3:D:1394:VAL:HG22	1.65	0.61
3:D:504:ASP:O	3:D:506:GLY:N	2.30	0.61
3:D:655:PRO:HA	3:D:658:LEU:HD12	1.82	0.61
3:D:704:ARG:NH1	3:D:743:ASP:OD2	2.30	0.61
5:F:209:PHE:HA	5:F:212:LEU:HD12	1.83	0.61
2:C:141:HIS:CE1	2:C:165:LEU:HD11	2.36	0.61
2:C:424:GLY:HA3	2:C:428:ARG:HE	1.65	0.61
3:D:108:VAL:HB	3:D:109:PRO:HD3	1.83	0.61
3:D:274:ARG:HB2	3:D:279:VAL:HG21	1.82	0.61
3:D:1104:GLU:OE1	3:D:1374:GLN:NE2	2.33	0.61
1:A:86:VAL:HG13	1:A:124:ASN:HB2	1.83	0.61
2:C:270:GLY:H	2:C:288:ARG:NH2	1.99	0.61
3:D:593:ASN:OD1	3:D:593:ASN:N	2.34	0.61
3:D:215:TYR:HE1	3:D:380:GLU:HB3	1.66	0.60
3:D:416:ALA:HB2	3:D:432:TYR:HA	1.83	0.60
3:D:781:PRO:HG2	3:D:911:LEU:HD23	1.83	0.60
3:D:800:LYS:HE2	3:D:830:ALA:HB3	1.82	0.60
3:D:660:LYS:HA	3:D:663:GLU:HG3	1.84	0.60
2:C:101:ILE:HG23	2:C:107:LEU:HB3	1.83	0.60
2:C:399:ASN:OD1	2:C:402:SER:OG	2.19	0.60
3:D:705:ALA:HB3	3:D:706:PRO:HD3	1.84	0.60
3:D:42:ASP:OD2	3:D:48:ARG:NH2	2.34	0.60
3:D:73:CYS:SG	3:D:74:GLU:N	2.75	0.60
3:D:782:SER:O	3:D:786:ILE:HD12	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:846:PRO:HB3	3:D:880:ILE:HD12	1.83	0.60
1:B:48:ILE:HG23	1:B:173:PRO:HD2	1.84	0.59
2:C:194:VAL:HG22	2:C:221:LEU:HD12	1.84	0.59
2:C:564:MET:HE1	2:C:846:LYS:HE2	1.84	0.59
1:A:206:THR:HG23	1:A:209:GLU:H	1.66	0.59
2:C:141:HIS:HE1	2:C:165:LEU:HD11	1.67	0.59
5:F:353:GLU:HG2	6:G:127:ARG:HB3	1.84	0.59
3:D:484:PRO:O	3:D:489:ARG:NH1	2.34	0.59
3:D:756:GLN:O	3:D:760:ARG:HG2	2.01	0.59
3:D:972:LEU:HD23	3:D:976:GLN:HE21	1.66	0.59
5:F:80:PRO:HA	5:F:83:GLN:HB2	1.84	0.59
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.02	0.59
6:H:56:GLU:HG3	6:H:64:ARG:HD2	1.83	0.59
1:B:143:ARG:NE	1:B:145:ASP:OD1	2.33	0.59
3:D:313:MET:HG3	3:D:314:PRO:HD2	1.85	0.59
2:C:1013:TYR:HA	2:C:1020:PRO:HA	1.84	0.59
1:B:206:THR:HG23	1:B:209:GLU:H	1.68	0.59
2:C:185:LYS:HA	2:C:189:ARG:O	2.02	0.59
3:D:238:PRO:HB3	3:D:317:VAL:O	2.02	0.59
3:D:259:VAL:HG11	3:D:293:VAL:HG12	1.84	0.59
3:D:569:ASN:ND2	5:F:84:TYR:OH	2.34	0.59
3:D:1154:GLU:HG2	3:D:1159:ARG:HG2	1.85	0.59
2:C:288:ARG:HA	2:C:288:ARG:NE	2.18	0.58
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.35	0.58
2:C:1076:VAL:HG22	3:D:752:SER:HB2	1.83	0.58
3:D:1152:GLU:OE1	3:D:1159:ARG:NH2	2.32	0.58
4:E:40:LEU:HD13	4:E:45:ARG:HD2	1.85	0.58
1:A:156:HIS:CD2	1:A:158:ILE:HG12	2.39	0.58
2:C:751:PRO:HG3	2:C:796:GLU:HA	1.84	0.58
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.38	0.58
1:A:168:ASP:OD1	1:A:168:ASP:N	2.36	0.58
3:D:1129:THR:HG23	3:D:1131:SER:HB3	1.85	0.58
2:C:285:LEU:HD12	2:C:301:GLU:HG2	1.85	0.58
3:D:902:LEU:HD23	3:D:902:LEU:H	1.68	0.58
3:D:1278:ASP:OD1	3:D:1278:ASP:N	2.36	0.58
2:C:987:ILE:HG23	3:D:948:THR:HG21	1.84	0.58
3:D:58:CYS:SG	3:D:60:CYS:N	2.76	0.58
3:D:84:ILE:HA	3:D:87:ARG:HG2	1.85	0.58
3:D:1379:VAL:O	3:D:1392:GLY:HA2	2.04	0.58
1:B:65:PHE:HE1	3:D:813:LEU:HD13	1.69	0.58
3:D:39:PRO:HG2	3:D:47:GLU:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ARG:HG2	1:B:231:ALA:HB3	1.85	0.58
3:D:812:ALA:O	3:D:816:HIS:HB2	2.04	0.58
2:C:711:GLU:HG2	2:C:822:VAL:HG12	1.86	0.57
2:C:721:ARG:NH2	6:G:95:ASN:OD1	2.37	0.57
2:C:1044:GLY:O	2:C:1046:ALA:N	2.37	0.57
3:D:841:TYR:HB2	3:D:864:VAL:HG13	1.86	0.57
4:E:40:LEU:HD21	4:E:67:GLU:HA	1.86	0.57
3:D:786:ILE:HG21	3:D:1027:GLY:H	1.69	0.57
2:C:197:LEU:HA	2:C:200:LEU:HD12	1.86	0.57
2:C:266:ARG:HD3	2:C:273:GLY:HA3	1.86	0.57
3:D:804:LEU:O	3:D:831:GLY:HA2	2.04	0.57
1:B:86:VAL:HG13	1:B:124:ASN:HB2	1.85	0.57
2:C:567:GLN:HB2	2:C:997:LEU:HD12	1.86	0.57
3:D:357:GLU:HA	3:D:387:LEU:HD11	1.87	0.57
3:D:1135:ARG:NH2	3:D:1350:GLU:OE2	2.37	0.57
3:D:547:LEU:HD11	3:D:578:VAL:HG23	1.86	0.57
3:D:242:LEU:HD22	3:D:285:PRO:HG3	1.86	0.57
3:D:1462:LEU:O	3:D:1466:VAL:HG23	2.05	0.57
3:D:1472:ILE:O	3:D:1477:GLY:HA3	2.05	0.57
2:C:1005:MET:O	2:C:1005:MET:HG3	2.02	0.57
2:C:1092:LEU:HD13	2:C:1099:VAL:HG11	1.86	0.57
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	1.87	0.57
3:D:539:ASP:OD2	3:D:598:ARG:NH2	2.38	0.57
2:C:861:LEU:HB2	2:C:865:THR:HG23	1.87	0.57
1:B:68:ILE:HB	1:B:71:VAL:HB	1.85	0.57
2:C:165:LEU:HA	2:C:166:PRO:O	2.05	0.57
3:D:1096:ARG:HH11	3:D:1096:ARG:HB2	1.70	0.56
1:A:178:ALA:HB2	2:C:864:GLY:H	1.70	0.56
2:C:604:ALA:HB3	2:C:612:VAL:HG12	1.87	0.56
3:D:892:ASP:OD2	3:D:894:LYS:HG2	2.06	0.56
1:A:56:VAL:HG13	1:A:142:VAL:HG12	1.87	0.56
2:C:290:LEU:HB2	2:C:300:ASP:HA	1.87	0.56
2:C:846:LYS:HB3	3:D:741:ASP:HB2	1.88	0.56
3:D:1472:ILE:HG22	3:D:1474:ALA:H	1.71	0.56
1:A:36:LEU:HD11	1:B:221:HIS:HB3	1.86	0.56
2:C:134:ARG:NH1	2:C:392:SER:OG	2.38	0.56
3:D:1207:TYR:HA	3:D:1214:PRO:HA	1.88	0.56
3:D:131:LYS:HG3	3:D:568:ARG:HG2	1.88	0.56
3:D:465:LEU:HD22	3:D:509:PRO:HB2	1.88	0.56
2:C:369:PRO:O	2:C:372:LEU:N	2.30	0.56
3:D:908:LYS:HB3	3:D:1027:GLY:HA3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1205:TYR:CE1	3:D:1366:LYS:HD3	2.41	0.56
4:E:46:PRO:HB3	4:E:54:LEU:HD13	1.88	0.56
2:C:89:THR:HG23	2:C:129:ILE:HA	1.88	0.56
1:A:38:ASN:H	1:A:39:PRO:HD2	1.70	0.55
1:A:48:ILE:HG22	1:A:173:PRO:HD2	1.88	0.55
3:D:843:PHE:HB2	3:D:866:VAL:HG13	1.88	0.55
4:E:54:LEU:HD22	4:E:63:TRP:HE1	1.71	0.55
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.88	0.55
2:C:606:VAL:HG12	2:C:611:ILE:HG12	1.89	0.55
3:D:1422:MET:HE2	3:D:1427:SER:HA	1.87	0.55
3:D:207:PHE:O	3:D:391:ALA:N	2.39	0.55
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.88	0.55
2:C:1084:SER:HB2	3:D:613:ARG:HH12	1.72	0.55
1:A:156:HIS:HD2	1:A:158:ILE:HG12	1.70	0.55
3:D:798:GLU:OE1	3:D:828:LYS:NZ	2.34	0.55
1:B:6:LEU:C	1:B:8:ALA:H	2.15	0.55
1:B:58:ILE:HD13	1:B:140:MET:HB3	1.89	0.55
2:C:6:PHE:CD1	2:C:909:ALA:HB2	2.42	0.55
3:D:207:PHE:HB2	3:D:391:ALA:HB3	1.89	0.55
3:D:215:TYR:CE1	3:D:380:GLU:HB3	2.42	0.55
5:F:392:VAL:HG12	5:F:393:THR:H	1.72	0.55
1:A:156:HIS:HE1	1:A:167:VAL:O	1.89	0.55
3:D:186:VAL:N	3:D:189:GLN:OE1	2.36	0.55
3:D:562:ALA:HB1	3:D:567:ILE:HD11	1.89	0.55
3:D:324:ALA:HB1	3:D:331:VAL:HG11	1.89	0.54
3:D:1137:ARG:H	3:D:1137:ARG:HD2	1.72	0.54
3:D:1486:VAL:HG11	4:E:22:VAL:HG13	1.89	0.54
5:F:394:ARG:O	5:F:397:ILE:HG13	2.07	0.54
3:D:1462:LEU:HD21	3:D:1472:ILE:HG23	1.89	0.54
2:C:95:TYR:HD2	2:C:114:PHE:HB3	1.72	0.54
3:D:539:ASP:OD1	5:F:316:SER:OG	2.14	0.54
3:D:820:GLU:HG2	3:D:825:ALA:O	2.08	0.54
2:C:358:ARG:HG2	2:C:371:LYS:O	2.07	0.54
2:C:143:SER:O	2:C:147:TYR:OH	2.17	0.54
5:F:223:ALA:HB2	5:F:242:TRP:HB2	1.90	0.54
2:C:25:SER:OG	2:C:337:GLY:N	2.38	0.54
2:C:598:GLU:HB2	2:C:615:TYR:HE1	1.71	0.54
2:C:794:PRO:HG3	2:C:1025:ALA:HA	1.89	0.54
3:D:112:ILE:HG13	3:D:113:GLY:N	2.22	0.54
3:D:782:SER:H	3:D:785:ILE:HD13	1.72	0.54
3:D:807:ALA:HB2	3:D:832:ARG:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:968:ASP:OD1	3:D:1058:ARG:NH2	2.41	0.54
5:F:126:LEU:O	5:F:130:VAL:HG23	2.08	0.54
3:D:408:GLU:HG2	3:D:421:LEU:O	2.07	0.54
3:D:465:LEU:HD12	3:D:513:ILE:HD11	1.89	0.54
3:D:811:GLU:O	3:D:815:ALA:HB3	2.06	0.54
3:D:843:PHE:CE1	3:D:864:VAL:HG11	2.43	0.54
4:E:33:HIS:O	4:E:37:ASN:ND2	2.41	0.54
1:B:65:PHE:CE1	3:D:813:LEU:HD13	2.43	0.54
3:D:206:ARG:HE	3:D:394:LEU:HB2	1.72	0.54
3:D:911:LEU:O	3:D:915:VAL:HG23	2.07	0.54
3:D:1263:PHE:CE2	3:D:1371:VAL:HG11	2.43	0.54
2:C:535:SER:OG	2:C:537:LYS:NZ	2.40	0.53
2:C:1041:GLU:HB3	3:D:1223:ILE:HD13	1.90	0.53
2:C:115:LEU:HD12	2:C:378:LEU:HD22	1.89	0.53
2:C:557:ARG:HA	2:C:560:MET:HG3	1.89	0.53
3:D:1003:VAL:O	3:D:1007:VAL:HG13	2.06	0.53
1:A:185:ARG:HB3	1:A:190:THR:HG23	1.91	0.53
1:B:73:GLU:CD	1:B:131:THR:H	2.16	0.53
2:C:1068:GLU:O	2:C:1072:LYS:HG2	2.07	0.53
3:D:1263:PHE:HE2	3:D:1371:VAL:HG11	1.74	0.53
3:D:1155:VAL:C	3:D:1157:GLY:H	2.16	0.53
2:C:1007:ALA:HB2	3:D:648:MET:HG3	1.90	0.53
3:D:412:GLY:N	3:D:435:VAL:O	2.39	0.53
3:D:785:ILE:HG13	3:D:939:PHE:CE2	2.44	0.53
3:D:1404:ASN:O	3:D:1409:ALA:HB3	2.08	0.53
2:C:627:ARG:HG3	2:C:628:PHE:N	2.24	0.53
5:F:79:ASP:HB3	5:F:80:PRO:HD3	1.90	0.53
1:B:161:ARG:HG3	1:B:163:ASN:H	1.73	0.53
2:C:863:ASP:OD1	2:C:863:ASP:N	2.41	0.53
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.91	0.53
3:D:1292:VAL:HG23	3:D:1305:LEU:HD11	1.90	0.53
3:D:568:ARG:HH11	3:D:571:LYS:HD2	1.74	0.53
3:D:792:ILE:HG21	3:D:941:PHE:CD1	2.44	0.53
2:C:410:ILE:HB	2:C:453:THR:O	2.08	0.53
3:D:237:LYS:HB3	3:D:238:PRO:HD2	1.91	0.53
5:F:371:LEU:HD22	5:F:375:LEU:HB2	1.91	0.53
2:C:41:ASN:OD1	2:C:41:ASN:N	2.39	0.52
3:D:86:ARG:HG2	3:D:522:PRO:HG2	1.89	0.52
3:D:1233:GLY:HA2	3:D:1236:LEU:HD12	1.91	0.52
1:A:229:GLN:HB3	1:B:12:THR:HG22	1.91	0.52
2:C:84:ARG:NH2	2:C:133:ASP:OD1	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:276:LYS:HE3	2:C:464:LEU:HD21	1.91	0.52
2:C:50:GLU:OE2	2:C:345:ARG:NH1	2.42	0.52
2:C:71:TYR:HA	2:C:96:ALA:HA	1.92	0.52
3:D:1164:ARG:NH2	3:D:1170:ASP:OD1	2.43	0.52
1:B:59:GLU:HG2	1:B:139:ASN:HB3	1.91	0.52
3:D:957:PRO:HG2	3:D:1007:VAL:HG12	1.90	0.52
3:D:12:LEU:HD21	3:D:104:PHE:HZ	1.73	0.52
3:D:546:ARG:NH2	3:D:576:GLU:OE2	2.42	0.52
1:A:42:ARG:HH12	2:C:857:ASP:HB3	1.73	0.52
2:C:1086:ARG:HG2	2:C:1111:ILE:HD12	1.91	0.52
2:C:1088:LEU:O	2:C:1092:LEU:HB2	2.10	0.52
3:D:1486:VAL:HA	4:E:74:VAL:O	2.09	0.52
2:C:100:LEU:HD22	2:C:372:LEU:HD21	1.91	0.52
2:C:433:THR:C	2:C:435:TYR:H	2.17	0.52
3:D:214:GLU:O	3:D:383:GLY:HA2	2.10	0.52
3:D:436:GLU:HG3	3:D:445:ARG:HB2	1.92	0.52
1:B:48:ILE:CG2	1:B:173:PRO:HD2	2.40	0.52
2:C:170:PRO:HG2	2:C:258:TYR:CD2	2.45	0.52
