



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:57 AM UTC

PDB ID : 5TMC / pdb_00005tmc
Title : Re-refinement of Thermus thermopiles DNA-directed RNA polymerase structure
Authors : Wang, J.
Deposited on : 2016-10-12
Resolution : 2.71 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

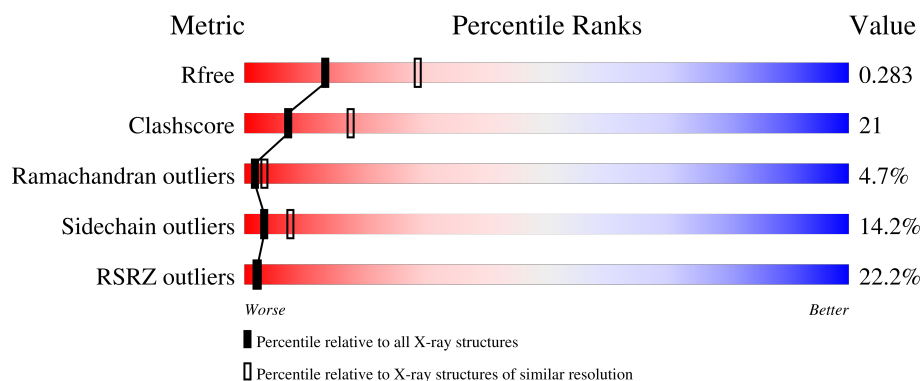
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	
1	B	315	
2	C	1119	
3	D	1524	
4	E	99	

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Mol	Chain	Length	Quality of chain
5	F	423	29% 53% 26% • 17%
6	Z	48	96% •

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 28419 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1816	1159	315	339	3			
1	B	238	Total	C	N	O	S	0	0	0
			1863	1188	322	350	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1504	Total	C	N	O	S	0	0	0
			11864	7518	2091	2219	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	conflict	UNP Q72ID6
E	92	ILE	LEU	conflict	UNP Q72ID6
E	95	GLY	VAL	conflict	UNP Q72ID6

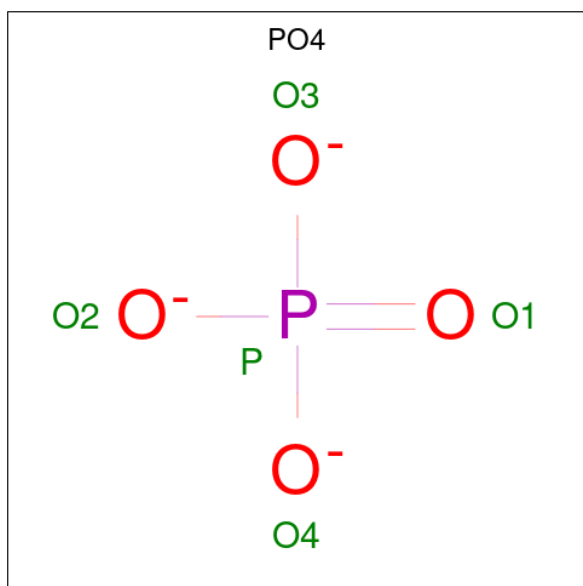
- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	351	Total	C	N	O	S	0	0	0
			2844	1794	515	531	4			

- Molecule 6 is a protein called unknown protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	Z	48	Total	C	N	O	0	0	0
			240	144	48	48			

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	P	0	0
			5	4	1		

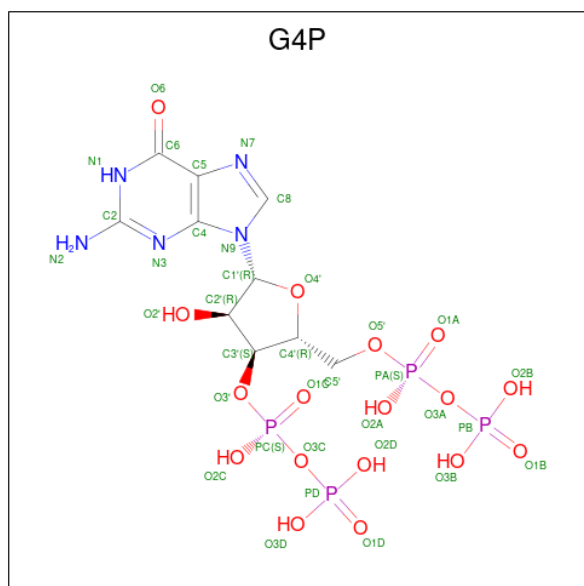
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Mg	0	0
			1	1		
8	D	3	Total	Mg	0	0
			3	3		

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 10 is GUANOSINE-5',3'-TETRAPHOSPHATE (CCD ID: G4P) (formula: $C_{10}H_{17}N_5O_{17}P_4$).



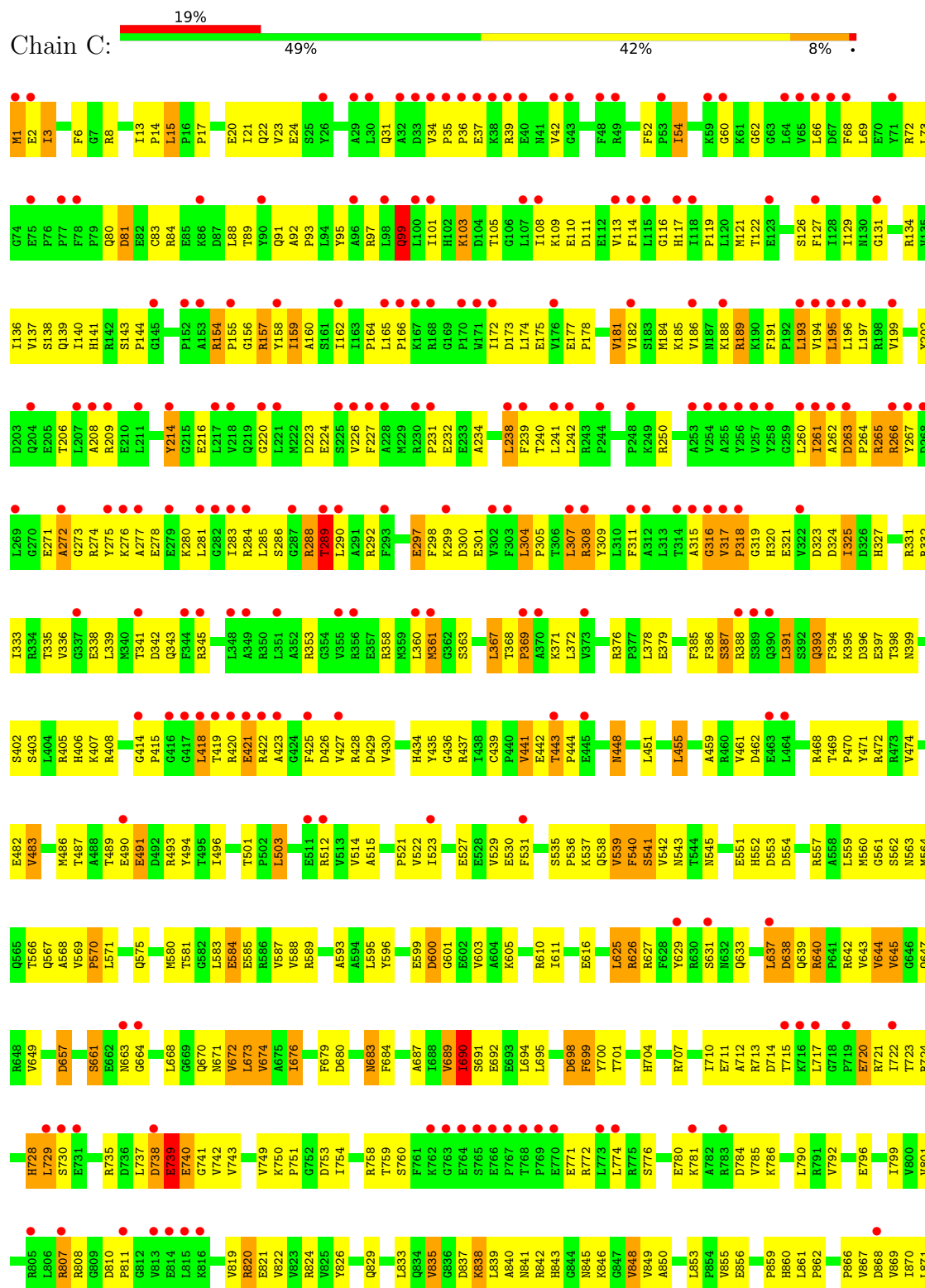
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	D	1	Total	C	N	O	P	0	0
			36	10	5	17	4		

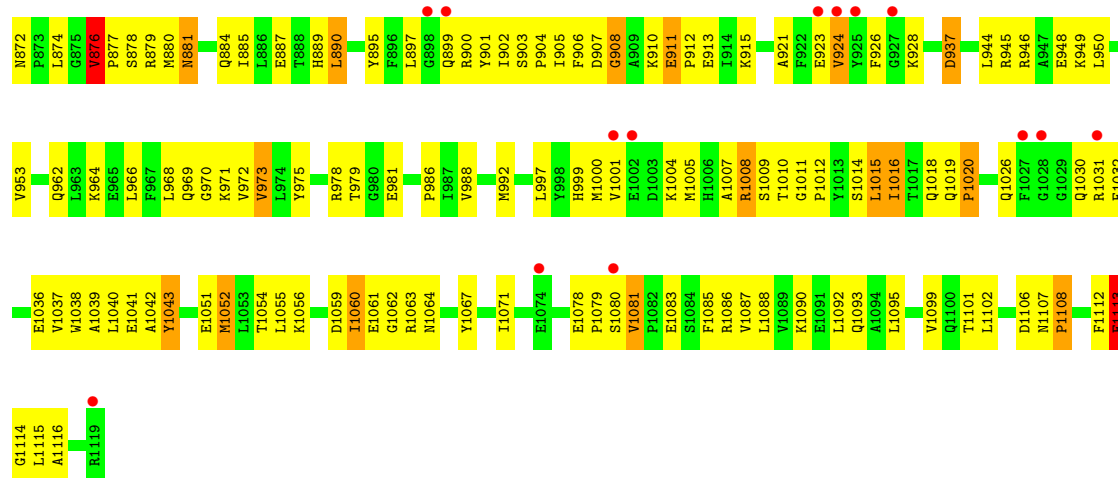
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	15	Total	O	0	0
			15	15		
11	B	2	Total	O	0	0
			2	2		
11	C	54	Total	O	0	0
			54	54		
11	D	62	Total	O	0	0
			62	62		
11	E	9	Total	O	0	0
			9	9		
11	F	5	Total	O	0	0
			5	5		