2:C:200:LEU:HD22	2:C:300:ASP:HB3	1.92	0.52
2:C:524:VAL:HG22	2:C:525:SER:H	1.75	0.52
3:D:413:ASP:OD1	5:F:178:ARG:NH1	2.36	0.52
2:C:94:LEU:O	2:C:114:PHE:HA	2.09	0.51
2:C:204:GLN:HE22	2:C:225:SER:HB3	1.75	0.51
3:D:754:PHE:O	3:D:758:GLU:HG2	2.10	0.51
3:D:1428:ALA:O	3:D:1431:THR:HG23	2.10	0.51
1:A:153:ALA:HA	1:A:156:HIS:CE1	2.44	0.51
3:D:376:GLU:O	3:D:378:ILE:HG13	2.10	0.51
3:D:611:GLN:O	3:D:616:GLN:HB2	2.10	0.51
2:C:235:LEU:HD21	2:C:251:ASP:O	2.11	0.51
2:C:312:ALA:HB1	2:C:318:PRO:HG3	1.91	0.51
2:C:368:THR:HB	2:C:369:PRO:HD3	1.93	0.51
2:C:1066:ALA:HA	2:C:1077:PRO:HD2	1.93	0.51
3:D:475:LYS:HA	3:D:478:LEU:HD12	1.91	0.51
3:D:835:SER:H	3:D:838:ARG:HE	1.58	0.51
2:C:578:VAL:HG23	2:C:579:VAL:HG12	1.92	0.51
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.45	0.51
3:D:206:ARG:HB3	3:D:207:PHE:CD1	2.46	0.51
3:D:222:GLY:HA2	3:D:333:LEU:O	2.10	0.51
3:D:813:LEU:HD12	3:D:814:ALA:N	2.25	0.51
1:A:188:GLN:HG2	1:A:189:ARG:HG2	1.93	0.51
1:B:4:SER:HA	1:B:7:LYS:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:17:PRO:O	2:C:20:GLU:HB3	2.11	0.51
2:C:1019:GLN:HB2	3:D:622:ARG:HB2	1.92	0.51
2:C:1101:THR:HG21	2:C:1111:ILE:HG21	1.93	0.51
3:D:701:LEU:HD21	3:D:763:MET:HE3	1.91	0.51
3:D:802:ALA:O	3:D:804:LEU:N	2.44	0.51
3:D:1264:GLU:OE2	3:D:1425:THR:OG1	2.25	0.51
4:E:41:GLU:O	4:E:42:PRO:C	2.53	0.51
6:H:18:ASP:OD1	6:H:60:LYS:NZ	2.36	0.51
3:D:1042:ARG:O	3:D:1057:VAL:HB	2.10	0.51
2:C:1095:LEU:O	2:C:1097:LEU:N	2.41	0.51
3:D:612:GLY:O	3:D:614:PHE:N	2.44	0.51
5:F:132:ARG:O	5:F:136:LEU:HG	2.11	0.51
1:A:7:LYS:HG2	1:A:9:PRO:HD3	1.93	0.51
1:B:124:ASN:HD21	1:B:127:LEU:HD22	1.76	0.51
2:C:540:PHE:HE1	2:C:906:PHE:HE1	1.59	0.51
2:C:726:ILE:HG12	2:C:787:ASP:HB2	1.93	0.51
3:D:165:LYS:HG3	3:D:397:LYS:HB3	1.93	0.51
3:D:931:LEU:HA	3:D:934:LEU:HD12	1.93	0.51
3:D:799:LYS:HE2	3:D:801:GLY:HA3	1.92	0.50
3:D:850:LEU:HA	3:D:853:VAL:HB	1.93	0.50
2:C:73:LEU:HA	2:C:93:PRO:O	2.11	0.50
3:D:90:MET:HG3	3:D:521:PRO:HD3	1.93	0.50
5:F:411:HIS:O	6:G:120:THR:OG1	2.16	0.50
3:D:84:ILE:HG12	3:D:85:VAL:N	2.25	0.50
3:D:1095:THR:O	3:D:1099:VAL:HG23	2.11	0.50
1:A:59:GLU:HG2	1:A:139:ASN:HB3	1.94	0.50
2:C:66:LEU:HD13	2:C:100:LEU:HB3	1.93	0.50
1:B:83:LYS:O	1:B:170:VAL:HG21	2.12	0.50
2:C:15:LEU:HD11	2:C:457:ALA:HB1	1.93	0.50
2:C:276:LYS:O	2:C:280:LYS:HD2	2.11	0.50
3:D:1125:PRO:HA	3:D:1131:SER:O	2.11	0.50
3:D:1479:ASP:HA	3:D:1482:ARG:HD3	1.94	0.50
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.94	0.50
3:D:504:ASP:C	3:D:506:GLY:N	2.67	0.50
2:C:575:GLN:HB2	2:C:670:GLN:HA	1.94	0.50
1:B:58:ILE:HB	1:B:61:VAL:HB	1.93	0.49
2:C:710:ILE:HB	2:C:790:LEU:HD22	1.93	0.49
3:D:371:ILE:HG13	3:D:372:ASP:H	1.76	0.49
2:C:11:GLU:HG2	2:C:535:SER:HB2	1.94	0.49
2:C:1002:GLU:C	2:C:1004:LYS:H	2.19	0.49
4:E:51:LEU:HD12	4:E:53:GLY:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:971:LYS:HA	2:C:988:VAL:HA	1.94	0.49
3:D:30:GLU:O	3:D:43:GLY:HA3	2.12	0.49
3:D:52:PRO:HD3	3:D:78:VAL:HG13	1.93	0.49
3:D:87:ARG:HB3	3:D:523:ASP:HB2	1.94	0.49
3:D:192:ALA:HB1	3:D:193:PRO:HD2	1.93	0.49
3:D:233:LYS:HD3	3:D:235:ALA:HB3	1.94	0.49
3:D:475:LYS:O	3:D:479:GLU:HG2	2.11	0.49
3:D:646:LYS:HB3	3:D:688:TRP:CH2	2.47	0.49
2:C:759:THR:HB	2:C:785:VAL:CG2	2.42	0.49
6:G:52:VAL:HG12	6:G:70:ILE:HA	1.94	0.49
1:A:41:ARG:HA	1:A:177:VAL:HG11	1.94	0.49
1:B:94:LEU:HD21	1:B:119:ASP:HB2	1.94	0.49
3:D:176:ASP:OD1	3:D:389:GLU:HG2	2.13	0.49
2:C:146:VAL:HG11	2:C:306:THR:HG22	1.94	0.49
3:D:136:ASP:HB3	3:D:137:PRO:CD	2.43	0.49
3:D:1046:GLN:HA	3:D:1052:THR:HA	1.95	0.49
3:D:1110:ALA:O	3:D:1202:GLN:HB2	2.12	0.49
5:F:346:THR:O	5:F:350:LEU:HB2	2.12	0.49
6:G:86:ALA:HA	6:G:107:LEU:HG	1.95	0.49
1:A:55:SER:HA	1:A:167:VAL:HG23	1.95	0.49
2:C:64:LEU:HB2	2:C:359:MET:HE3	1.94	0.49
3:D:303:PRO:O	3:D:305:ALA:N	2.45	0.49
3:D:1031:ASN:HB3	3:D:1034:GLN:HG3	1.92	0.49
3:D:1112:CYS:HB2	3:D:1195:GLN:HB3	1.95	0.49
3:D:1286:THR:HB	3:D:1289:LYS:O	2.13	0.49
6:G:31:LEU:HA	6:G:51:PRO:HB2	1.95	0.49
1:A:44:LEU:O	1:A:174:VAL:HG21	2.12	0.49
1:A:57:TYR:CE1	1:A:163:ASN:HB2	2.48	0.49
2:C:913:GLU:O	2:C:917:LEU:HD12	2.12	0.49
1:A:134:GLU:CD	1:A:134:GLU:H	2.19	0.49
1:B:86:VAL:CG1	1:B:124:ASN:HB2	2.43	0.49
3:D:764:LEU:HD23	3:D:767:HIS:CE1	2.48	0.49
2:C:725:ASP:HB2	6:G:99:HIS:HE1	1.78	0.49
3:D:584:ASN:CG	3:D:590:PRO:HD2	2.38	0.49
3:D:959:GLU:HG3	3:D:1006:ALA:HB1	1.95	0.49
2:C:541:SER:O	2:C:545:ASN:HB2	2.13	0.48
3:D:1462:LEU:HD23	3:D:1472:ILE:HD12	1.94	0.48
1:A:213:GLN:O	1:A:217:ILE:HG13	2.14	0.48
1:B:128:HIS:NE2	1:B:131:THR:HG23	2.28	0.48
2:C:108:ILE:HB	2:C:368:THR:HG23	1.95	0.48
3:D:440:VAL:HG23	3:D:441:ARG:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:376:ILE:HG22	5:F:377:ASP:HB2	1.95	0.48
1:B:13:VAL:HG22	1:B:23:PHE:HD1	1.78	0.48
1:B:80:LEU:HD11	3:D:842:VAL:HG12	1.94	0.48
2:C:75:GLU:O	2:C:93:PRO:HD3	2.13	0.48
2:C:922:PHE:CD2	2:C:964:LYS:HD2	2.48	0.48
3:D:39:PRO:HB3	3:D:45:PHE:O	2.13	0.48
3:D:41:ARG:HB2	3:D:42:ASP:H	1.53	0.48
3:D:1349:VAL:HA	3:D:1368:ILE:HG21	1.94	0.48
3:D:1364:HIS:NE2	3:D:1366:LYS:HE3	2.28	0.48
5:F:355:GLU:HA	5:F:358:LEU:HB3	1.95	0.48
2:C:2:GLU:O	2:C:899:GLN:HB2	2.14	0.48
2:C:712:ALA:O	2:C:820:ARG:HB2	2.13	0.48
3:D:56:TYR:O	3:D:80:VAL:HG21	2.13	0.48
1:A:122:ILE:HG22	1:A:124:ASN:H	1.78	0.48
1:A:178:ALA:HB2	2:C:864:GLY:N	2.29	0.48
3:D:481:MET:SD	3:D:489:ARG:HB2	2.53	0.48
2:C:350:ARG:HG2	2:C:353:ARG:NH1	2.29	0.48
3:D:351:MET:HG3	3:D:370:ALA:HB2	1.95	0.48
3:D:804:LEU:HD22	3:D:825:ALA:HB1	1.95	0.48
2:C:151:ASP:HB2	2:C:157:ARG:O	2.13	0.48
2:C:266:ARG:HD2	2:C:266:ARG:N	2.28	0.48
3:D:1330:ILE:HG21	3:D:1335:LEU:HD12	1.95	0.48
4:E:33:HIS:C	4:E:37:ASN:HD21	2.21	0.48
5:F:114:LYS:O	5:F:117:SER:OG	2.25	0.48
5:F:152:ASP:HB2	5:F:153:PRO:HD3	1.95	0.48
3:D:592:THR:O	3:D:593:ASN:C	2.56	0.48
3:D:770:LEU:HA	3:D:777:PRO:HA	1.94	0.48
3:D:838:ARG:HD3	3:D:874:GLU:HB3	1.96	0.48
2:C:502:PRO:HB2	2:C:509:ALA:HB3	1.96	0.48
4:E:60:ALA:O	4:E:63:TRP:HB2	2.12	0.48
1:B:81:ASN:O	1:B:127:LEU:HD21	2.14	0.48
2:C:151:ASP:HB3	2:C:154:ARG:O	2.13	0.48
2:C:863:ASP:O	2:C:865:THR:N	2.41	0.48
3:D:1381:VAL:HG23	3:D:1391:GLU:HB2	1.95	0.48
2:C:165:LEU:HA	2:C:166:PRO:C	2.39	0.47
2:C:250:ARG:HE	2:C:250:ARG:HB3	1.46	0.47
3:D:45:PHE:HB3	3:D:86:ARG:HH22	1.79	0.47
3:D:764:LEU:HD12	3:D:765:SER:N	2.29	0.47
3:D:1172:HIS:HA	3:D:1175:ILE:HD12	1.96	0.47
3:D:1192:LEU:HG	3:D:1369:GLU:HB3	1.95	0.47
1:B:30:ARG:HE	2:C:854:PRO:HB3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ASN:HB3	1:B:39:PRO:HD3	1.96	0.47
2:C:343:GLN:HG2	2:C:385:PHE:HB2	1.96	0.47
3:D:817:GLU:O	3:D:821:VAL:HG23	2.13	0.47
3:D:877:PRO:O	3:D:880:ILE:HG22	2.14	0.47
1:A:46:SER:OG	1:A:47:SER:N	2.46	0.47
2:C:346:VAL:O	2:C:350:ARG:HG3	2.14	0.47
5:F:94:LEU:HB3	5:F:97:GLU:HB2	1.96	0.47
2:C:798:GLY:H	2:C:827:VAL:HG12	1.79	0.47
3:D:117:ASP:HB3	3:D:150:ARG:HD3	1.96	0.47
3:D:413:ASP:OD1	3:D:413:ASP:N	2.47	0.47
5:F:232:ARG:HA	5:F:232:ARG:HD2	1.78	0.47
2:C:780:GLU:O	2:C:781:LYS:HB3	2.15	0.47
4:E:27:ALA:HB2	4:E:61:GLU:HA	1.96	0.47
4:E:70:THR:HB	4:E:72:ARG:HG3	1.96	0.47
1:A:86:VAL:HG22	1:A:123:MET:HB2	1.96	0.47
3:D:227:LEU:HD13	3:D:328:GLY:C	2.40	0.47
3:D:686:GLU:H	3:D:686:GLU:HG3	1.36	0.47
3:D:804:LEU:HD21	3:D:829:VAL:HG21	1.96	0.47
3:D:850:LEU:HD21	3:D:881:LEU:HB2	1.96	0.47
5:F:88:ILE:HD13	5:F:193:ARG:HB2	1.96	0.47
6:G:34:LEU:HD13	6:G:134:HIS:CE1	2.50	0.47
2:C:264:PRO:HB2	2:C:289:THR:HG21	1.96	0.47
2:C:717:LEU:O	2:C:783:ARG:NH1	2.37	0.47
3:D:62:LYS:HE2	3:D:75:ARG:HD3	1.95	0.47
3:D:135:LEU:HD22	3:D:137:PRO:O	2.14	0.47
3:D:348:GLN:HB2	3:D:351:MET:SD	2.54	0.47
3:D:632:VAL:O	3:D:727:GLN:HA	2.14	0.47
3:D:800:LYS:HB2	3:D:829:VAL:HB	1.96	0.47
3:D:860:LEU:HD23	3:D:877:PRO:HB2	1.96	0.47
3:D:889:ALA:HB1	3:D:930:LEU:HA	1.96	0.47
3:D:1278:ASP:HA	3:D:1319:VAL:O	2.15	0.47
6:H:21:THR:HG22	6:H:22:GLU:N	2.30	0.47
2:C:25:SER:OG	2:C:335:THR:HB	2.15	0.47
2:C:97:ARG:HA	2:C:111:ASP:O	2.15	0.47
2:C:584:GLU:O	2:C:588:VAL:HG13	2.15	0.47
3:D:9:ARG:HB2	3:D:1456:LYS:HG2	1.96	0.47
3:D:130:SER:HB3	3:D:132:TYR:HD2	1.79	0.47
3:D:254:GLU:O	3:D:255:GLU:HB2	2.13	0.47
3:D:433:GLY:HA2	3:D:449:SER:H	1.79	0.47
3:D:800:LYS:HG2	3:D:802:ALA:O	2.15	0.47
3:D:892:ASP:OD2	3:D:895:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1122:LEU:HD11	3:D:1186:VAL:HG23	1.97	0.47
3:D:1412:LYS:O	3:D:1414:PRO:HD3	2.15	0.47
1:B:62:LEU:HD12	1:B:63:HIS:H	1.79	0.47
3:D:269:PHE:HD1	3:D:283:PHE:HD1	1.63	0.47
3:D:719:VAL:O	3:D:721:VAL:HG13	2.15	0.47
5:F:405:LEU:HA	5:F:408:LEU:HD23	1.96	0.47
2:C:1029:GLY:HA3	3:D:623:VAL:O	2.14	0.47
2:C:1081:VAL:HG11	2:C:1086:ARG:HG3	1.97	0.47
3:D:259:VAL:HG21	3:D:293:VAL:HG12	1.97	0.47
1:A:83:LYS:HE2	1:A:168:ASP:HB2	1.97	0.46
3:D:36:THR:C	3:D:38:LYS:H	2.23	0.46
3:D:1106:VAL:HG12	3:D:1107:VAL:H	1.81	0.46
3:D:1481:VAL:HG12	4:E:21:VAL:HG21	1.97	0.46
5:F:93:LEU:HD13	5:F:99:GLU:HG2	1.96	0.46
2:C:149:THR:HG22	2:C:150:PRO:O	2.15	0.46
2:C:302:VAL:O	2:C:305:PRO:HD2	2.14	0.46
2:C:739:GLU:OE1	6:G:61:ARG:HB2	2.15	0.46
3:D:546:ARG:O	3:D:550:ARG:HG2	2.15	0.46
3:D:1271:LYS:HE3	3:D:1334:GLN:HE22	1.80	0.46
3:D:495:ARG:O	3:D:498:VAL:HG13	2.15	0.46
3:D:565:ILE:HD12	3:D:566:ILE:HG13	1.97	0.46
6:G:63:VAL:HG12	6:G:93:GLY:HA2	1.97	0.46
1:B:75:VAL:HA	1:B:78:ILE:HD12	1.97	0.46
2:C:1076:VAL:HA	2:C:1077:PRO:HD3	1.69	0.46
3:D:635:PRO:HG2	3:D:636:GLN:HG2	1.96	0.46
3:D:1282:ARG:HA	3:D:1315:ASP:OD1	2.16	0.46
1:B:54:THR:OG1	1:B:158:ILE:HG13	2.16	0.46
1:B:80:LEU:HG	3:D:844:ALA:HB2	1.98	0.46
2:C:395:LYS:HE2	2:C:403:SER:HB2	1.98	0.46
2:C:792:VAL:HA	2:C:793:PRO:HD3	1.76	0.46
3:D:1493:LYS:O	3:D:1496:GLU:HB3	2.14	0.46
2:C:431:HIS:ND1	2:C:433:THR:OG1	2.42	0.46
2:C:598:GLU:HB2	2:C:615:TYR:CE1	2.50	0.46
3:D:130:SER:O	3:D:568:ARG:NH2	2.49	0.46
3:D:1317:ASP:N	3:D:1317:ASP:OD1	2.48	0.46
3:D:845:ASN:HB2	3:D:848:GLU:HB2	1.98	0.46
3:D:1440:PHE:O	3:D:1442:ASN:N	2.42	0.46
5:F:388:ALA:HB3	5:F:397:ILE:HD13	1.97	0.46
6:H:95:ASN:OD1	6:H:95:ASN:N	2.48	0.46
3:D:90:MET:HG2	3:D:519:VAL:O	2.15	0.46
1:B:191:ASP:OD1	1:B:191:ASP:N	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:49:ARG:HH11	2:C:49:ARG:HB2	1.81	0.46
2:C:787:ASP:OD1	2:C:789:SER:OG	2.33	0.46
3:D:123:LEU:HD23	3:D:152:LEU:HD13	1.96	0.46
1:B:73:GLU:OE2	1:B:131:THR:OG1	2.29	0.46
2:C:177:GLU:HG3	2:C:179:ASN:H	1.81	0.46
2:C:424:GLY:O	2:C:428:ARG:HG3	2.16	0.46
3:D:30:GLU:HB3	3:D:40:GLU:HG2	1.97	0.46
3:D:566:ILE:HD13	5:F:217:ASN:HB3	1.98	0.46
3:D:835:SER:H	3:D:838:ARG:NE	2.15	0.45
3:D:1272:ALA:HA	3:D:1326:THR:HB	1.99	0.45
6:G:11:ARG:HH21	6:H:17:PRO:HG2	1.81	0.45
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.97	0.45
3:D:510:GLU:O	3:D:513:ILE:HD12	2.17	0.45
3:D:529:GLN:NE2	3:D:532:GLY:O	2.48	0.45
3:D:729:HIS:HA	3:D:730:PRO:HD2	1.81	0.45
3:D:1118:ILE:HD11	3:D:1346:ARG:HD2	1.98	0.45
5:F:369:LEU:HD13	5:F:373:LYS:HE3	1.97	0.45
6:H:7:GLU:N	6:H:8:PRO:HD2	2.30	0.45
3:D:840:LYS:HD3	3:D:841:TYR:CE1	2.52	0.45
3:D:959:GLU:OE1	3:D:959:GLU:N	2.48	0.45
3:D:1036:ARG:HH21	3:D:1042:ARG:HA	1.82	0.45
6:H:23:LEU:HB3	6:H:59:ARG:HH12	1.82	0.45
1:A:18:ARG:HH22	1:A:88:ARG:NH2	2.08	0.45
1:A:42:ARG:HD2	2:C:978:ARG:HA	1.97	0.45
1:B:175:ARG:N	1:B:200:TRP:O	2.27	0.45
2:C:810:ASP:HA	2:C:811:PRO:HD3	1.79	0.45
3:D:102:ILE:O	3:D:102:ILE:HG13	2.17	0.45
3:D:266:GLU:O	3:D:314:PRO:HG3	2.17	0.45
4:E:40:LEU:HG	4:E:67:GLU:HG2	1.97	0.45
1:A:62:LEU:HD12	1:A:62:LEU:H	1.81	0.45
2:C:95:TYR:HA	2:C:113:VAL:O	2.15	0.45
3:D:161:LEU:O	3:D:449:SER:HB2	2.17	0.45
3:D:408:GLU:HG3	3:D:422:ALA:HA	1.99	0.45
3:D:612:GLY:O	3:D:615:ARG:N	2.50	0.45
3:D:1258:ARG:NH1	3:D:1261:GLU:OE2	2.50	0.45
3:D:1432:LYS:HD2	3:D:1433:SER:H	1.82	0.45
5:F:108:GLU:HB3	5:F:176:ILE:HG23	1.99	0.45
5:F:355:GLU:HG3	5:F:358:LEU:HD22	1.99	0.45
1:B:19:GLU:O	1:B:200:TRP:HA	2.16	0.45
2:C:446:GLY:O	2:C:449:ILE:HG13	2.17	0.45
2:C:627:ARG:HG3	2:C:628:PHE:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:725:ASP:HB2	6:G:99:HIS:CE1	2.51	0.45
2:C:815:LEU:HD21	2:C:821:GLU:HA	1.98	0.45
3:D:8:VAL:HG12	3:D:1434:TRP:CH2	2.51	0.45
3:D:939:PHE:O	3:D:943:THR:HG23	2.16	0.45
3:D:1259:VAL:O	3:D:1263:PHE:HD1	1.97	0.45
2:C:190:LYS:HE2	2:C:190:LYS:HB3	1.66	0.45
2:C:309:TYR:HA	2:C:312:ALA:HB3	1.98	0.45
2:C:439:CYS:HA	2:C:440:PRO:HD3	1.75	0.45
2:C:782:ALA:HB1	6:G:34:LEU:HD12	1.99	0.45
3:D:22:SER:HB2	3:D:92:HIS:HB3	1.98	0.45
3:D:828:LYS:O	3:D:828:LYS:HG2	2.16	0.45
3:D:907:GLU:HG2	3:D:908:LYS:H	1.82	0.45
2:C:479:VAL:N	2:C:506:ASN:O	2.42	0.45
2:C:1008:ARG:NH1	3:D:624:ASP:OD1	2.49	0.45
3:D:553:ARG:NH1	3:D:570:GLU:OE1	2.49	0.45
1:A:88:ARG:HD3	1:A:90:LEU:HD23	1.99	0.45
1:B:132:LEU:HD12	1:B:132:LEU:HA	1.71	0.45
2:C:1016:ILE:HG13	2:C:1017:THR:H	1.81	0.45
3:D:177:ALA:HB3	3:D:191:LEU:O	2.17	0.45
3:D:709:HIS:HA	3:D:1227:GLN:HB3	1.99	0.45
3:D:800:LYS:HG3	3:D:804:LEU:HG	1.98	0.45
3:D:809:PRO:O	3:D:812:ALA:HB3	2.17	0.45
3:D:907:GLU:HG3	3:D:1025:GLN:O	2.17	0.45
5:F:399:GLN:O	5:F:403:LYS:HG2	2.17	0.45
1:A:19:GLU:O	1:A:201:THR:N	2.50	0.45
1:A:212:ASN:O	1:A:215:VAL:HG22	2.17	0.45
2:C:110:GLU:HG2	2:C:369:PRO:HB3	1.99	0.45
2:C:214:TYR:CE1	2:C:311:PHE:HB3	2.52	0.45
2:C:721:ARG:NH2	6:G:94:ASP:OD1	2.50	0.45
2:C:1024:LYS:H	2:C:1026:GLN:HE22	1.65	0.45
2:C:1043:TYR:CE1	3:D:710:ARG:HB2	2.52	0.45
3:D:879:ARG:NE	3:D:902:LEU:O	2.31	0.45
3:D:1377:LYS:HE3	3:D:1394:VAL:HG13	1.99	0.45
4:E:26:ARG:O	4:E:30:LEU:HB2	2.16	0.45
2:C:352:ALA:HA	2:C:355:VAL:HG12	2.00	0.44
3:D:202:VAL:HG12	3:D:204:LEU:HD12	1.98	0.44
3:D:229:ALA:O	3:D:231:VAL:HG22	2.17	0.44
3:D:759:ALA:HA	3:D:763:MET:HE2	1.98	0.44
3:D:1434:TRP:CZ3	3:D:1457:ASP:HB2	2.52	0.44
1:A:70:GLY:HA3	1:A:136:GLY:HA2	1.98	0.44
1:B:48:ILE:HA	1:B:49:PRO:HD3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ALA:HA	1:B:156:HIS:HE1	1.82	0.44
3:D:415:VAL:O	3:D:416:ALA:HB2	2.17	0.44
1:B:99:LEU:HD13	1:B:99:LEU:HA	1.85	0.44
2:C:432:ARG:NH1	2:C:492:ASP:OD2	2.49	0.44
2:C:565:GLN:CG	2:C:995:MET:HE1	2.47	0.44
5:F:368:VAL:HG12	5:F:369:LEU:N	2.31	0.44
1:B:39:PRO:O	1:B:43:ILE:HG12	2.18	0.44
2:C:433:THR:C	2:C:435:TYR:N	2.75	0.44
2:C:492:ASP:HB3	2:C:518:LYS:HB3	1.99	0.44
2:C:1044:GLY:HA2	3:D:1475:GLY:HA3	1.99	0.44
3:D:1412:LYS:HD2	3:D:1414:PRO:HG3	1.99	0.44
6:H:57:ILE:HG22	6:H:58:LYS:HG2	1.99	0.44
1:A:115:LEU:HA	1:A:116:PRO:HD3	1.87	0.44
1:B:87:VAL:HG12	1:B:122:ILE:HG23	1.99	0.44
2:C:411:SER:OG	2:C:413:LEU:HD12	2.17	0.44
2:C:444:PRO:HA	2:C:563:ASN:HD21	1.82	0.44
2:C:472:ARG:HD3	2:C:534:VAL:HA	2.00	0.44
2:C:517:ARG:O	2:C:518:LYS:C	2.59	0.44
3:D:7:LYS:HG2	3:D:1458:GLU:OE2	2.17	0.44
3:D:219:GLU:HG2	3:D:220:ARG:H	1.83	0.44
1:A:100:LEU:HD13	1:A:115:LEU:HD21	1.98	0.44
1:B:176:ARG:HD3	3:D:884:ARG:HH22	1.83	0.44
2:C:263:ASP:HB2	2:C:264:PRO:HD3	1.98	0.44
2:C:614:ARG:HH11	2:C:620:LEU:HD12	1.83	0.44
3:D:601:ARG:NH2	3:D:605:ASP:O	2.51	0.44
6:G:38:MET:HE1	6:G:68:VAL:HG11	2.00	0.44
6:H:18:ASP:HB3	6:H:61:ARG:NH2	2.33	0.44
1:B:221:HIS:HA	1:B:224:TYR:CD2	2.53	0.44
2:C:170:PRO:HG2	2:C:258:TYR:HD2	1.82	0.44
2:C:363:SER:O	2:C:364:GLU:HG3	2.18	0.44
2:C:560:MET:O	2:C:564:MET:HB2	2.18	0.44
3:D:31:THR:C	3:D:32:ILE:HG13	2.43	0.44
3:D:46:ASP:OD2	3:D:48:ARG:N	2.51	0.44
3:D:136:ASP:HB3	3:D:137:PRO:HD3	2.00	0.44
3:D:644:LEU:HA	3:D:645:PRO:HD3	1.82	0.44
3:D:875:THR:HG23	3:D:876:SER:O	2.18	0.44
3:D:999:THR:O	3:D:1003:VAL:HG13	2.17	0.44
3:D:1123:PHE:HE2	3:D:1184:GLN:HA	1.82	0.44
4:E:30:LEU:HD12	4:E:30:LEU:HA	1.86	0.44
3:D:256:GLU:HG2	3:D:299:GLU:HG2	1.99	0.44
6:H:88:ALA:HB2	6:H:104:PRO:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:VAL:HG21	1:B:82:LEU:HB3	2.00	0.43
2:C:52:PHE:CG	2:C:68:PHE:HB2	2.52	0.43
2:C:396:ASP:O	2:C:402:SER:HB2	2.18	0.43
2:C:778:PHE:O	2:C:779:GLY:C	2.61	0.43
2:C:946:ARG:NH1	3:D:861:GLN:OE1	2.51	0.43
3:D:256:GLU:HB3	3:D:299:GLU:HG2	2.00	0.43
3:D:825:ALA:HA	3:D:826:PRO:HD3	1.74	0.43
1:A:58:ILE:O	1:A:59:GLU:C	2.60	0.43
1:B:100:LEU:O	1:B:115:LEU:HG	2.18	0.43
2:C:742:VAL:HG22	2:C:756:VAL:HG22	1.99	0.43
2:C:957:LYS:HG2	2:C:961:GLU:OE1	2.18	0.43
3:D:214:GLU:HA	3:D:341:GLU:O	2.18	0.43
3:D:562:ALA:C	3:D:567:ILE:HD11	2.43	0.43
4:E:43:GLU:HG3	4:E:44:GLU:H	1.83	0.43
2:C:879:ARG:O	2:C:881:ASN:N	2.51	0.43
3:D:503:LEU:HD23	3:D:503:LEU:HA	1.78	0.43
3:D:783:ARG:H	3:D:783:ARG:HG2	1.53	0.43
5:F:369:LEU:HA	5:F:372:ARG:HB3	1.99	0.43
1:A:218:LEU:O	1:A:222:LEU:HD22	2.19	0.43
1:B:206:THR:HG22	1:B:209:GLU:CD	2.43	0.43
2:C:121:MET:HB2	2:C:127:PHE:HE2	1.84	0.43
2:C:194:VAL:HG21	2:C:221:LEU:O	2.18	0.43
2:C:200:LEU:HD13	2:C:300:ASP:HB3	2.01	0.43
2:C:1015:LEU:HD22	2:C:1015:LEU:HA	1.79	0.43
3:D:135:LEU:HD23	3:D:453:ASP:O	2.18	0.43
3:D:760:ARG:NH1	4:E:61:GLU:OE2	2.52	0.43
3:D:943:THR:OG1	3:D:944:THR:N	2.51	0.43
1:B:23:PHE:HB2	1:B:197:LEU:HD23	2.00	0.43
1:B:85:LEU:HA	1:B:124:ASN:HD22	1.84	0.43
2:C:20:GLU:O	2:C:24:GLU:HB2	2.18	0.43
2:C:227:PHE:CE2	2:C:237:ARG:HD3	2.54	0.43
3:D:984:THR:HG23	3:D:987:GLU:H	1.84	0.43
5:F:397:ILE:HG13	5:F:398:ARG:H	1.83	0.43
1:A:65:PHE:CE1	2:C:799:ILE:HD11	2.54	0.43
2:C:64:LEU:HD22	2:C:359:MET:HG3	2.01	0.43
2:C:456:ALA:HB1	2:C:538:GLN:O	2.19	0.43
2:C:1058:ASP:HB2	3:D:621:LYS:HE3	2.01	0.43
3:D:495:ARG:O	3:D:499:VAL:HG23	2.18	0.43
4:E:6:ILE:HD12	4:E:6:ILE:HA	1.83	0.43
5:F:166:LEU:HA	5:F:167:PRO:HD3	1.89	0.43
5:F:253:ASP:OD2	5:F:253:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1057:SER:OG	2:C:1058:ASP:N	2.51	0.43
3:D:167:GLU:O	3:D:206:ARG:NH2	2.51	0.43
3:D:921:ARG:HH11	3:D:921:ARG:HB3	1.84	0.43
4:E:54:LEU:HG	4:E:58:PRO:HB2	2.00	0.43
1:A:179:PHE:HA	1:A:197:LEU:HA	2.01	0.43
1:B:102:LYS:HB2	1:B:139:ASN:OD1	2.19	0.43
2:C:1018:GLN:HG3	2:C:1060:ILE:HD11	2.01	0.43
3:D:289:THR:O	3:D:305:ALA:HA	2.18	0.43
5:F:329:TYR:CE2	5:F:333:ILE:HD11	2.54	0.43
2:C:264:PRO:O	2:C:266:ARG:NH1	2.52	0.43
2:C:288:ARG:HA	2:C:288:ARG:CZ	2.48	0.43
2:C:497:ALA:N	2:C:531:PHE:O	2.44	0.43
3:D:31:THR:O	3:D:32:ILE:HG13	2.19	0.43
3:D:133:ILE:HD11	3:D:456:MET:HE3	2.01	0.43
3:D:301:GLY:C	3:D:303:PRO:HD2	2.43	0.43
3:D:639:LEU:HD23	3:D:639:LEU:HA	1.84	0.43
3:D:829:VAL:H	3:D:835:SER:HB2	1.82	0.43
3:D:895:VAL:O	3:D:898:GLU:N	2.52	0.43
1:A:75:VAL:O	1:A:79:ILE:HG23	2.18	0.43
1:A:109:VAL:HG12	1:A:129:ILE:HB	2.01	0.43
1:A:159:LYS:O	6:H:21:THR:HG23	2.18	0.43
2:C:717:LEU:H	2:C:717:LEU:HG	1.62	0.43
2:C:766:GLU:H	2:C:766:GLU:HG3	1.67	0.43
3:D:12:LEU:HD23	3:D:12:LEU:HA	1.85	0.43
6:H:37:ARG:HH11	6:H:37:ARG:HA	1.82	0.43
1:A:57:TYR:HE1	1:A:163:ASN:HB2	1.84	0.42
1:B:18:ARG:O	1:B:207:PRO:HD3	2.19	0.42
1:B:40:LEU:HD21	1:B:215:VAL:HG12	2.00	0.42
2:C:13:ILE:HA	2:C:14:PRO:HD3	1.79	0.42
3:D:778:LEU:HD12	3:D:778:LEU:HA	1.81	0.42
3:D:1389:LEU:HD23	3:D:1389:LEU:H	1.84	0.42
3:D:1394:VAL:HB	3:D:1397:LYS:HB2	2.01	0.42