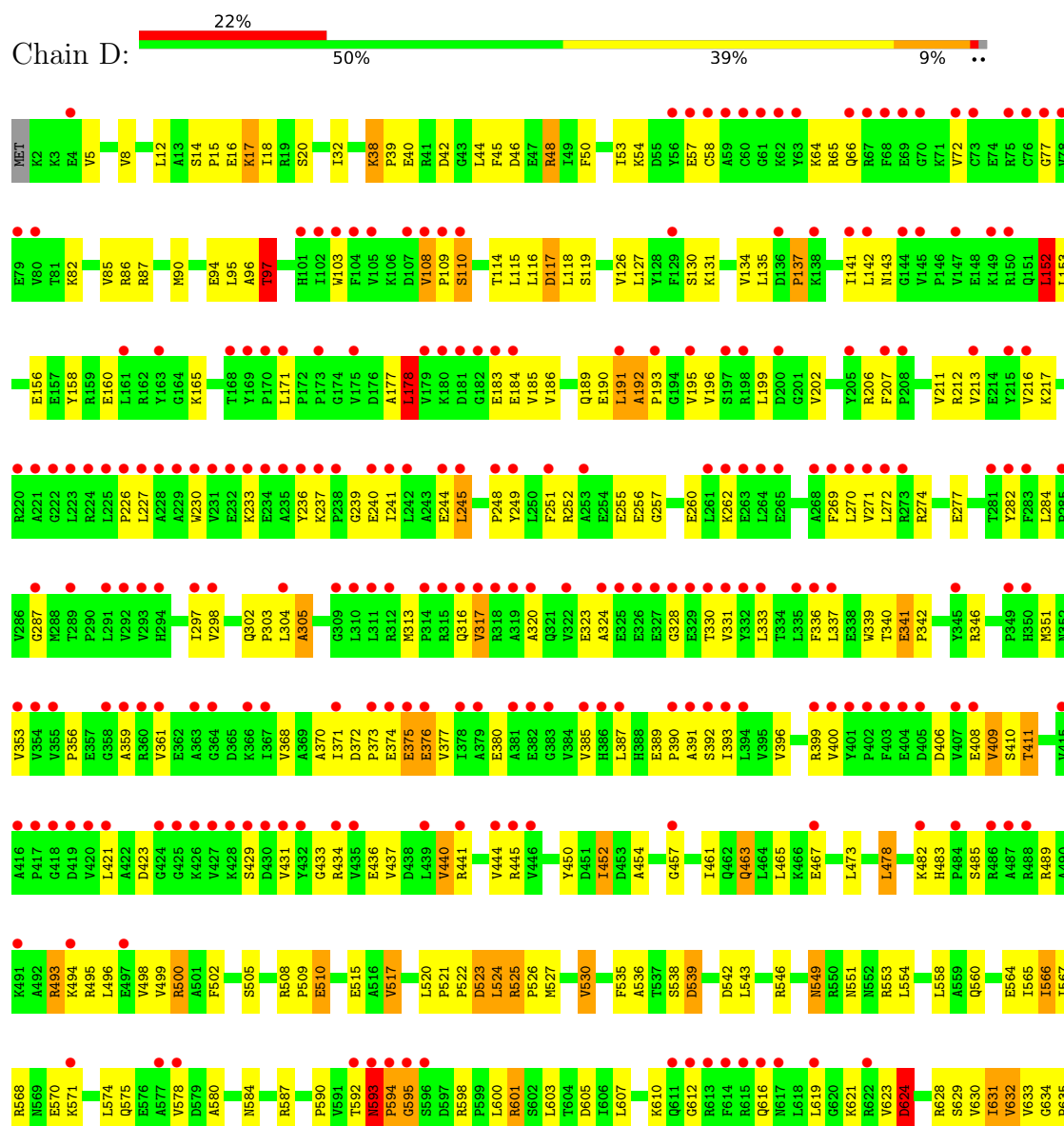
PRO GLY ILE GLY GLU ARG SER LEU GLU GLU ILE LYS GLU ALA LEU GLU LYS LYS GLY PHE THR LEU LYS GLU

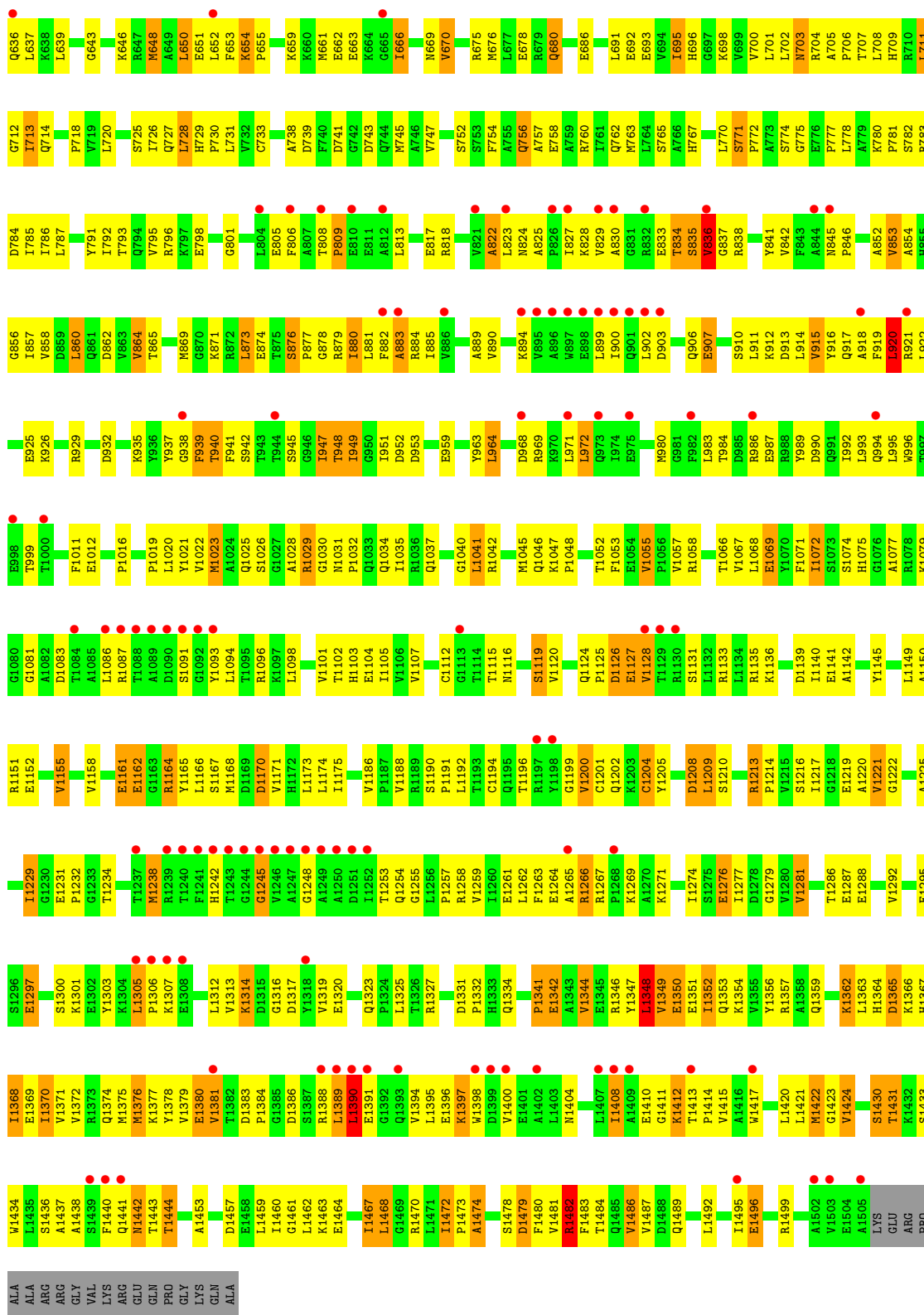
- Molecule 2: DNA-directed RNA polymerase subunit beta

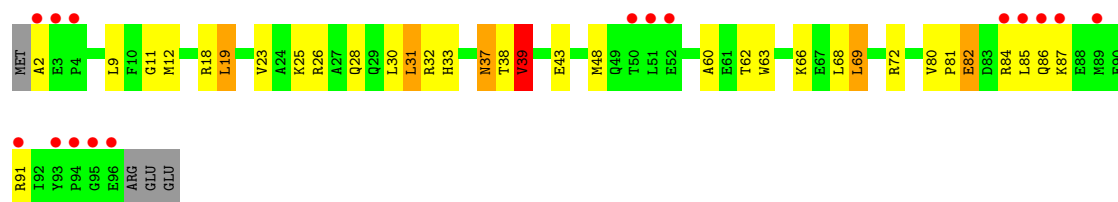




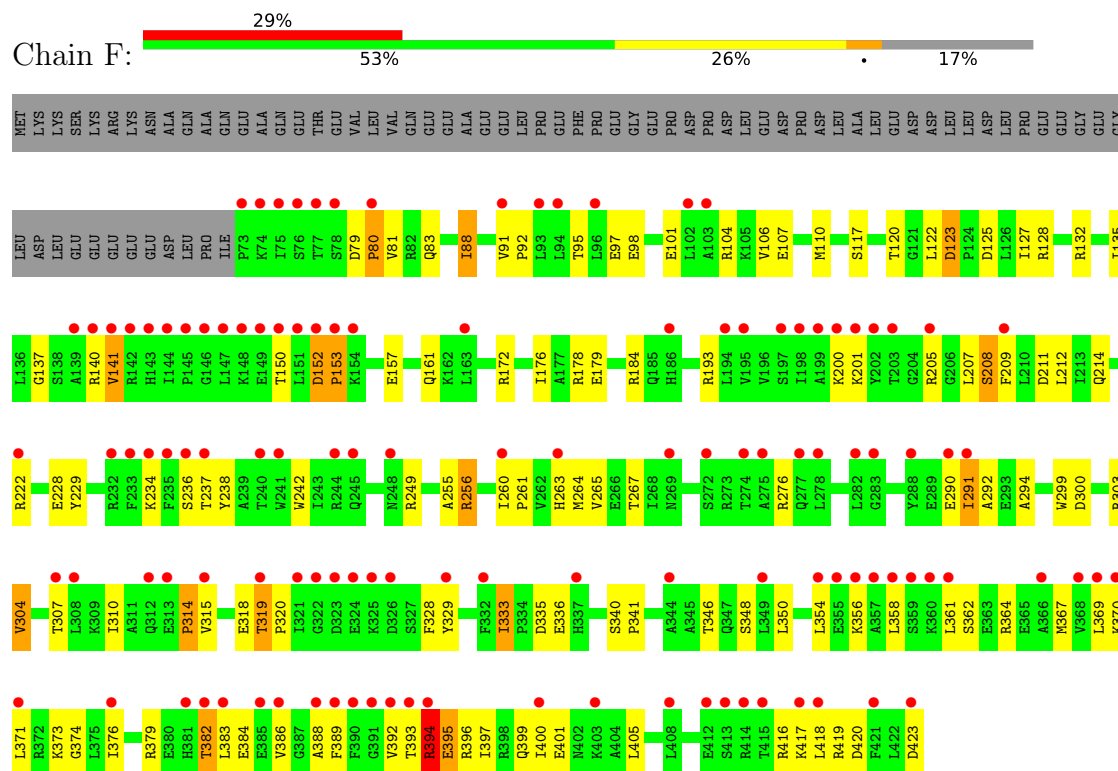
• Molecule 3: DNA-directed RNA polymerase subunit beta'