3:D:1434:TRP:CD1	3:D:1434:TRP:C	2.97	0.42
6:H:27:TYR:OH	6:H:34:LEU:O	2.37	0.42
2:C:29:ALA:HB2	2:C:337:GLY:CA	2.49	0.42
2:C:740:GLU:OE1	2:C:805:ARG:NH1	2.51	0.42
3:D:21:TRP:HE3	3:D:90:MET:HE1	1.83	0.42
3:D:181:ASP:C	3:D:183:GLU:N	2.77	0.42
3:D:469:ASP:HB3	3:D:472:ALA:HB3	2.01	0.42
3:D:907:GLU:CD	3:D:909:ASN:HD22	2.28	0.42
4:E:54:LEU:CD2	4:E:63:TRP:HE1	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:147:LEU:HD23	5:F:147:LEU:HA	1.79	0.42
6:G:38:MET:HE3	6:G:98:LEU:HD12	2.01	0.42
6:H:20:GLU:HA	6:H:61:ARG:CD	2.46	0.42
2:C:540:PHE:CE1	2:C:906:PHE:HE1	2.37	0.42
2:C:448:ASN:HA	2:C:451:LEU:HD12	2.01	0.42
2:C:1036:GLU:OE1	2:C:1036:GLU:N	2.45	0.42
1:A:91:ASN:HA	1:A:92:PRO:HD3	1.85	0.42
2:C:1098:ASP:HB2	3:D:13:ALA:HB2	2.00	0.42
3:D:39:PRO:HG2	3:D:47:GLU:CG	2.47	0.42
3:D:525:ARG:NE	3:D:541:ASN:OD1	2.47	0.42
3:D:535:PHE:HB2	5:F:314:PRO:HB3	2.02	0.42
3:D:1197:ARG:HB2	3:D:1396:GLU:CD	2.45	0.42
3:D:1271:LYS:NZ	3:D:1334:GLN:OE1	2.47	0.42
3:D:1377:LYS:HE2	3:D:1378:TYR:CZ	2.54	0.42
2:C:881:ASN:OD1	2:C:884:GLN:NE2	2.46	0.42
3:D:313:MET:HG3	3:D:314:PRO:CD	2.49	0.42
3:D:703:ASN:HB2	3:D:713:ILE:HG12	2.01	0.42
3:D:1112:CYS:HB3	3:D:1196:THR:HG23	2.02	0.42
3:D:1149:LEU:HD23	3:D:1149:LEU:HA	1.78	0.42
3:D:1170:ASP:O	3:D:1173:LEU:HB3	2.20	0.42
3:D:1372:VAL:HG22	3:D:1375:MET:HE3	2.00	0.42
5:F:105:LYS:HB3	5:F:180:GLY:HA2	2.02	0.42
5:F:249:ARG:HG3	5:F:250:ALA:N	2.35	0.42
1:B:75:VAL:O	1:B:79:ILE:HG23	2.19	0.42
2:C:404:LEU:O	2:C:408:ARG:HG2	2.19	0.42
2:C:422:ARG:H	2:C:422:ARG:HG3	1.54	0.42
3:D:256:GLU:HB2	3:D:296:GLU:CG	2.50	0.42
3:D:667:ALA:HA	3:D:668:PRO:HD3	1.89	0.42
3:D:1171:VAL:O	3:D:1175:ILE:HG13	2.19	0.42
3:D:1209:LEU:HD12	3:D:1209:LEU:HA	1.89	0.42
3:D:1262:LEU:HD12	3:D:1262:LEU:HA	1.89	0.42
2:C:470:PRO:HA	2:C:485:TYR:HA	2.01	0.42
2:C:717:LEU:HD13	2:C:763:GLY:HA2	2.01	0.42
2:C:988:VAL:HG12	3:D:948:THR:OG1	2.20	0.42
2:C:1051:GLU:OE2	3:D:752:SER:HB3	2.20	0.42
3:D:178:LEU:O	3:D:181:ASP:HB2	2.20	0.42
3:D:550:ARG:NH1	3:D:573:MET:HB3	2.35	0.42
3:D:881:LEU:O	3:D:885:ILE:HG13	2.19	0.42
3:D:1106:VAL:HG12	3:D:1107:VAL:N	2.35	0.42
6:G:134:HIS:CD2	6:G:134:HIS:N	2.88	0.42
2:C:97:ARG:HE	2:C:97:ARG:HB3	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:143:SER:HB2	2:C:332:ARG:HB2	2.01	0.42
2:C:239:PHE:HZ	2:C:253:ALA:HB3	1.83	0.42
3:D:250:LEU:HD11	3:D:304:LEU:HB3	2.01	0.42
3:D:349:PRO:HB3	5:F:96:LEU:HB3	2.02	0.42
3:D:623:VAL:HG12	3:D:626:SER:HB3	2.01	0.42
3:D:764:LEU:HD12	3:D:765:SER:H	1.84	0.42
3:D:1364:HIS:CE1	3:D:1366:LYS:HB2	2.54	0.42
5:F:82:ARG:O	5:F:86:HIS:HB2	2.19	0.42
1:A:173:PRO:O	1:A:201:THR:HG23	2.20	0.42
1:B:40:LEU:HD23	1:B:40:LEU:HA	1.86	0.42
2:C:30:LEU:HD22	2:C:118:ILE:HD11	2.02	0.42
2:C:80:GLN:HG3	2:C:90:TYR:CE1	2.55	0.42
2:C:576:ALA:HA	2:C:577:PRO:HD3	1.90	0.42
3:D:440:VAL:HG23	3:D:441:ARG:N	2.34	0.42
3:D:690:ALA:O	3:D:694:VAL:HG23	2.20	0.42
3:D:806:PHE:O	3:D:808:THR:N	2.52	0.42
3:D:840:LYS:HD3	3:D:841:TYR:CZ	2.55	0.42
3:D:1463:LYS:O	3:D:1467:ILE:HG13	2.20	0.42
1:A:42:ARG:NH2	1:B:31:GLY:O	2.53	0.41
1:A:161:ARG:HG2	1:A:162:ILE:N	2.35	0.41
2:C:48:PHE:HD1	2:C:48:PHE:HA	1.75	0.41
2:C:137:VAL:HG12	2:C:138:SER:N	2.35	0.41
3:D:223:LEU:HD12	3:D:223:LEU:HA	1.83	0.41
3:D:808:THR:HB	3:D:809:PRO:HD3	2.01	0.41
3:D:1348:LEU:HD12	3:D:1348:LEU:HA	1.85	0.41
5:F:135:ILE:HD11	5:F:178:ARG:HD3	2.02	0.41
3:D:792:ILE:HG13	3:D:793:THR:N	2.33	0.41
2:C:548:PRO:HA	2:C:581:THR:HG22	2.02	0.41
3:D:31:THR:HG23	3:D:45:PHE:CD2	2.55	0.41
3:D:33:ASN:HB3	3:D:35:ARG:HG3	2.03	0.41
3:D:292:VAL:HG12	3:D:293:VAL:HG13	2.02	0.41
3:D:758:GLU:O	3:D:762:GLN:HG3	2.19	0.41
3:D:1396:GLU:O	3:D:1400:VAL:HG23	2.19	0.41
3:D:1403:LEU:HD23	3:D:1407:LEU:HD13	2.01	0.41
3:D:1494:ALA:HB1	4:E:88:GLU:OE2	2.20	0.41
1:B:23:PHE:CE2	1:B:199:ILE:HD12	2.55	0.41
1:B:57:TYR:CE1	1:B:163:ASN:HB2	2.55	0.41
2:C:44:ILE:HG23	2:C:344:PHE:CE1	2.55	0.41
2:C:580:MET:HB3	2:C:584:GLU:CD	2.45	0.41
2:C:670:GLN:O	2:C:993:PHE:HA	2.21	0.41
2:C:803:THR:HG22	2:C:825:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:943:VAL:HG11	2:C:973:VAL:HG13	2.01	0.41
3:D:36:THR:C	3:D:38:LYS:N	2.78	0.41
3:D:104:PHE:N	3:D:104:PHE:CD2	2.88	0.41
3:D:450:TYR:O	3:D:452:ILE:N	2.53	0.41
3:D:1117:TYR:O	3:D:1193:THR:HG21	2.20	0.41
6:G:125:TYR:CE2	6:G:129:MET:HE3	2.55	0.41
1:B:26:GLU:HB2	1:B:194:LYS:HA	2.01	0.41
1:B:219:ARG:O	1:B:223:THR:HG23	2.21	0.41
2:C:176:VAL:HG12	2:C:182:VAL:HG22	2.01	0.41
2:C:424:GLY:HA3	2:C:428:ARG:NE	2.34	0.41
2:C:511:GLU:O	2:C:526:PRO:HD3	2.21	0.41
2:C:515:ALA:C	2:C:516:ARG:HE	2.29	0.41
2:C:1009:SER:HB2	3:D:651:GLU:O	2.20	0.41
3:D:543:LEU:HD21	3:D:600:LEU:HD12	2.02	0.41
3:D:654:LYS:HB3	3:D:655:PRO:HD3	2.03	0.41
3:D:786:ILE:HD13	3:D:908:LYS:HB3	2.02	0.41
3:D:1209:LEU:HD21	3:D:1216:SER:HB2	2.01	0.41
1:B:99:LEU:HD12	1:B:100:LEU:H	1.86	0.41
2:C:52:PHE:CD2	2:C:68:PHE:HB2	2.56	0.41
2:C:517:ARG:HH21	2:C:524:VAL:CG2	2.33	0.41
2:C:984:GLU:HG3	3:D:944:THR:O	2.21	0.41
3:D:299:GLU:O	3:D:301:GLY:N	2.50	0.41
3:D:659:LYS:O	3:D:663:GLU:HG2	2.21	0.41
3:D:706:PRO:O	3:D:708:LEU:HG	2.21	0.41
3:D:894:LYS:CD	3:D:894:LYS:H	2.33	0.41
6:H:107:LEU:HD23	6:H:107:LEU:HA	1.92	0.41
1:B:106:PRO:HA	1:B:132:LEU:O	2.20	0.41
1:B:192:LEU:HA	1:B:192:LEU:HD23	1.74	0.41
2:C:273:GLY:HA2	2:C:276:LYS:NZ	2.36	0.41
2:C:319:GLY:N	2:C:321:GLU:OE1	2.38	0.41
2:C:435:TYR:C	2:C:437:ARG:H	2.29	0.41
2:C:754:ILE:H	2:C:754:ILE:HG12	1.60	0.41
2:C:906:PHE:HZ	3:D:1070:TYR:HD2	1.69	0.41
2:C:950:LEU:HA	2:C:950:LEU:HD13	1.60	0.41
1:A:211:LEU:O	1:A:215:VAL:HG13	2.21	0.41
1:B:36:LEU:O	1:B:39:PRO:HD2	2.21	0.41
2:C:113:VAL:O	2:C:115:LEU:HD23	2.20	0.41
3:D:361:VAL:O	3:D:382:GLU:HA	2.20	0.41
3:D:421:LEU:HD13	3:D:429:SER:H	1.85	0.41
3:D:629:SER:HB2	3:D:648:MET:HE1	2.03	0.41
3:D:919:PHE:C	3:D:919:PHE:CD2	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:936:TYR:C	3:D:936:TYR:CD2	2.98	0.41
3:D:957:PRO:HB2	3:D:959:GLU:HG2	2.02	0.41
5:F:360:LYS:HA	5:F:360:LYS:HD3	1.87	0.41
1:B:6:LEU:C	1:B:8:ALA:N	2.77	0.41
1:B:8:ALA:HA	1:B:9:PRO:HD3	1.87	0.41
2:C:184:MET:HG3	2:C:193:LEU:HD23	2.03	0.41
2:C:227:PHE:CD2	2:C:237:ARG:HD3	2.56	0.41
2:C:274:ARG:HB2	2:C:288:ARG:HH12	1.85	0.41
2:C:517:ARG:HH21	2:C:524:VAL:HG23	1.85	0.41
2:C:724:ARG:NH2	2:C:734:LEU:O	2.54	0.41
2:C:758:ARG:HB3	2:C:788:THR:O	2.21	0.41
2:C:1015:LEU:HD23	5:F:334:PRO:O	2.20	0.41
3:D:172:PRO:O	3:D:174:GLY:N	2.54	0.41
3:D:260:GLU:HB2	3:D:271:VAL:O	2.21	0.41
3:D:422:ALA:C	3:D:424:GLY:H	2.28	0.41
3:D:556:LYS:HB3	3:D:556:LYS:HE2	1.94	0.41
3:D:890:VAL:HG12	3:D:926:LYS:HG2	2.02	0.41
4:E:42:PRO:HB2	4:E:45:ARG:HH21	1.86	0.41
5:F:125:ASP:O	5:F:129:GLU:HG2	2.20	0.41
5:F:188:ILE:O	5:F:192:LEU:HD12	2.21	0.41
5:F:371:LEU:HD13	5:F:375:LEU:HD22	2.03	0.41
6:H:16:ILE:HG21	6:H:63:VAL:HG21	2.03	0.41
6:H:37:ARG:HA	6:H:37:ARG:NH1	2.36	0.41
1:B:122:ILE:C	1:B:124:ASN:H	2.29	0.41
2:C:101:ILE:HG22	2:C:102:HIS:H	1.86	0.41
2:C:172:ILE:HG23	2:C:186:VAL:HG13	2.03	0.41
2:C:177:GLU:CD	2:C:178:PRO:HD2	2.46	0.41
2:C:222:MET:HE3	2:C:222:MET:HB2	1.98	0.41
2:C:270:GLY:O	2:C:274:ARG:HD3	2.21	0.41
2:C:1035:MET:HE3	2:C:1035:MET:HB2	1.85	0.41
3:D:162:ARG:HD2	3:D:162:ARG:HA	1.90	0.41
3:D:806:PHE:O	3:D:807:ALA:C	2.63	0.41
3:D:933:ALA:O	3:D:937:TYR:HD1	2.04	0.41
3:D:1148:VAL:HG21	3:D:1203:LYS:HA	2.01	0.41
5:F:228:GLU:HB3	5:F:230:LYS:HE3	2.03	0.41
2:C:911:GLU:O	2:C:915:LYS:HG2	2.21	0.40
3:D:41:ARG:H	3:D:41:ARG:HG2	1.56	0.40
3:D:736:PHE:O	3:D:738:ALA:N	2.54	0.40
3:D:996:TRP:HB2	3:D:1044:LEU:HD11	2.02	0.40
3:D:1422:MET:HE3	3:D:1426:LYS:HG2	2.03	0.40
3:D:1485:GLN:O	4:E:75:PHE:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:181:GLU:O	5:F:184:ARG:HB3	2.21	0.40
2:C:52:PHE:CD1	2:C:68:PHE:HB2	2.56	0.40
2:C:501:THR:HA	2:C:502:PRO:HD3	1.80	0.40
2:C:666:LEU:HG	2:C:668:LEU:HD11	2.03	0.40
3:D:307:ALA:HB1	3:D:311:LEU:HD11	2.03	0.40
3:D:785:ILE:H	3:D:785:ILE:HD12	1.86	0.40
3:D:828:LYS:HD2	3:D:862:ASP:OD2	2.21	0.40
3:D:920:LEU:HD12	3:D:920:LEU:HA	1.95	0.40
3:D:1472:ILE:HA	3:D:1473:PRO:HD3	1.89	0.40
1:A:101:LEU:HB2	1:A:114:PHE:CE2	2.56	0.40
1:B:65:PHE:O	1:B:66:SER:C	2.64	0.40
2:C:76:PRO:HA	2:C:77:PRO:HD3	1.93	0.40
2:C:610:ARG:HB3	2:C:624:PRO:HA	2.03	0.40
2:C:953:VAL:HG13	2:C:966:LEU:HD13	2.03	0.40
3:D:128:TYR:CZ	3:D:461:ILE:HG13	2.57	0.40
3:D:919:PHE:C	3:D:919:PHE:HD2	2.29	0.40
3:D:1092:GLY:O	3:D:1096:ARG:N	2.52	0.40
3:D:1168:MET:HE3	3:D:1171:VAL:HB	2.04	0.40
5:F:198:ILE:HD11	5:F:240:THR:HA	2.04	0.40
2:C:433:THR:HG21	2:C:488:ALA:HB1	2.02	0.40
3:D:12:LEU:O	3:D:507:ASN:ND2	2.54	0.40
3:D:148:GLU:HB3	3:D:151:GLN:HB2	2.04	0.40
3:D:237:LYS:HB3	3:D:238:PRO:CD	2.52	0.40
3:D:392:SER:C	3:D:393:ILE:HG13	2.46	0.40
3:D:421:LEU:HB3	3:D:422:ALA:H	1.78	0.40
3:D:788:GLY:O	3:D:792:ILE:HG23	2.21	0.40
5:F:174:LEU:HD13	5:F:175:HIS:N	2.37	0.40
5:F:323:ASP:O	5:F:325:LYS:N	2.54	0.40
5:F:365:GLU:H	5:F:365:GLU:HG3	1.59	0.40
2:C:129:ILE:HD11	2:C:386:PHE:HD2	1.87	0.40
2:C:208:ALA:HB2	2:C:222:MET:SD	2.62	0.40
2:C:860:HIS:HA	2:C:866:PRO:HA	2.03	0.40
3:D:129:PHE:O	3:D:572:ARG:HG3	2.21	0.40
3:D:471:GLU:O	3:D:474:GLU:HB3	2.22	0.40
3:D:972:LEU:HD23	3:D:976:GLN:NE2	2.35	0.40
3:D:1096:ARG:HB2	3:D:1096:ARG:NH1	2.34	0.40
5:F:98:GLU:O	5:F:102:LEU:HG	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