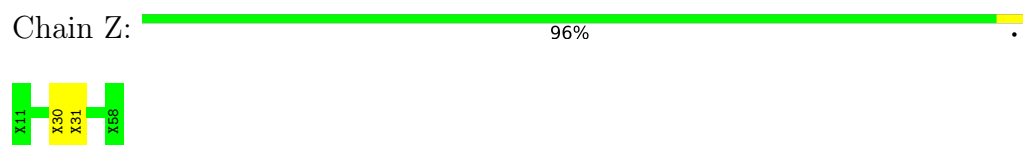




- Molecule 5: RNA polymerase sigma factor SigA



- Molecule 6: unknown protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	236.35Å 236.35Å 249.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.51 – 2.71 48.51 – 2.71	Depositor EDS
% Data completeness (in resolution range)	96.9 (48.51-2.71) 97.1 (48.51-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.265 , 0.286 0.262 , 0.283	Depositor DCC
R_{free} test set	7447 reflections (3.51%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 102.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.086 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.875 for H, K, L 0.125 for -H-K, K, -L	Depositor
Outliers	1 of 206105 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	28419	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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: MG, PO4, ZN, G4P

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	0.62	0/1848	0.96	1/2512 (0.0%)
1	B	0.54	0/1896	0.90	2/2579 (0.1%)
2	C	0.61	1/8997 (0.0%)	0.96	15/12164 (0.1%)
3	D	0.59	0/12073	0.97	23/16324 (0.1%)
4	E	0.58	0/783	0.95	2/1054 (0.2%)
5	F	0.47	0/2890	0.91	4/3888 (0.1%)
All	All	0.58	1/28487 (0.0%)	0.95	47/38521 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	690	ILE	CA-CB	5.82	1.61	1.54

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	771	SER	CA-C-N	9.97	129.73	119.56
3	D	771	SER	C-N-CA	9.97	129.73	119.56
2	C	1052	MET	N-CA-C	-9.82	101.42	113.50
3	D	1397	LYS	N-CA-C	-7.49	102.67	112.41
5	F	333	ILE	CA-C-N	7.41	127.32	120.21
5	F	333	ILE	C-N-CA	7.41	127.32	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1127	GLU	N-CA-C	-7.33	103.93	114.12
2	C	905	ILE	N-CA-C	7.30	118.06	110.62
3	D	1126	ASP	N-CA-C	6.97	118.37	108.54
2	C	320	HIS	N-CA-C	6.79	120.91	111.74
3	D	775	GLY	N-CA-C	-6.73	105.91	113.79
2	C	876	VAL	CA-C-N	-6.61	111.58	119.84
2	C	876	VAL	C-N-CA	-6.61	111.58	119.84
3	D	1279	GLY	N-CA-C	6.15	118.25	110.38
2	C	781	LYS	N-CA-C	-6.09	104.19	111.69
1	B	48	ILE	CA-C-N	5.90	127.21	119.84
1	B	48	ILE	C-N-CA	5.90	127.21	119.84
3	D	433	GLY	N-CA-C	5.83	118.97	110.63
2	C	601	GLY	N-CA-C	5.83	118.44	110.69
2	C	188	LYS	N-CA-C	-5.77	106.28	113.38
2	C	323	ASP	N-CA-C	5.70	118.54	110.50
3	D	767	HIS	N-CA-C	-5.67	107.36	114.56
2	C	418	LEU	N-CA-C	5.61	117.57	108.26
2	C	1019	GLN	CA-C-N	5.59	126.83	119.84
2	C	1019	GLN	C-N-CA	5.59	126.83	119.84
5	F	340	SER	CA-C-N	5.51	126.73	119.84
5	F	340	SER	C-N-CA	5.51	126.73	119.84
2	C	494	TYR	N-CA-C	5.48	117.31	109.14
3	D	517	VAL	N-CA-C	5.43	112.50	107.56
3	D	277	GLU	CA-C-N	5.39	126.58	119.84
3	D	277	GLU	C-N-CA	5.39	126.58	119.84
3	D	97	THR	CA-C-N	-5.35	114.45	119.85
3	D	97	THR	C-N-CA	-5.35	114.45	119.85
4	E	32	ARG	N-CA-C	-5.29	105.90	112.93
3	D	1069	GLU	N-CA-C	-5.28	105.70	111.82
3	D	920	LEU	N-CA-C	-5.25	105.70	112.68
4	E	38	THR	N-CA-C	5.24	117.01	108.63
3	D	624	ASP	N-CA-C	5.21	119.62	113.16
3	D	880	ILE	CB-CA-C	-5.14	105.29	112.02
2	C	238	LEU	N-CA-C	-5.13	108.77	114.62
3	D	793	THR	N-CA-C	-5.11	106.73	113.12
3	D	152	LEU	N-CA-C	5.10	118.03	110.48
3	D	1474	ALA	N-CA-C	5.08	115.24	108.38
3	D	631	ILE	N-CA-C	5.08	115.28	108.17
3	D	639	LEU	N-CA-C	5.07	118.93	112.34
1	A	140	MET	N-CA-C	5.07	116.69	109.14
2	C	540	PHE	N-CA-C	5.05	117.06	109.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	1126	ASP	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	1816	0	1871	92	0
1	B	1863	0	1914	59	0
2	C	8829	0	8933	423	0
3	D	11864	0	12094	578	0
4	E	769	0	775	24	0
5	F	2844	0	2926	78	0
6	Z	240	0	50	1	0
7	A	5	0	0	0	0
8	C	1	0	0	0	0
8	D	3	0	0	0	0
9	D	2	0	0	0	0
10	D	36	0	11	1	0
11	A	15	0	0	0	0
11	B	2	0	0	2	0
11	C	54	0	0	4	0
11	D	62	0	0	7	0
11	E	9	0	0	1	0
11	F	5	0	0	0	0
All	All	28419	0	28574	1175	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 21.