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	190/273 (70%)	152 (80%)	38 (20%)	1	8
1	B	200/273 (73%)	163 (82%)	37 (18%)	1	10
2	C	887/941 (94%)	704 (79%)	183 (21%)	1	8
3	D	1254/1279 (98%)	1007 (80%)	247 (20%)	1	8
4	E	83/87 (95%)	68 (82%)	15 (18%)	2	11
5	F	241/371 (65%)	199 (83%)	42 (17%)	2	12
6	G	107/121 (88%)	87 (81%)	20 (19%)	1	10
6	H	79/121 (65%)	72 (91%)	7 (9%)	9	33
All	All	3041/3466 (88%)	2452 (81%)	589 (19%)	1	9

All (589) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	19	GLU
1	A	26	GLU
1	A	43	ILE
1	A	54	THR
1	A	56	VAL
1	A	58	ILE
1	A	59	GLU
1	A	62	LEU
1	A	67	THR
1	A	73	GLU
1	A	76	VAL

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Mol	Chain	Res	Type
1	A	82	LEU
1	A	84	GLU
1	A	86	VAL
1	A	87	VAL
1	A	95	GLN
1	A	96	THR
1	A	104	GLU
1	A	126	ASP
1	A	131	THR
1	A	132	LEU
1	A	134	GLU
1	A	143	ARG
1	A	160	ASP
1	A	165	ILE
1	A	167	VAL
1	A	168	ASP
1	A	174	VAL
1	A	186	LEU
1	A	189	ARG
1	A	196	THR
1	A	216	GLU
1	A	222	LEU
1	A	223	THR
1	A	226	SER
1	A	227	ASN
1	A	229	GLN
1	B	5	LYS
1	B	7	LYS
1	B	10	VAL
1	B	26	GLU
1	B	30	ARG
1	B	34	VAL
1	B	45	LEU
1	B	48	ILE
1	B	54	THR
1	B	59	GLU
1	B	62	LEU
1	B	73	GLU
1	B	76	VAL
1	B	77	GLU
1	B	79	ILE
1	B	80	LEU