All (1175) 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:1265:ALA:HA	3:D:1266:ARG:CB	1.60	1.29
3:D:1265:ALA:HA	3:D:1266:ARG:HB2	1.23	1.13
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.32	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:93:PRO:HA	2:C:117:HIS:HB2	1.36	1.06
2:C:567:GLN:HB2	2:C:997:LEU:HD22	1.41	1.01
3:D:703:ASN:HA	3:D:712:GLY:O	1.59	1.01
3:D:728:LEU:HD13	3:D:745:MET:HE1	1.43	0.99
3:D:836:VAL:H	3:D:837:GLY:HA3	1.26	0.97
3:D:1213:ARG:HG2	3:D:1213:ARG:HH11	1.26	0.96
3:D:964:LEU:HD21	3:D:1058:ARG:HG2	1.45	0.95
3:D:1265:ALA:HA	3:D:1266:ARG:HB3	1.49	0.95
3:D:8:VAL:HG12	3:D:1434:TRP:HZ2	1.32	0.94
2:C:838:LYS:HG3	2:C:997:LEU:HB2	1.48	0.93
2:C:881:ASN:H	2:C:881:ASN:ND2	1.67	0.93
2:C:676:ILE:O	3:D:948:THR:HG22	1.69	0.91
2:C:881:ASN:HD22	2:C:881:ASN:N	1.62	0.91
3:D:1496:GLU:HA	3:D:1499:ARG:HB2	1.50	0.91
2:C:1093:GLN:HB3	3:D:90:MET:HE2	1.53	0.90
3:D:1265:ALA:CA	3:D:1266:ARG:HB2	2.01	0.90
3:D:845:ASN:HB2	3:D:846:PRO:HD2	1.53	0.90
2:C:724:ARG:HE	2:C:738:ASP:HA	1.35	0.89
2:C:263:ASP:H	2:C:264:PRO:CD	1.86	0.88
2:C:575:GLN:NE2	2:C:671:ASN:H	1.71	0.88
3:D:192:ALA:HB1	3:D:193:PRO:HD2	1.55	0.88
2:C:199:VAL:HG21	2:C:238:LEU:HD11	1.56	0.88
2:C:22:GLN:HG3	2:C:407:LYS:HB3	1.55	0.87
2:C:889:HIS:HE1	3:D:951:ILE:H	1.21	0.87
2:C:396:ASP:HA	2:C:633:GLN:HE22	1.40	0.87
3:D:493:ARG:HH12	3:D:1390:LEU:H	1.23	0.86
3:D:675:ARG:HA	3:D:678:GLU:OE1	1.76	0.86
2:C:469:THR:HG22	2:C:538:GLN:HE21	1.37	0.85
2:C:1059:ASP:OD1	2:C:1062:GLY:N	2.10	0.85
1:B:2:LEU:N	1:B:3:ASP:HA	1.91	0.85
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.58	0.85
3:D:1258:ARG:CZ	3:D:1262:LEU:HD21	2.07	0.85
3:D:1377:LYS:HD2	3:D:1378:TYR:CE2	2.12	0.84
3:D:584:ASN:OD1	3:D:590:PRO:HD2	1.78	0.84
3:D:1047:LYS:HB3	3:D:1048:PRO:HD2	1.60	0.83
3:D:1091:SER:C	3:D:1093:TYR:H	1.87	0.83
1:A:128:HIS:HE1	1:A:131:THR:HG23	1.43	0.82
1:B:167:VAL:HG12	1:B:168:ASP:H	1.44	0.82
2:C:881:ASN:H	2:C:881:ASN:HD22	0.84	0.82
2:C:34:VAL:N	2:C:35:PRO:HD2	1.93	0.82
5:F:370:LYS:HA	5:F:374:GLY:HA3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:984:THR:HG22	3:D:987:GLU:HG3	1.61	0.81
3:D:730:PRO:O	11:D:1701:HOH:O	1.97	0.81
3:D:1094:LEU:O	3:D:1098:LEU:HD13	1.80	0.81
2:C:263:ASP:H	2:C:264:PRO:HD3	1.44	0.81
2:C:157:ARG:HG3	2:C:158:TYR:H	1.44	0.81
3:D:580:ALA:O	3:D:584:ASN:HB2	1.80	0.80
3:D:907:GLU:OE2	3:D:910:SER:HB3	1.81	0.80
2:C:93:PRO:HA	2:C:117:HIS:CB	2.10	0.80
2:C:581:THR:HA	2:C:903:SER:O	1.81	0.80
3:D:1042:ARG:HH11	3:D:1042:ARG:HB3	1.45	0.80
3:D:96:ALA:CB	3:D:554:LEU:HD23	2.09	0.80
2:C:13:ILE:HD12	2:C:14:PRO:HD2	1.63	0.80
3:D:1011:PHE:HB3	3:D:1021:TYR:CD2	2.16	0.80
2:C:1081:VAL:HG13	2:C:1086:ARG:HE	1.46	0.79
3:D:117:ASP:HB2	3:D:495:ARG:HH12	1.47	0.79
3:D:964:LEU:O	3:D:968:ASP:HB2	1.82	0.79
2:C:971:LYS:HA	2:C:988:VAL:HA	1.65	0.79
3:D:1434:TRP:NE1	3:D:1457:ASP:HB2	1.98	0.78
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	1.63	0.78
3:D:836:VAL:N	3:D:837:GLY:HA3	1.96	0.78
2:C:737:LEU:O	2:C:739:GLU:N	2.16	0.78
3:D:152:LEU:HD23	3:D:152:LEU:H	1.49	0.78
2:C:695:LEU:HD21	2:C:833:LEU:HB3	1.65	0.78
2:C:1083:GLU:OE1	3:D:87:ARG:NH1	2.18	0.77
1:B:86:VAL:HG13	1:B:123:MET:HB2	1.66	0.77
3:D:1312:LEU:HD13	3:D:1327:ARG:HG2	1.67	0.76
3:D:1201:CYS:SG	3:D:1204:CYS:HB2	2.25	0.76
1:A:128:HIS:CE1	1:A:131:THR:HG23	2.18	0.76
2:C:878:SER:N	11:C:1301:HOH:O	2.07	0.76
2:C:436:GLY:HA2	2:C:538:GLN:O	1.86	0.76
1:A:23:PHE:HE2	1:A:208:LEU:HD13	1.51	0.75
3:D:1041:LEU:HD12	3:D:1058:ARG:HA	1.66	0.75
3:D:1031:ASN:H	3:D:1034:GLN:HE21	1.34	0.75
4:E:26:ARG:HH21	4:E:30:LEU:HD13	1.52	0.75
3:D:8:VAL:HG12	3:D:1434:TRP:CZ2	2.18	0.75
3:D:632:VAL:O	3:D:727:GLN:HA	1.87	0.75
2:C:859:PRO:O	2:C:867:VAL:HG22	1.87	0.74
3:D:1496:GLU:HA	3:D:1499:ARG:CB	2.16	0.74
2:C:490:GLU:HG2	2:C:493:ARG:HH21	1.51	0.74
3:D:97:THR:HG21	3:D:571:LYS:HD3	1.69	0.74
1:B:58:ILE:HD12	1:B:61:VAL:HB	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:351:MET:HG2	3:D:370:ALA:HA	1.69	0.74
3:D:885:ILE:HG21	3:D:937:TYR:HD1	1.53	0.74
2:C:261:ILE:O	2:C:264:PRO:HD3	1.88	0.73
3:D:907:GLU:O	3:D:911:LEU:HD12	1.89	0.73
2:C:325:ILE:HD12	2:C:325:ILE:H	1.54	0.73
1:A:96:THR:HB	1:A:145:ASP:OD2	1.88	0.72
2:C:776:SER:HA	2:C:780:GLU:HB2	1.69	0.72
3:D:698:LYS:HA	3:D:756:GLN:HE22	1.53	0.72
3:D:947:ILE:HG13	3:D:948:THR:N	2.04	0.72
3:D:1378:TYR:HD1	3:D:1422:MET:SD	2.11	0.72
5:F:152:ASP:N	5:F:153:PRO:HD3	2.05	0.72
5:F:208:SER:O	5:F:212:LEU:HG	1.88	0.72
2:C:674:VAL:HG11	2:C:992:MET:HE3	1.70	0.71
3:D:1368:ILE:HD12	3:D:1368:ILE:H	1.55	0.71
2:C:738:ASP:O	2:C:740:GLU:N	2.22	0.71
3:D:646:LYS:HA	3:D:720:LEU:HD22	1.72	0.71
3:D:1459:LEU:HA	3:D:1464:GLU:HG3	1.72	0.71
3:D:661:MET:HA	3:D:666:ILE:HD12	1.71	0.70
3:D:1380:GLU:HB2	3:D:1420:LEU:HD11	1.73	0.70
1:B:38:ASN:ND2	2:C:979:THR:HA	2.06	0.70
2:C:181:VAL:HA	2:C:220:GLY:HA2	1.74	0.70
2:C:214:TYR:CE1	2:C:311:PHE:HB3	2.26	0.70
5:F:135:ILE:HD11	5:F:178:ARG:HA	1.72	0.70
3:D:1208:ASP:O	3:D:1209:LEU:HB2	1.90	0.70
2:C:15:LEU:HD12	2:C:15:LEU:H	1.57	0.70
2:C:425:PHE:O	2:C:429:ASP:HB2	1.92	0.69
2:C:724:ARG:NE	2:C:738:ASP:HA	2.07	0.69
3:D:158:TYR:HE1	3:D:454:ALA:HB3	1.57	0.69
2:C:277:ALA:HA	2:C:280:LYS:HB2	1.74	0.69
3:D:984:THR:HG22	3:D:987:GLU:CG	2.22	0.69
2:C:672:VAL:HG22	2:C:868:ASP:CB	2.23	0.69
2:C:536:PRO:O	2:C:539:VAL:HG23	1.92	0.69
2:C:848:VAL:CG1	3:D:632:VAL:HG23	2.23	0.69
3:D:791:TYR:CE2	3:D:945:SER:HB2	2.28	0.69
3:D:1213:ARG:HH11	3:D:1213:ARG:CG	2.05	0.69
2:C:430:VAL:HG13	3:D:1075:HIS:HD2	1.58	0.68
2:C:850:ALA:HA	3:D:632:VAL:CG2	2.23	0.68
2:C:850:ALA:HA	3:D:632:VAL:HG22	1.75	0.68
3:D:631:ILE:HG21	3:D:745:MET:HG3	1.75	0.68
3:D:1139:ASP:O	3:D:1142:ALA:HB3	1.94	0.68
2:C:838:LYS:CG	2:C:997:LEU:HB2	2.21	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:263:ASP:N	2:C:264:PRO:HD3	2.10	0.67
2:C:193:LEU:HD21	2:C:307:LEU:HD21	1.76	0.67
2:C:840:ALA:HA	2:C:845:ASN:O	1.95	0.67
2:C:305:PRO:HA	2:C:308:ARG:HG2	1.76	0.67
3:D:1397:LYS:C	3:D:1398:TRP:HE3	2.03	0.67
3:D:317:VAL:HG23	3:D:337:LEU:HA	1.76	0.67
3:D:482:LYS:H	3:D:489:ARG:HG3	1.60	0.67
3:D:592:THR:HG23	3:D:600:LEU:HD21	1.76	0.67
2:C:1008:ARG:NH2	2:C:1020:PRO:HB3	2.09	0.67
5:F:222:ARG:HG2	5:F:242:TRP:CZ3	2.30	0.67
2:C:704:HIS:HB3	11:C:1308:HOH:O	1.95	0.66
2:C:843:HIS:HE1	2:C:887:GLU:OE1	1.78	0.66
3:D:1351:GLU:HA	3:D:1354:LYS:HD3	1.76	0.66
3:D:836:VAL:H	3:D:837:GLY:CA	2.05	0.66
1:B:45:LEU:HD11	11:B:401:HOH:O	1.95	0.66
3:D:1261:GLU:O	3:D:1265:ALA:HB2	1.96	0.66
3:D:630:VAL:HG13	3:D:725:SER:HB3	1.76	0.66
3:D:964:LEU:CD2	3:D:1058:ARG:HG2	2.23	0.66
5:F:370:LYS:HA	5:F:374:GLY:CA	2.25	0.66
3:D:1225:ALA:O	3:D:1229:ILE:HG13	1.96	0.65
3:D:1397:LYS:HB2	3:D:1398:TRP:CZ3	2.32	0.65
3:D:1442:ASN:HD21	3:D:1444:THR:HB	1.60	0.65
2:C:1102:LEU:HB3	2:C:1106:ASP:HA	1.78	0.65
3:D:108:VAL:HG12	3:D:109:PRO:HA	1.79	0.65
2:C:140:ILE:HD12	2:C:331:ARG:NH2	2.12	0.65
2:C:846:LYS:HE2	3:D:741:ASP:O	1.97	0.65
3:D:838:ARG:HD3	3:D:874:GLU:CD	2.22	0.65
3:D:885:ILE:CG2	3:D:937:TYR:HD1	2.10	0.65
3:D:1258:ARG:NH2	3:D:1262:LEU:HD21	2.10	0.65
3:D:702:LEU:O	3:D:713:ILE:HA	1.96	0.65
3:D:1265:ALA:CA	3:D:1266:ARG:CB	2.51	0.65
2:C:949:LYS:HD2	3:D:796:ARG:NH2	2.11	0.65
2:C:91:GLN:HB3	2:C:119:PRO:HA	1.79	0.64
2:C:399:ASN:ND2	2:C:568:ALA:HB3	2.12	0.64
2:C:673:LEU:HD11	2:C:895:TYR:CZ	2.31	0.64
1:A:38:ASN:O	1:A:41:ARG:N	2.30	0.64
2:C:317:VAL:N	2:C:318:PRO:HD3	2.13	0.64
2:C:1086:ARG:HD3	2:C:1112:PHE:CD2	2.33	0.64
2:C:588:VAL:HG13	2:C:593:ALA:HB3	1.79	0.64
3:D:633:VAL:HG13	3:D:635:PRO:HD3	1.78	0.64
2:C:707:ARG:HG3	2:C:826:TYR:CE2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:379:ARG:HD3	5:F:382:THR:HB	1.78	0.64
1:A:200:TRP:HE3	1:A:200:TRP:H	1.45	0.64
2:C:1081:VAL:CG1	2:C:1086:ARG:HE	2.09	0.64
2:C:116:GLY:HA3	2:C:378:LEU:HD23	1.78	0.64
2:C:911:GLU:N	2:C:912:PRO:HD2	2.11	0.64
2:C:1090:LYS:HA	2:C:1093:GLN:HB2	1.80	0.64
3:D:659:LYS:HE3	3:D:663:GLU:HG3	1.77	0.64
3:D:1102:THR:HG21	3:D:1371:VAL:HG22	1.79	0.64
3:D:1232:PRO:HG2	3:D:1356:TYR:HE2	1.63	0.64
3:D:574:LEU:O	3:D:578:VAL:HG23	1.98	0.63
3:D:1376:MET:HE3	3:D:1421:LEU:HD12	1.79	0.63
2:C:640:ARG:HH11	2:C:642:ARG:HH22	1.46	0.63
3:D:183:GLU:O	3:D:202:VAL:HG13	1.98	0.63
2:C:1052:MET:HG3	3:D:623:VAL:HG21	1.79	0.63
3:D:791:TYR:CD2	3:D:945:SER:HB2	2.34	0.63
2:C:1009:SER:HB3	3:D:651:GLU:OE2	1.98	0.63
3:D:941:PHE:O	3:D:945:SER:HB3	1.98	0.63
1:A:111:ALA:HB2	1:A:127:LEU:HD23	1.79	0.63
3:D:885:ILE:CG2	3:D:937:TYR:CD1	2.82	0.63
5:F:367:MET:HA	5:F:370:LYS:HB2	1.80	0.63
1:A:24:VAL:HG13	1:A:196:THR:HG23	1.80	0.63
2:C:575:GLN:NE2	2:C:670:GLN:HG2	2.14	0.63
2:C:304:LEU:HB3	2:C:305:PRO:HD3	1.81	0.62
1:A:73:GLU:HB3	1:A:78:ILE:HG12	1.81	0.62
3:D:1440:PHE:HE2	3:D:1463:LYS:HZ3	1.47	0.62
3:D:535:PHE:O	5:F:314:PRO:HB2	1.99	0.62
3:D:969:ARG:O	3:D:972:LEU:HB2	1.99	0.62
2:C:202:TYR:HE2	2:C:300:ASP:HB3	1.63	0.62
2:C:396:ASP:HA	2:C:633:GLN:NE2	2.11	0.62
2:C:1012:PRO:HD3	2:C:1026:GLN:HG2	1.81	0.62
2:C:710:ILE:HB	2:C:790:LEU:HD22	1.80	0.62
3:D:45:PHE:O	3:D:86:ARG:NH2	2.32	0.62
1:A:38:ASN:O	1:A:39:PRO:C	2.41	0.62
2:C:363:SER:H	2:C:367:LEU:HD21	1.64	0.62
3:D:1127:GLU:HB3	3:D:1131:SER:HB3	1.82	0.62
1:A:110:LYS:HB2	1:A:112:ARG:HG2	1.81	0.62
2:C:430:VAL:HG13	3:D:1075:HIS:CD2	2.34	0.62
2:C:1018:GLN:HG3	2:C:1060:ILE:HD11	1.80	0.62
3:D:1372:VAL:HA	3:D:1375:MET:HE3	1.81	0.62
3:D:845:ASN:HB2	3:D:846:PRO:CD	2.29	0.62
3:D:1091:SER:C	3:D:1093:TYR:N	2.55	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:THR:HG22	1:A:208:LEU:H	1.65	0.61
2:C:575:GLN:HE21	2:C:671:ASN:H	1.48	0.61
3:D:1074:SER:HA	3:D:1077:ALA:HB3	1.81	0.61
3:D:1341:PRO:HD2	3:D:1342:GLU:OE2	2.00	0.61
2:C:441:VAL:O	2:C:441:VAL:CG2	2.48	0.61
2:C:1087:VAL:HG22	3:D:524:LEU:HD22	1.81	0.61
2:C:194:VAL:HA	2:C:197:LEU:HD12	1.81	0.61
3:D:1152:GLU:HG3	3:D:1161:GLU:HA	1.83	0.61
2:C:843:HIS:CE1	2:C:887:GLU:OE1	2.53	0.61
2:C:1030:GLN:OE1	3:D:628:ARG:HB2	2.00	0.61
3:D:703:ASN:HB2	3:D:713:ILE:HG12	1.81	0.61
2:C:720:GLU:HB3	2:C:760:SER:HA	1.83	0.61
3:D:838:ARG:HH11	3:D:874:GLU:HB3	1.66	0.61
2:C:759:THR:HB	2:C:785:VAL:HB	1.82	0.61
3:D:703:ASN:ND2	3:D:707:THR:OG1	2.33	0.61
3:D:520:LEU:O	3:D:525:ARG:NH1	2.34	0.60
3:D:616:GLN:HA	3:D:619:LEU:HD12	1.81	0.60
3:D:711:LEU:HD13	3:D:778:LEU:HD23	1.82	0.60
2:C:469:THR:HG22	2:C:538:GLN:NE2	2.12	0.60
2:C:971:LYS:HB2	2:C:986:PRO:HB2	1.83	0.60
2:C:711:GLU:O	2:C:758:ARG:NH1	2.32	0.60
2:C:553:ASP:OD1	2:C:843:HIS:CD2	2.54	0.60
3:D:781:PRO:HG2	3:D:911:LEU:HD22	1.84	0.60
2:C:1039:ALA:HB2	3:D:707:THR:HG21	1.84	0.60
1:B:124:ASN:HD22	1:B:127:LEU:HD13	1.67	0.60
2:C:469:THR:CG2	2:C:538:GLN:HE21	2.10	0.60
2:C:807:ARG:HA	2:C:821:GLU:HB2	1.84	0.60
4:E:25:LYS:HA	4:E:28:GLN:OE1	2.01	0.60
3:D:1433:SER:HA	3:D:1457:ASP:OD2	2.01	0.60
2:C:807:ARG:CZ	2:C:807:ARG:HB3	2.31	0.60
3:D:729:HIS:HE1	3:D:932:ASP:OD1	1.85	0.60
3:D:795:VAL:HG12	3:D:876:SER:HB3	1.84	0.60
3:D:885:ILE:HG23	3:D:937:TYR:CE1	2.36	0.60
2:C:772:ARG:HG2	5:F:373:LYS:HD3	1.84	0.59
2:C:885:ILE:HG22	2:C:889:HIS:CE1	2.36	0.59
3:D:64:LYS:HB3	5:F:376:ILE:HB	1.84	0.59
3:D:1145:TYR:CE2	3:D:1168:MET:HB2	2.36	0.59
2:C:91:GLN:CB	2:C:119:PRO:HA	2.33	0.59
2:C:177:GLU:HG2	2:C:178:PRO:HD2	1.84	0.59
2:C:551:GLU:HG2	2:C:552:HIS:CD2	2.37	0.59
5:F:101:GLU:HG3	5:F:104:ARG:HH12	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:877:PRO:HG3	3:D:1023:MET:CE	2.32	0.59
3:D:808:THR:N	3:D:809:PRO:HD2	2.17	0.59
3:D:1140:ILE:HD13	3:D:1175:ILE:HG12	1.83	0.59
10:D:1605:G4P:O3C	10:D:1605:G4P:H4'	2.02	0.59
1:B:209:GLU:O	1:B:213:GLN:HG2	2.01	0.59
3:D:1127:GLU:HB3	3:D:1131:SER:CB	2.32	0.59
1:B:226:SER:O	1:B:228:PRO:HD3	2.02	0.59
1:A:138:LEU:HD11	1:A:140:MET:HE2	1.83	0.59
2:C:3:ILE:HG22	2:C:900:ARG:HB2	1.84	0.59
3:D:17:LYS:O	3:D:20:SER:HB3	2.03	0.59
3:D:709:HIS:ND1	3:D:1231:GLU:HG3	2.18	0.59
1:A:42:ARG:HH21	2:C:978:ARG:HG3	1.67	0.59
2:C:1009:SER:HB2	3:D:651:GLU:O	2.02	0.59
3:D:1352:ILE:HG21	3:D:1368:ILE:HG21	1.85	0.59
1:B:66:SER:O	1:B:75:VAL:HG23	2.03	0.59
3:D:770:LEU:HA	3:D:777:PRO:HA	1.85	0.59
3:D:890:VAL:O	3:D:926:LYS:HD3	2.02	0.59
3:D:628:ARG:HG2	3:D:629:SER:N	2.18	0.58
1:A:58:ILE:HB	1:A:61:VAL:HG22	1.85	0.58
3:D:558:LEU:HD23	3:D:567:ILE:HD12	1.85	0.58
5:F:79:ASP:N	5:F:80:PRO:HD2	2.18	0.58
3:D:527:MET:O	3:D:527:MET:HG3	2.03	0.58
5:F:319:THR:O	5:F:329:TYR:N	2.32	0.58
2:C:640:ARG:NH1	2:C:642:ARG:HH22	2.01	0.58
2:C:1032:PHE:HZ	2:C:1040:LEU:HD11	1.67	0.58
2:C:405:ARG:HD2	2:C:442:GLU:OE2	2.03	0.58
2:C:971:LYS:CB	2:C:986:PRO:HB2	2.34	0.58
3:D:65:ARG:HG3	3:D:66:GLN:H	1.67	0.58
3:D:1378:TYR:CE1	3:D:1430:SER:HB2	2.39	0.58
2:C:435:TYR:HA	3:D:1071:PHE:HE2	1.69	0.58