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Mol	Chain	Res	Type
1	B	84	GLU
1	B	86	VAL
1	B	90	LEU
1	B	96	THR
1	B	97	VAL
1	B	99	LEU
1	B	101	LEU
1	B	112	ARG
1	B	122	ILE
1	B	132	LEU
1	B	133	GLU
1	B	138	LEU
1	B	145	ASP
1	B	151	VAL
1	B	167	VAL
1	B	175	ARG
1	B	184	THR
1	B	196	THR
1	B	201	THR
1	B	205	VAL
1	B	215	VAL
2	C	5	ARG
2	C	13	ILE
2	C	20	GLU
2	C	30	LEU
2	C	33	ASP
2	C	41	ASN
2	C	48	PHE
2	C	49	ARG
2	C	51	THR
2	C	52	PHE
2	C	55	GLU
2	C	67	ASP
2	C	71	TYR
2	C	73	LEU
2	C	82	GLU
2	C	88	LEU
2	C	95	TYR
2	C	100	LEU
2	C	101	ILE
2	C	104	ASP
2	C	107	LEU

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Mol	Chain	Res	Type
2	C	108	ILE
2	C	113	VAL
2	C	115	LEU
2	C	120	LEU
2	C	122	THR
2	C	135	VAL
2	C	140	ILE
2	C	142	ARG
2	C	146	VAL
2	C	161	SER
2	C	163	ILE
2	C	165	LEU
2	C	167	LYS
2	C	172	ILE
2	C	174	LEU
2	C	181	VAL
2	C	184	MET
2	C	186	VAL
2	C	190	LYS
2	C	194	VAL
2	C	203	ASP
2	C	205	GLU
2	C	207	LEU
2	C	223	ASP
2	C	230	ARG
2	C	232	GLU
2	C	239	PHE
2	C	242	LEU
2	C	243	ARG
2	C	254	VAL
2	C	256	TYR
2	C	257	VAL
2	C	288	ARG
2	C	289	THR
2	C	292	ARG
2	C	294	GLU
2	C	301	GLU
2	C	309	TYR
2	C	322	VAL
2	C	331	ARG
2	C	332	ARG
2	C	333	ILE

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Mol	Chain	Res	Type
2	C	335	THR
2	C	341	THR
2	C	345	ARG
2	C	351	LEU
2	C	359	MET
2	C	360	LEU
2	C	366	SER
2	C	368	THR
2	C	372	LEU
2	C	376	ARG
2	C	387	SER
2	C	391	LEU
2	C	393	GLN
2	C	402	SER
2	C	407	LYS
2	C	408	ARG
2	C	413	LEU
2	C	418	LEU
2	C	420	ARG
2	C	422	ARG
2	C	432	ARG
2	C	433	THR
2	C	438	ILE
2	C	443	THR
2	C	452	ILE
2	C	472	ARG
2	C	474	VAL
2	C	480	THR
2	C	482	GLU
2	C	483	VAL
2	C	484	VAL
2	C	486	MET
2	C	489	THR
2	C	498	GLN
2	C	500	ASN
2	C	503	LEU
2	C	513	VAL
2	C	514	VAL
2	C	516	ARG
2	C	525	SER
2	C	535	SER
2	C	537	LYS

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Mol	Chain	Res	Type
2	C	542	VAL
2	C	551	GLU
2	C	559	LEU
2	C	560	MET
2	C	564	MET
2	C	569	VAL
2	C	578	VAL
2	C	579	VAL
2	C	584	GLU
2	C	585	GLU
2	C	586	ARG
2	C	588	VAL
2	C	589	ARG
2	C	590	ASP
2	C	595	LEU
2	C	606	VAL
2	C	607	ASP
2	C	617	ASP
2	C	628	PHE
2	C	670	GLN
2	C	713	ARG
2	C	715	THR
2	C	717	LEU
2	C	742	VAL
2	C	754	ILE
2	C	755	LEU
2	C	780	GLU
2	C	781	LYS
2	C	787	ASP
2	C	789	SER
2	C	808	ARG
2	C	813	VAL
2	C	815	LEU
2	C	820	ARG
2	C	824	ARG
2	C	825	VAL
2	C	827	VAL
2	C	834	GLN
2	C	837	ASP
2	C	845	ASN
2	C	853	LEU
2	C	855	VAL

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Mol	Chain	Res	Type
2	C	856	GLU
2	C	858	MET
2	C	865	THR
2	C	900	ARG
2	C	903	SER
2	C	911	GLU
2	C	914	ILE
2	C	917	LEU
2	C	918	LEU
2	C	928	LYS
2	C	936	VAL
2	C	940	GLU
2	C	950	LEU
2	C	958	THR
2	C	960	GLU
2	C	971	LYS
2	C	972	VAL
2	C	979	THR
2	C	984	GLU
2	C	988	VAL
2	C	1000	MET
2	C	1001	VAL
2	C	1002	GLU
2	C	1005	MET
2	C	1015	LEU
2	C	1021	LEU
2	C	1024	LYS
2	C	1026	GLN
2	C	1052	MET
2	C	1053	LEU
2	C	1056	LYS
2	C	1078	GLU
2	C	1095	LEU
2	C	1097	LEU
2	C	1104	GLU
2	C	1115	LEU
3	D	2	LYS
3	D	5	VAL
3	D	8	VAL
3	D	33	ASN
3	D	36	THR
3	D	41	ARG

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Mol	Chain	Res	Type
3	D	47	GLU
3	D	53	ILE
3	D	55	ASP
3	D	65	ARG
3	D	68	PHE
3	D	81	THR
3	D	84	ILE
3	D	85	VAL
3	D	89	ARG
3	D	90	MET
3	D	102	ILE
3	D	111	LYS
3	D	112	ILE
3	D	114	THR
3	D	118	LEU
3	D	122	GLU
3	D	127	LEU
3	D	134	VAL
3	D	135	LEU
3	D	141	ILE
3	D	142	LEU
3	D	145	VAL
3	D	149	LYS
3	D	152	LEU
3	D	154	THR
3	D	156	GLU
3	D	165	LYS
3	D	175	VAL
3	D	185	VAL
3	D	191	LEU
3	D	199	LEU
3	D	204	LEU
3	D	227	LEU
3	D	232	GLU
3	D	259	VAL
3	D	264	LEU
3	D	266	GLU
3	D	269	PHE
3	D	297	ILE
3	D	298	VAL
3	D	313	MET
3	D	336	PHE

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Mol	Chain	Res	Type
3	D	338	GLU
3	D	347	VAL
3	D	350	HIS
3	D	351	MET
3	D	361	VAL
3	D	365	ASP
3	D	378	ILE
3	D	380	GLU
3	D	388	HIS
3	D	400	VAL
3	D	408	GLU
3	D	411	THR
3	D	413	ASP
3	D	415	VAL
3	D	420	VAL
3	D	421	LEU
3	D	434	ARG
3	D	436	GLU
3	D	441	ARG
3	D	452	ILE
3	D	468	LEU
3	D	486	ARG
3	D	488	ARG
3	D	498	VAL
3	D	504	ASP
3	D	510	GLU
3	D	511	TRP
3	D	512	MET
3	D	513	ILE
3	D	525	ARG
3	D	528	VAL
3	D	554	LEU
3	D	557	LEU
3	D	565	ILE
3	D	578	VAL
3	D	581	LEU
3	D	587	ARG
3	D	592	THR
3	D	593	ASN
3	D	598	ARG
3	D	600	LEU
3	D	606	ILE

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Mol	Chain	Res	Type
3	D	611	GLN
3	D	619	LEU
3	D	621	LYS
3	D	623	VAL
3	D	630	VAL
3	D	637	LEU
3	D	639	LEU
3	D	647	ARG
3	D	651	GLU
3	D	652	LEU
3	D	659	LYS
3	D	660	LYS
3	D	661	MET
3	D	662	GLU
3	D	663	GLU
3	D	679	ARG
3	D	686	GLU
3	D	700	VAL
3	D	702	LEU
3	D	704	ARG
3	D	717	GLN
3	D	725	SER
3	D	726	ILE
3	D	732	VAL
3	D	747	VAL
3	D	754	PHE
3	D	758	GLU
3	D	762	GLN
3	D	763	MET
3	D	783	ARG
3	D	784	ASP
3	D	787	LEU
3	D	792	ILE
3	D	793	THR
3	D	794	GLN
3	D	796	ARG
3	D	810	GLU
3	D	818	ARG
3	D	828	LYS
3	D	832	ARG
3	D	836	VAL
3	D	851	LEU