3:D:1400:VAL:HG12	3:D:1404:ASN:HD21	1.69	0.58
2:C:395:LYS:HE2	2:C:403:SER:OG	2.04	0.58
2:C:281:LEU:HB3	2:C:305:PRO:HB2	1.86	0.57
3:D:374:GLU:HB3	3:D:376:GLU:HG3	1.86	0.57
5:F:367:MET:O	5:F:371:LEU:HG	2.04	0.57
1:B:151:VAL:HB	1:B:169:ALA:HB3	1.84	0.57
3:D:1362:LYS:HD3	11:D:1752:HOH:O	2.04	0.57
3:D:1481:VAL:CG1	4:E:18:ARG:HA	2.34	0.57
5:F:350:LEU:O	5:F:354:LEU:HG	2.03	0.57
2:C:140:ILE:HD12	2:C:331:ARG:HH22	1.67	0.57
3:D:860:LEU:HA	3:D:877:PRO:HD2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:634:GLY:O	3:D:637:LEU:HB2	2.03	0.57
3:D:852:ALA:HB1	3:D:857:ILE:HG12	1.85	0.57
3:D:1042:ARG:NH1	3:D:1045:MET:HE1	2.19	0.57
3:D:1205:TYR:CZ	3:D:1221:VAL:HG22	2.39	0.57
3:D:1481:VAL:O	3:D:1482:ARG:C	2.47	0.57
3:D:108:VAL:HA	3:D:109:PRO:C	2.30	0.57
2:C:441:VAL:O	2:C:441:VAL:HG23	2.03	0.57
3:D:568:ARG:O	3:D:571:LYS:N	2.37	0.57
3:D:992:ILE:O	3:D:995:LEU:HB3	2.03	0.57
3:D:1115:THR:O	3:D:1151:ARG:NH2	2.38	0.57
3:D:1295:GLU:HG2	3:D:1300:SER:HA	1.86	0.57
1:A:41:ARG:HG3	1:A:45:LEU:HD12	1.86	0.57
3:D:770:LEU:HD11	3:D:919:PHE:CE1	2.39	0.57
3:D:262:LYS:HD3	3:D:269:PHE:HD2	1.70	0.57
3:D:549:ASN:O	3:D:553:ARG:HB2	2.04	0.57
1:A:181:VAL:HG12	1:A:181:VAL:O	2.05	0.56
3:D:320:ALA:HB3	3:D:336:PHE:HD1	1.70	0.56
2:C:271:GLU:H	2:C:274:ARG:HD3	1.70	0.56
2:C:274:ARG:HD2	2:C:285:LEU:HB3	1.87	0.56
2:C:728:HIS:NE2	2:C:730:SER:O	2.38	0.56
2:C:889:HIS:CD2	2:C:970:GLY:HA3	2.41	0.56
3:D:421:LEU:HD22	3:D:429:SER:HB2	1.85	0.56
1:B:167:VAL:HG12	1:B:168:ASP:N	2.17	0.56
2:C:712:ALA:HB3	2:C:821:GLU:H	1.70	0.56
2:C:713:ARG:HG2	2:C:819:VAL:HG22	1.86	0.56
2:C:890:LEU:HG	2:C:901:TYR:CD1	2.40	0.56
3:D:1155:VAL:HG11	3:D:1174:LEU:HD23	1.88	0.56
2:C:501:THR:O	2:C:503:LEU:HD13	2.06	0.56
5:F:417:LYS:HB2	5:F:418:LEU:HD12	1.87	0.56
2:C:6:PHE:HB2	2:C:902:ILE:O	2.06	0.56
2:C:712:ALA:O	2:C:820:ARG:N	2.38	0.56
2:C:877:PRO:HG3	3:D:1023:MET:HE3	1.87	0.56
2:C:1008:ARG:HH21	2:C:1020:PRO:HB3	1.68	0.56
3:D:935:LYS:HG2	3:D:939:PHE:CE1	2.41	0.56
2:C:17:PRO:O	2:C:20:GLU:HB2	2.05	0.56
2:C:234:ALA:O	2:C:238:LEU:HG	2.05	0.56
2:C:469:THR:HG22	2:C:470:PRO:HD2	1.88	0.56
3:D:917:GLN:C	3:D:919:PHE:H	2.14	0.56
2:C:695:LEU:HD21	2:C:833:LEU:CB	2.36	0.56
3:D:408:GLU:O	3:D:409:VAL:HG22	2.06	0.56
3:D:1190:SER:OG	3:D:1191:PRO:HD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:VAL:HG22	1:B:123:MET:HG3	1.88	0.56
2:C:99:GLN:HB2	2:C:109:LYS:HA	1.88	0.56
3:D:400:VAL:HG12	3:D:445:ARG:HG2	1.86	0.56
3:D:729:HIS:CD2	3:D:730:PRO:HD2	2.41	0.56
3:D:824:ASN:ND2	3:D:862:ASP:OD2	2.39	0.56
3:D:127:LEU:HD11	3:D:461:ILE:HG13	1.87	0.56
3:D:1030:GLY:HA2	3:D:1034:GLN:NE2	2.21	0.56
3:D:1379:VAL:HG13	3:D:1395:LEU:HB2	1.87	0.56
2:C:426:ASP:O	2:C:428:ARG:N	2.38	0.55
3:D:879:ARG:HB3	3:D:902:LEU:CD1	2.36	0.55
3:D:916:TYR:CE2	3:D:920:LEU:HD21	2.40	0.55
2:C:368:THR:HB	2:C:369:PRO:HD3	1.86	0.55
2:C:835:VAL:HA	2:C:849:VAL:O	2.05	0.55
2:C:1015:LEU:HA	5:F:335:ASP:HB2	1.89	0.55
3:D:711:LEU:HD13	3:D:778:LEU:CD2	2.35	0.55
2:C:881:ASN:O	2:C:884:GLN:HG2	2.06	0.55
3:D:272:LEU:HG	3:D:282:TYR:HE1	1.71	0.55
2:C:496:ILE:HG12	2:C:531:PHE:HB2	1.88	0.55
3:D:1342:GLU:CD	3:D:1342:GLU:H	2.15	0.55
5:F:207:LEU:HB3	5:F:212:LEU:HD21	1.88	0.55
1:A:139:ASN:C	1:A:139:ASN:OD1	2.50	0.55
2:C:625:LEU:O	2:C:626:ARG:C	2.50	0.55
2:C:672:VAL:HG22	2:C:868:ASP:HB2	1.89	0.55
2:C:99:GLN:H	2:C:110:GLU:HB2	1.71	0.55
1:A:32:PHE:HA	1:A:35:THR:HB	1.88	0.55
2:C:557:ARG:HD3	2:C:879:ARG:HG3	1.89	0.55
2:C:1032:PHE:CE1	2:C:1052:MET:HG2	2.42	0.55
3:D:522:PRO:HA	3:D:525:ARG:NH1	2.21	0.55
3:D:798:GLU:HG3	3:D:824:ASN:HB2	1.89	0.55
4:E:39:VAL:O	4:E:72:ARG:HD2	2.07	0.55
2:C:23:VAL:HG12	2:C:121:MET:HE1	1.89	0.55
2:C:553:ASP:OD1	2:C:843:HIS:HD2	1.89	0.55
3:D:728:LEU:HD13	3:D:745:MET:CE	2.27	0.55
2:C:1081:VAL:HG13	2:C:1086:ARG:NE	2.20	0.55
3:D:634:GLY:HA3	3:D:637:LEU:HD12	1.88	0.55
3:D:770:LEU:HB2	3:D:1210:SER:HA	1.87	0.55
3:D:1229:ILE:O	3:D:1229:ILE:HG22	2.06	0.55
3:D:1353:GLN:O	3:D:1357:ARG:HG2	2.06	0.55
3:D:1127:GLU:HB3	3:D:1131:SER:OG	2.07	0.54
2:C:595:LEU:HD12	2:C:639:GLN:NE2	2.22	0.54
3:D:939:PHE:O	3:D:940:THR:C	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1047:LYS:HB3	3:D:1048:PRO:CD	2.30	0.54
1:A:181:VAL:N	2:C:937:ASP:OD2	2.32	0.54
3:D:50:PHE:CD2	3:D:522:PRO:HD3	2.42	0.54
2:C:34:VAL:N	2:C:35:PRO:CD	2.68	0.54
3:D:216:VAL:HG22	3:D:340:THR:HG22	1.87	0.54
3:D:980:MET:HE2	3:D:980:MET:HA	1.89	0.54
3:D:1314:LYS:HB3	3:D:1317:ASP:OD2	2.07	0.54
2:C:83:CYS:HB3	2:C:88:LEU:O	2.07	0.54
2:C:164:PRO:HB2	2:C:166:PRO:HD3	1.89	0.54
2:C:512:ARG:HD3	2:C:523:ILE:HD12	1.90	0.54
3:D:570:GLU:OE2	5:F:214:GLN:NE2	2.36	0.54
3:D:835:SER:N	3:D:838:ARG:HE	2.06	0.54
3:D:1369:GLU:O	3:D:1372:VAL:HG12	2.08	0.54
3:D:822:ALA:HB3	3:D:825:ALA:HB2	1.88	0.54
2:C:108:ILE:HD12	2:C:368:THR:HG21	1.90	0.54
3:D:1145:TYR:HE2	3:D:1168:MET:HB2	1.71	0.54
2:C:181:VAL:HG12	2:C:182:VAL:H	1.73	0.54
3:D:436:GLU:HB2	3:D:445:ARG:HB2	1.88	0.54
3:D:835:SER:H	3:D:838:ARG:HE	1.56	0.54
3:D:1459:LEU:HD12	3:D:1470:ARG:HH11	1.73	0.54
2:C:637:LEU:O	2:C:638:ASP:HB3	2.08	0.54
2:C:698:ASP:OD1	2:C:701:THR:OG1	2.20	0.54
3:D:353:VAL:HG12	3:D:368:VAL:HG22	1.90	0.54
1:A:38:ASN:O	1:A:40:LEU:N	2.41	0.53
1:A:24:VAL:HG11	1:A:194:LYS:HE2	1.90	0.53
4:E:33:HIS:HB2	4:E:37:ASN:HD21	1.72	0.53
5:F:200:LYS:HA	5:F:209:PHE:CE1	2.44	0.53
2:C:657:ASP:CG	2:C:663:ASN:H	2.16	0.53
3:D:1332:PRO:HB2	3:D:1421:LEU:CD2	2.38	0.53
5:F:300:ASP:HB3	5:F:303:ARG:HB2	1.89	0.53
1:A:23:PHE:CE2	1:A:208:LEU:HD13	2.39	0.53
2:C:861:LEU:CD2	2:C:972:VAL:HG21	2.38	0.53
2:C:897:LEU:HB3	2:C:899:GLN:OE1	2.08	0.53
1:B:85:LEU:HA	1:B:124:ASN:HD21	1.72	0.53
2:C:89:THR:HG23	2:C:129:ILE:HA	1.90	0.53
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.89	0.53
2:C:393:GLN:OE1	2:C:406:HIS:HE1	1.92	0.53
2:C:1114:GLY:O	2:C:1116:ALA:N	2.41	0.53
3:D:1066:THR:HB	3:D:1069:GLU:H	1.74	0.53
2:C:1020:PRO:HG3	3:D:624:ASP:OD1	2.09	0.53
3:D:38:LYS:HG3	3:D:39:PRO:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:698:LYS:HA	3:D:756:GLN:NE2	2.22	0.53
3:D:1012:GLU:HA	3:D:1012:GLU:OE1	2.08	0.53
3:D:1264:GLU:HA	3:D:1423:GLY:HA3	1.91	0.53
5:F:117:SER:HB2	5:F:122:LEU:O	2.09	0.53
2:C:84:ARG:HA	2:C:131:GLY:HA2	1.90	0.53
2:C:455:LEU:HG	2:C:459:ALA:HB3	1.89	0.53
2:C:862:PRO:HA	2:C:975:TYR:HE1	1.74	0.53