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Mol	Chain	Res	Type
3	D	857	ILE
3	D	858	VAL
3	D	861	GLN
3	D	863	VAL
3	D	865	THR
3	D	875	THR
3	D	876	SER
3	D	879	ARG
3	D	880	ILE
3	D	888	GLU
3	D	890	VAL
3	D	891	GLU
3	D	894	LYS
3	D	897	TRP
3	D	899	LEU
3	D	904	VAL
3	D	910	SER
3	D	912	LYS
3	D	919	PHE
3	D	921	ARG
3	D	926	LYS
3	D	947	ILE
3	D	951	ILE
3	D	956	ILE
3	D	964	LEU
3	D	971	LEU
3	D	972	LEU
3	D	976	GLN
3	D	984	THR
3	D	988	ARG
3	D	990	ASP
3	D	991	GLN
3	D	1002	LYS
3	D	1005	GLN
3	D	1007	VAL
3	D	1020	LEU
3	D	1033	GLN
3	D	1041	LEU
3	D	1042	ARG
3	D	1045	MET
3	D	1049	SER
3	D	1052	THR

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Mol	Chain	Res	Type
3	D	1063	GLU
3	D	1066	THR
3	D	1067	VAL
3	D	1068	LEU
3	D	1078	ARG
3	D	1095	THR
3	D	1096	ARG
3	D	1102	THR
3	D	1109	GLU
3	D	1111	ASP
3	D	1115	THR
3	D	1130	ARG
3	D	1136	LYS
3	D	1137	ARG
3	D	1154	GLU
3	D	1155	VAL
3	D	1161	GLU
3	D	1166	LEU
3	D	1183	ILE
3	D	1194	CYS
3	D	1197	ARG
3	D	1200	VAL
3	D	1201	CYS
3	D	1209	LEU
3	D	1210	SER
3	D	1211	MET
3	D	1216	SER
3	D	1223	ILE
3	D	1234	THR
3	D	1238	MET
3	D	1260	ILE
3	D	1262	LEU
3	D	1278	ASP
3	D	1295	GLU
3	D	1296	SER
3	D	1302	GLU
3	D	1307	LYS
3	D	1311	LEU
3	D	1312	LEU
3	D	1314	LYS
3	D	1319	VAL
3	D	1325	LEU

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Mol	Chain	Res	Type
3	D	1335	LEU
3	D	1337	GLU
3	D	1339	LYS
3	D	1346	ARG
3	D	1359	GLN
3	D	1373	ARG
3	D	1379	VAL
3	D	1381	VAL
3	D	1382	THR
3	D	1389	LEU
3	D	1403	LEU
3	D	1412	LYS
3	D	1415	VAL
3	D	1422	MET
3	D	1424	VAL
3	D	1425	THR
3	D	1426	LYS
3	D	1429	LEU
3	D	1432	LYS
3	D	1434	TRP
3	D	1435	LEU
3	D	1447	LEU
3	D	1455	LYS
3	D	1457	ASP
3	D	1462	LEU
3	D	1464	GLU
3	D	1465	ASN
3	D	1468	LEU
3	D	1486	VAL
3	D	1488	ASP
3	D	1501	GLU
4	E	31	LEU
4	E	38	THR
4	E	42	PRO
4	E	47	LYS
4	E	48	MET
4	E	49	GLN
4	E	51	LEU
4	E	54	LEU
4	E	56	ASP
4	E	62	THR
4	E	66	LYS

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Mol	Chain	Res	Type
4	E	70	THR
4	E	74	VAL
4	E	79	LEU
4	E	85	LEU
5	F	77	THR
5	F	85	LEU
5	F	86	HIS
5	F	94	LEU
5	F	108	GLU
5	F	120	THR
5	F	123	ASP
5	F	125	ASP
5	F	126	LEU
5	F	144	ILE
5	F	147	LEU
5	F	149	GLU
5	F	157	GLU
5	F	174	LEU
5	F	176	ILE
5	F	192	LEU
5	F	194	LEU
5	F	197	SER
5	F	210	LEU
5	F	224	VAL
5	F	225	GLU
5	F	249	ARG
5	F	321	ILE
5	F	335	ASP
5	F	338	LEU
5	F	347	GLN
5	F	350	LEU
5	F	355	GLU
5	F	358	LEU
5	F	362	SER
5	F	365	GLU
5	F	367	MET
5	F	375	LEU
5	F	386	VAL
5	F	390	PHE
5	F	392	VAL
5	F	393	THR
5	F	396	ARG

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Mol	Chain	Res	Type
5	F	397	ILE
5	F	398	ARG
5	F	405	LEU
5	F	408	LEU
6	G	5	PHE
6	G	16	ILE
6	G	25	THR
6	G	28	ASP
6	G	31	LEU
6	G	32	ASP
6	G	42	SER
6	G	47	THR
6	G	61	ARG
6	G	72	ARG
6	G	75	HIS
6	G	76	VAL
6	G	78	LEU
6	G	105	VAL
6	G	106	VAL
6	G	119	VAL
6	G	127	ARG
6	G	128	LEU
6	G	135	VAL
6	G	136	ASP
6	H	6	VAL
6	H	22	GLU
6	H	32	ASP
6	H	37	ARG
6	H	47	THR
6	H	59	ARG
6	H	95	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	156	HIS
1	A	212	ASN
1	A	213	GLN
1	B	63	HIS
1	B	124	ASN
1	B	212	ASN

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Mol	Chain	Res	Type
2	C	31	GLN
2	C	45	GLN
2	C	187	ASN
2	C	327	HIS
2	C	390	GLN
2	C	563	ASN
2	C	567	GLN
2	C	728	HIS
2	C	1018	GLN
3	D	386	HIS
3	D	549	ASN
3	D	640	HIS
3	D	909	ASN
3	D	1195	GLN
4	E	29	GLN
5	F	399	GLN
6	G	75	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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 1 ligands modelled in this entry, 1 is 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	225/315 (71%)	-0.47	0	100	100	11, 37, 83, 144	0
1	B	232/315 (73%)	-0.36	0	100	100	14, 47, 104, 158	0
2	C	1053/1119 (94%)	-0.06	31 (2%)	53	30	8, 61, 154, 222	0
3	D	1488/1524 (97%)	0.17	82 (5%)	30	18	8, 85, 179, 244	0
4	E	95/99 (95%)	0.25	3 (3%)	50	29	40, 74, 183, 242	0
5	F	278/423 (65%)	0.48	20 (7%)	21	14	44, 119, 192, 255	0
6	G	127/141 (90%)	-0.16	0	100	100	27, 73, 137, 179	0
6	H	91/141 (64%)	0.26	1 (1%)	78	52	73, 113, 161, 175	0
All	All	3589/4077 (88%)	0.05	137 (3%)	44	25	8, 76, 171, 255	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	57	ASP	11.3
3	D	294	HIS	7.9
3	D	298	VAL	7.1
4	E	56	ASP	6.9
3	D	297	ILE	6.1
2	C	267	TYR	6.1
3	D	450	TYR	6.0
3	D	83	SER	5.8
3	D	64	LYS	5.2
3	D	230	TRP	5.1
3	D	449	SER	5.1
5	F	89	GLY	5.1
3	D	420	VAL	5.0
3	D	802	ALA	4.8
3	D	488	ARG	4.7
3	D	293	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
2	C	61	LYS	4.4
3	D	226	PRO	4.2
3	D	456	MET	4.1
2	C	716	LYS	4.0
3	D	78	VAL	4.0
2	C	516	ARG	3.9
3	D	1388	ARG	3.9
3	D	810	GLU	3.9
3	D	131	LYS	3.9
5	F	378	GLY	3.8
2	C	262	ALA	3.7
3	D	259	VAL	3.7
3	D	79	GLU	3.7
3	D	533	GLY	3.5
3	D	808	THR	3.5
5	F	255	ALA	3.5
5	F	386	VAL	3.5
3	D	81	THR	3.3
2	C	223	ASP	3.2
3	D	1195	GLN	3.2
2	C	269	LEU	3.2
3	D	448	GLU	3.1
3	D	163	TYR	3.1
3	D	175	VAL	3.1
3	D	505	SER	3.1
5	F	320	PRO	3.1
3	D	160	GLU	3.1
3	D	303	PRO	3.1
2	C	60	GLY	3.1
5	F	339	PRO	3.0
3	D	137	PRO	3.0
5	F	342	VAL	3.0
3	D	190	GLU	2.9
3	D	244	GLU	2.9
3	D	1405	GLU	2.9
3	D	147	VAL	2.9
3	D	180	LYS	2.9
3	D	59	ALA	2.9
3	D	140	ALA	2.8
3	D	252	ARG	2.8
5	F	321	ILE	2.8
5	F	145	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	178	PRO	2.7
2	C	359	MET	2.7
3	D	1414	PRO	2.7
3	D	205	TYR	2.7
3	D	57	GLU	2.7
3	D	142	LEU	2.7
4	E	33	HIS	2.6
2	C	226	VAL	2.6
3	D	316	GLN	2.6
3	D	77	GLY	2.6
3	D	72	VAL	2.6
2	C	271	GLU	2.6
5	F	143	HIS	2.6
5	F	371	LEU	2.6
3	D	811	GLU	2.5
3	D	419	ASP	2.5
3	D	203	ALA	2.5
3	D	295	GLY	2.5
3	D	805	GLU	2.5
3	D	493	ARG	2.5
3	D	1188	VAL	2.5
3	D	491	LYS	2.5
5	F	331	ASP	2.5
3	D	1128	VAL	2.5
2	C	252	LYS	2.4
2	C	242	LEU	2.4
2	C	256	TYR	2.4
5	F	373	LYS	2.4
3	D	1408	ILE	2.4
3	D	304	LEU	2.4
3	D	63	TYR	2.4
3	D	1111	ASP	2.4
3	D	76	CYS	2.3
3	D	258	VAL	2.3
3	D	326	GLU	2.3
5	F	90	GLN	2.3
2	C	425	PHE	2.3
3	D	371	ILE	2.3
3	D	1210	SER	2.3
5	F	341	PRO	2.3
5	F	344	ALA	2.3
3	D	136	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	293	PHE	2.2
2	C	224	GLU	2.2
2	C	416	GLY	2.2
3	D	1503	VAL	2.2
2	C	105	THR	2.2
2	C	1003	ASP	2.2
3	D	250	LEU	2.2
2	C	1016	ILE	2.2
2	C	506	ASN	2.2
3	D	1198	TYR	2.2
3	D	400	VAL	2.2
3	D	128	TYR	2.2
3	D	594	PRO	2.2
6	H	86	ALA	2.2
3	D	1398	TRP	2.2
2	C	415	PRO	2.2
2	C	781	LYS	2.2
5	F	254	GLN	2.1
5	F	323	ASP	2.1
3	D	34	TYR	2.1
3	D	73	CYS	2.1
3	D	197	SER	2.1
2	C	64	LEU	2.1
5	F	367	MET	2.1
3	D	824	ASN	2.1
3	D	454	ALA	2.1
3	D	409	VAL	2.1
2	C	270	GLY	2.0
3	D	1027	GLY	2.0
2	C	166	PRO	2.0
2	C	168	ARG	2.0
3	D	53	ILE	2.0
3	D	1401	GLU	2.0
3	D	257	GLY	2.0
2	C	290	LEU	2.0
2	C	418	LEU	2.0
5	F	181	GLU	2.0

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

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
7	ZN	D	1601	1/1	0.99	0.03	110,110,110,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.