3:D:15:PRO:HA	3:D:18:ILE:HD12	1.90	0.53
3:D:695:ILE:O	3:D:696:HIS:C	2.51	0.53
3:D:1046:GLN:N	11:D:1702:HOH:O	2.29	0.53
2:C:468:ARG:HE	2:C:487:THR:HG23	1.73	0.53
3:D:792:ILE:O	3:D:878:GLY:HA3	2.08	0.53
3:D:165:LYS:HD3	3:D:199:LEU:HD11	1.90	0.53
3:D:925:GLU:HG3	4:E:2:ALA:HB3	1.91	0.53
3:D:1397:LYS:HB2	3:D:1398:TRP:HZ3	1.73	0.53
5:F:152:ASP:N	5:F:153:PRO:CD	2.72	0.53
5:F:416:ARG:HG2	5:F:419:ARG:HD2	1.91	0.53
1:A:70:GLY:HA2	1:A:133:GLU:HG2	1.90	0.52
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.91	0.52
3:D:1276:GLU:H	3:D:1303:TYR:HH	1.52	0.52
3:D:1370:ILE:HG22	3:D:1371:VAL:N	2.22	0.52
5:F:172:ARG:O	5:F:176:ILE:HG12	2.09	0.52
3:D:885:ILE:HG23	3:D:937:TYR:CD1	2.43	0.52
3:D:1042:ARG:HB3	3:D:1042:ARG:NH1	2.19	0.52
3:D:1140:ILE:O	3:D:1141:GLU:C	2.52	0.52
3:D:1462:LEU:HD23	3:D:1473:PRO:HG2	1.91	0.52
3:D:1481:VAL:HG11	4:E:18:ARG:HA	1.92	0.52
2:C:292:ARG:HB2	2:C:299:LYS:H	1.75	0.52
2:C:444:PRO:HG2	2:C:448:ASN:O	2.09	0.52
3:D:270:LEU:O	3:D:282:TYR:HB2	2.09	0.52
2:C:1092:LEU:CD1	2:C:1099:VAL:HG21	2.34	0.52
3:D:72:VAL:HG13	3:D:77:GLY:HA2	1.90	0.52
5:F:137:GLY:HA2	5:F:140:ARG:HB3	1.91	0.52
2:C:333:ILE:HD11	2:C:461:VAL:HG11	1.90	0.52
3:D:94:GLU:O	3:D:551:ASN:ND2	2.43	0.52
3:D:871:LYS:HD3	3:D:873:LEU:HD21	1.91	0.52
2:C:1063:ARG:HG3	5:F:341:PRO:HG3	1.92	0.52
3:D:1372:VAL:O	3:D:1375:MET:HB3	2.10	0.52
3:D:1379:VAL:HG11	3:D:1395:LEU:HD13	1.90	0.52
5:F:263:HIS:O	5:F:267:THR:HG23	2.10	0.52
3:D:730:PRO:HA	3:D:733:CYS:SG	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:704:ARG:CD	3:D:738:ALA:HB2	2.40	0.52
3:D:1213:ARG:HG2	3:D:1213:ARG:NH1	2.05	0.52
5:F:157:GLU:O	5:F:161:GLN:N	2.43	0.52
2:C:551:GLU:HB3	2:C:906:PHE:CD2	2.45	0.52
2:C:603:VAL:HG21	2:C:643:VAL:HG11	1.91	0.51
1:A:225:PHE:HD2	1:B:11:PHE:CE1	2.28	0.51
2:C:521:PRO:HG2	3:D:1055:VAL:HG21	1.93	0.51
3:D:948:THR:O	3:D:949:ILE:CG1	2.58	0.51
3:D:1381:VAL:HG13	3:D:1389:LEU:O	2.10	0.51
1:B:177:VAL:HB	11:B:401:HOH:O	2.11	0.51
2:C:72:ARG:HG3	2:C:95:TYR:HB2	1.92	0.51
2:C:157:ARG:HG3	2:C:158:TYR:N	2.21	0.51
2:C:1008:ARG:HD3	2:C:1010:THR:HA	1.92	0.51
3:D:1489:GLN:HA	3:D:1492:LEU:HD12	1.92	0.51
2:C:545:ASN:HB3	2:C:583:LEU:HD12	1.91	0.51
3:D:57:GLU:HG2	3:D:58:CYS:H	1.76	0.51
3:D:96:ALA:HB3	3:D:554:LEU:CD2	2.22	0.51
3:D:158:TYR:C	3:D:160:GLU:H	2.18	0.51
1:A:106:PRO:HG3	1:A:134:GLU:HG2	1.93	0.51
2:C:496:ILE:O	2:C:515:ALA:HB1	2.11	0.51
3:D:361:VAL:HG21	3:D:385:VAL:HG23	1.93	0.51
3:D:899:LEU:HD22	3:D:917:GLN:HB3	1.93	0.51
4:E:12:MET:HE1	4:E:69:LEU:HA	1.91	0.51
2:C:81:ASP:HB3	2:C:626:ARG:HH22	1.76	0.51
2:C:387:SER:HB3	2:C:388:ARG:HD3	1.92	0.51
2:C:1052:MET:HG3	3:D:623:VAL:CG2	2.41	0.51
3:D:440:VAL:HG23	3:D:441:ARG:H	1.75	0.51
5:F:95:THR:HB	5:F:98:GLU:H	1.75	0.51
2:C:603:VAL:HG23	2:C:647:GLN:O	2.10	0.51
2:C:1067:TYR:CE2	2:C:1071:ILE:HG13	2.45	0.51
2:C:162:ILE:HB	2:C:172:ILE:HB	1.91	0.51
2:C:1112:PHE:O	2:C:1113:GLU:C	2.52	0.51
2:C:443:THR:HG22	2:C:559:LEU:HD11	1.93	0.51
2:C:810:ASP:N	2:C:811:PRO:CD	2.74	0.51
2:C:1031:ARG:HA	3:D:621:LYS:O	2.10	0.51
3:D:593:ASN:CB	3:D:594:PRO:HD3	2.40	0.51
3:D:654:LYS:HB3	3:D:655:PRO:CD	2.35	0.51
3:D:1281:VAL:HB	3:D:1316:GLY:H	1.75	0.51
1:A:56:VAL:HG22	1:A:142:VAL:HG22	1.93	0.51
1:A:156:HIS:HD2	1:A:158:ILE:HB	1.76	0.51
3:D:95:LEU:HD21	3:D:517:VAL:HG23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:651:GLU:O	3:D:654:LYS:HB2	2.11	0.51
3:D:778:LEU:HG	3:D:778:LEU:O	2.11	0.51
2:C:585:GLU:HA	2:C:664:GLY:O	2.11	0.50
2:C:672:VAL:HG22	2:C:868:ASP:HB3	1.93	0.50
3:D:731:LEU:HA	11:D:1701:HOH:O	2.11	0.50
3:D:1292:VAL:HG11	3:D:1325:LEU:HD22	1.93	0.50
2:C:657:ASP:OD1	2:C:661:SER:OG	2.29	0.50
2:C:742:VAL:HG12	2:C:743:VAL:N	2.25	0.50
2:C:923:GLU:O	2:C:924:VAL:C	2.54	0.50
1:A:228:PRO:O	1:A:229:GLN:HB2	2.10	0.50
1:B:63:HIS:CE1	3:D:809:PRO:HB3	2.47	0.50
2:C:141:HIS:CE1	2:C:332:ARG:NH1	2.80	0.50
3:D:127:LEU:CD1	3:D:461:ILE:HG13	2.41	0.50
3:D:1397:LYS:HB2	3:D:1398:TRP:CE3	2.45	0.50
5:F:120:THR:HB	5:F:122:LEU:HG	1.92	0.50
2:C:842:ARG:NH1	11:C:1302:HOH:O	2.29	0.50
3:D:137:PRO:HA	3:D:452:ILE:HG23	1.92	0.50
3:D:860:LEU:HB3	3:D:878:GLY:N	2.25	0.50
2:C:728:HIS:CG	2:C:729:LEU:H	2.29	0.50
3:D:1347:TYR:CZ	3:D:1351:GLU:HG3	2.47	0.50
2:C:1036:GLU:HG3	3:D:703:ASN:ND2	2.27	0.50
3:D:192:ALA:HB1	3:D:193:PRO:CD	2.33	0.50
3:D:704:ARG:HD3	3:D:738:ALA:HB2	1.92	0.50
2:C:1036:GLU:O	2:C:1039:ALA:HB3	2.11	0.50
2:C:1083:GLU:O	2:C:1087:VAL:HB	2.12	0.50
3:D:44:LEU:HB3	3:D:525:ARG:HH21	1.77	0.50
3:D:206:ARG:HB2	3:D:392:SER:O	2.11	0.50
2:C:285:LEU:HD23	2:C:285:LEU:H	1.76	0.50
2:C:589:ARG:HA	2:C:596:TYR:HE1	1.75	0.50
1:A:42:ARG:O	1:A:43:ILE:C	2.54	0.50
2:C:23:VAL:HA	2:C:121:MET:HE1	1.93	0.50
2:C:536:PRO:HB3	2:C:906:PHE:HB2	1.92	0.50
2:C:754:ILE:N	2:C:754:ILE:HD12	2.27	0.50
3:D:539:ASP:OD2	3:D:598:ARG:NH2	2.43	0.50
3:D:1372:VAL:O	3:D:1375:MET:CB	2.60	0.50
2:C:266:ARG:HH11	2:C:273:GLY:H	1.60	0.49
2:C:881:ASN:ND2	2:C:881:ASN:N	2.36	0.49
3:D:939:PHE:O	3:D:942:SER:N	2.45	0.49
3:D:1481:VAL:O	3:D:1483:PHE:N	2.45	0.49
5:F:79:ASP:HB3	5:F:83:GLN:HB2	1.93	0.49
1:A:22:GLU:C	1:A:23:PHE:CD1	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:448:ASN:HA	2:C:451:LEU:HD12	1.94	0.49
2:C:753:ASP:O	2:C:792:VAL:HG23	2.12	0.49
2:C:904:PRO:HD2	2:C:908:GLY:CA	2.42	0.49
3:D:854:ALA:C	3:D:856:GLY:H	2.20	0.49
3:D:1101:VAL:HG11	3:D:1424:VAL:HG12	1.94	0.49
5:F:386:VAL:HG12	5:F:388:ALA:H	1.78	0.49
3:D:543:LEU:HD23	3:D:546:ARG:HD3	1.95	0.49
2:C:15:LEU:HD21	2:C:583:LEU:HD22	1.94	0.49
2:C:196:LEU:HD23	2:C:238:LEU:HD22	1.93	0.49
2:C:580:MET:SD	2:C:584:GLU:HG3	2.53	0.49
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.44	0.49
3:D:493:ARG:HH21	3:D:494:LYS:HZ3	1.59	0.49
1:A:185:ARG:HB2	1:A:190:THR:HG22	1.94	0.49
2:C:267:TYR:HB2	2:C:272:ALA:HB3	1.94	0.49
2:C:545:ASN:HB3	2:C:583:LEU:CD1	2.42	0.49
3:D:828:LYS:HB3	3:D:833:GLU:HG2	1.94	0.49
3:D:853:VAL:HG12	3:D:858:VAL:HG13	1.93	0.49
3:D:1463:LYS:O	3:D:1467:ILE:HG22	2.13	0.49
3:D:1213:ARG:HB2	3:D:1214:PRO:CD	2.42	0.49
3:D:1167:SER:HB3	3:D:1170:ASP:OD2	2.12	0.49
3:D:1320:GLU:O	3:D:1323:GLN:HB2	2.12	0.49
5:F:393:THR:HG22	5:F:397:ILE:HD11	1.93	0.49
2:C:713:ARG:HH11	2:C:713:ARG:HB2	1.78	0.49
2:C:1101:THR:HB	3:D:5:VAL:HG21	1.93	0.49
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.93	0.49
3:D:1378:TYR:HE2	3:D:1394:VAL:HG22	1.75	0.49
1:A:206:THR:O	1:A:207:PRO:C	2.55	0.49
3:D:117:ASP:CB	3:D:495:ARG:HH12	2.23	0.49
3:D:915:VAL:HG12	3:D:916:TYR:N	2.27	0.49
2:C:1090:LYS:HE2	2:C:1112:PHE:CZ	2.48	0.48
3:D:1434:TRP:HE1	3:D:1457:ASP:HB2	1.76	0.48
1:B:11:PHE:HZ	1:B:211:LEU:HD21	1.78	0.48
1:B:100:LEU:HB2	1:B:115:LEU:HD13	1.94	0.48
2:C:881:ASN:OD1	2:C:884:GLN:NE2	2.46	0.48
1:B:59:GLU:HB2	1:B:139:ASN:H	1.79	0.48
3:D:605:ASP:HA	3:D:610:LYS:HB2	1.94	0.48
2:C:595:LEU:HB2	2:C:639:GLN:HE21	1.79	0.48
4:E:87:LYS:HE2	4:E:91:ARG:HH22	1.78	0.48
5:F:152:ASP:H	5:F:153:PRO:HD3	1.79	0.48
2:C:724:ARG:HG3	2:C:738:ASP:O	2.13	0.48
3:D:1045:MET:O	3:D:1053:PHE:HD1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1281:VAL:HG23	3:D:1317:ASP:O	2.14	0.48
3:D:1443:THR:O	3:D:1444:THR:C	2.57	0.48
1:A:216:GLU:CD	1:A:219:ARG:HH21	2.22	0.48
2:C:92:ALA:O	2:C:117:HIS:HB2	2.12	0.48
2:C:561:GLY:O	2:C:562:SER:C	2.55	0.48
2:C:759:THR:HA	2:C:786:LYS:O	2.13	0.48
2:C:1085:PHE:O	2:C:1088:LEU:HB3	2.13	0.48
3:D:444:VAL:O	3:D:444:VAL:HG23	2.14	0.48
3:D:629:SER:OG	3:D:630:VAL:N	2.46	0.48
1:A:11:PHE:HB2	1:B:224:TYR:O	2.13	0.48
2:C:603:VAL:HG21	2:C:643:VAL:CG1	2.44	0.48
2:C:629:TYR:HD2	11:C:1330:HOH:O	1.96	0.48
2:C:850:ALA:HA	3:D:632:VAL:HG21	1.96	0.48
2:C:904:PRO:HD2	2:C:908:GLY:H	1.79	0.48
2:C:1051:GLU:O	2:C:1056:LYS:HD3	2.14	0.48
3:D:156:GLU:CD	3:D:156:GLU:H	2.22	0.48
3:D:233:LYS:HB2	3:D:236:TYR:HD1	1.79	0.48
3:D:356:PRO:HB3	3:D:441:ARG:HG3	1.96	0.48
3:D:785:ILE:HG23	3:D:935:LYS:HA	1.96	0.48
3:D:1028:ALA:O	3:D:1029:ARG:HB2	2.12	0.48
2:C:434:HIS:O	2:C:435:TYR:C	2.56	0.48
2:C:683:ASN:CG	2:C:872:ASN:HB2	2.38	0.48
2:C:874:LEU:CD2	3:D:1023:MET:SD	3.02	0.48
3:D:852:ALA:HB1	3:D:857:ILE:CG1	2.44	0.48
3:D:1263:PHE:CE2	3:D:1371:VAL:HG11	2.49	0.48
1:A:39:PRO:O	1:A:43:ILE:HG13	2.14	0.48
2:C:267:TYR:CD2	2:C:271:GLU:HB2	2.48	0.48
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.54	0.48
3:D:754:PHE:O	3:D:757:ALA:HB3	2.13	0.48
3:D:798:GLU:O	3:D:825:ALA:HA	2.13	0.48
3:D:853:VAL:HA	3:D:858:VAL:O	2.14	0.48
3:D:860:LEU:HB3	3:D:878:GLY:CA	2.44	0.48
3:D:1165:TYR:CZ	3:D:1214:PRO:HB3	2.49	0.48
3:D:1404:ASN:OD1	3:D:1408:ILE:HB	2.14	0.48
1:B:23:PHE:HE1	1:B:199:ILE:HD12	1.79	0.48
2:C:343:GLN:OE1	2:C:343:GLN:HA	2.13	0.48
3:D:131:LYS:HD3	3:D:152:LEU:HD12	1.95	0.48
3:D:757:ALA:O	3:D:758:GLU:C	2.56	0.48
3:D:947:ILE:CG1	3:D:948:THR:N	2.73	0.48
2:C:272:ALA:O	2:C:275:TYR:HB3	2.13	0.47
2:C:672:VAL:CG2	2:C:868:ASP:HB3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1005:MET:HG2	3:D:629:SER:HB2	1.96	0.47
3:D:233:LYS:HB2	3:D:236:TYR:CD1	2.49	0.47
3:D:351:MET:HE2	3:D:368:VAL:HG12	1.96	0.47
3:D:508:ARG:C	3:D:510:GLU:H	2.21	0.47
3:D:883:ALA:HA	3:D:900:ILE:HD13	1.96	0.47
1:A:38:ASN:HB3	1:A:39:PRO:CD	2.44	0.47
2:C:3:ILE:HA	2:C:900:ARG:O	2.13	0.47
2:C:154:ARG:HH21	2:C:156:GLY:HA3	1.79	0.47
2:C:238:LEU:C	2:C:240:THR:H	2.21	0.47
2:C:946:ARG:O	2:C:950:LEU:HG	2.14	0.47
3:D:42:ASP:HB2	11:D:1731:HOH:O	2.14	0.47
3:D:48:ARG:HB3	3:D:48:ARG:CZ	2.44	0.47
3:D:406:ASP:HB2	3:D:423:ASP:HA	1.95	0.47
3:D:1021:TYR:CE1	3:D:1025:GLN:HG3	2.49	0.47
3:D:1231:GLU:N	3:D:1232:PRO:CD	2.77	0.47
4:E:37:ASN:H	4:E:37:ASN:ND2	2.13	0.47
5:F:384:GLU:HA	5:F:397:ILE:HD12	1.96	0.47
1:A:55:SER:HB2	1:A:158:ILE:HG21	1.95	0.47
1:B:59:GLU:HB3	1:B:138:LEU:HG	1.96	0.47
3:D:834:THR:HG23	3:D:838:ARG:HB2	1.96	0.47
3:D:1042:ARG:NH1	3:D:1045:MET:CE	2.77	0.47
1:A:39:PRO:HG3	1:B:39:PRO:CG	2.44	0.47
1:A:151:VAL:HA	1:A:152:PRO:HD3	1.80	0.47
1:B:161:ARG:H	1:B:164:ALA:HB3	1.79	0.47
1:B:175:ARG:HE	1:B:202:ASP:HA	1.79	0.47
2:C:700:TYR:CB	2:C:833:LEU:HD13	2.44	0.47
2:C:953:VAL:HG13	2:C:966:LEU:HD13	1.96	0.47
3:D:889:ALA:O	3:D:929:ARG:NH1	2.47	0.47
2:C:944:LEU:HD22	2:C:962:GLN:HB3	1.96	0.47
2:C:1007:ALA:HB2	3:D:648:MET:HG2	1.97	0.47
3:D:1158:VAL:HG11	3:D:1173:LEU:HD21	1.96	0.47
5:F:292:ALA:C	5:F:294:ALA:H	2.22	0.47
1:A:84:GLU:O	1:A:85:LEU:C	2.58	0.47
2:C:144:PRO:CB	2:C:266:ARG:HB3	2.45	0.47
2:C:191:PHE:HZ	2:C:196:LEU:HD11	1.80	0.47
2:C:575:GLN:HE22	2:C:671:ASN:H	1.56	0.47
2:C:1001:VAL:O	2:C:1004:LYS:HB3	2.14	0.47
3:D:339:TRP:CZ3	3:D:341:GLU:HB2	2.50	0.47
3:D:351:MET:HE3	3:D:370:ALA:HB2	1.96	0.47
3:D:835:SER:H	3:D:838:ARG:NE	2.12	0.47
3:D:1150:ALA:C	3:D:1151:ARG:HG2	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:LEU:HB2	1:A:63:HIS:HD2	1.80	0.47
2:C:889:HIS:CE1	3:D:951:ILE:H	2.13	0.47
2:C:1107:ASN:O	2:C:1108:PRO:C	2.58	0.47
3:D:324:ALA:HA	3:D:331:VAL:HG13	1.97	0.47
3:D:917:GLN:O	3:D:919:PHE:N	2.48	0.47
3:D:989:TYR:CZ	3:D:993:LEU:HD11	2.49	0.47
5:F:256:ARG:NH2	5:F:310:ILE:O	2.48	0.47
1:A:154:GLU:H	1:A:154:GLU:CD	2.22	0.47
1:A:221:HIS:HA	1:A:224:TYR:CE1	2.50	0.47
1:B:2:LEU:H	1:B:3:ASP:HA	1.76	0.47
2:C:563:ASN:O	2:C:566:THR:HB	2.15	0.47
2:C:679:PHE:CE2	2:C:853:LEU:HD11	2.49	0.47
2:C:707:ARG:HD2	2:C:824:ARG:HH11	1.79	0.47
2:C:876:VAL:O	2:C:877:PRO:C	2.55	0.47
3:D:601:ARG:HB2	5:F:318:GLU:HG2	1.97	0.47
1:A:152:PRO:O	1:A:153:ALA:C	2.57	0.47
1:A:177:VAL:HG22	1:A:199:ILE:HG12	1.97	0.47
1:B:29:GLU:O	1:B:30:ARG:C	2.58	0.47
2:C:1:MET:HE3	2:C:900:ARG:HG3	1.96	0.47
2:C:689:VAL:HG22	2:C:870:ILE:HB	1.97	0.47
2:C:897:LEU:HG	2:C:921:ALA:HB2	1.96	0.47
2:C:904:PRO:HD2	2:C:908:GLY:N	2.29	0.47
3:D:141:ILE:C	3:D:143:ASN:H	2.23	0.47
3:D:1098:LEU:O	3:D:1102:THR:HG23	2.15	0.47
2:C:676:ILE:O	3:D:948:THR:CG2	2.53	0.47
3:D:478:LEU:HD12	3:D:478:LEU:HA	1.80	0.47
3:D:705:ALA:HA	3:D:706:PRO:HA	1.59	0.47
3:D:1058:ARG:N	3:D:1069:GLU:OE2	2.48	0.47
5:F:234:LYS:HD2	5:F:236:SER:HB3	1.96	0.47
2:C:265:ARG:HG2	2:C:288:ARG:HD2	1.97	0.46
2:C:644:VAL:HG12	2:C:645:VAL:H	1.80	0.46
3:D:538:SER:OG	3:D:539:ASP:N	2.47	0.46
3:D:567:ILE:O	3:D:571:LYS:HG3	2.15	0.46
3:D:913:ASP:O	3:D:914:LEU:C	2.58	0.46
1:A:224:TYR:CD1	1:B:9:PRO:HG2	2.49	0.46
3:D:1232:PRO:HG2	3:D:1356:TYR:CE2	2.47	0.46
5:F:392:VAL:HG11	5:F:396:ARG:HH11	1.80	0.46
1:B:47:SER:O	1:B:148:VAL:HG11	2.16	0.46
2:C:910:LYS:C	2:C:912:PRO:HD2	2.40	0.46
3:D:134:VAL:HA	3:D:454:ALA:HA	1.97	0.46
3:D:505:SER:HB3	3:D:1453:ALA:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:643:GLY:N	3:D:727:GLN:O	2.46	0.46
3:D:654:LYS:CB	3:D:655:PRO:HD3	2.40	0.46
3:D:911:LEU:O	3:D:912:LYS:C	2.59	0.46
2:C:683:ASN:HB2	2:C:687:ALA:O	2.16	0.46
2:C:1008:ARG:NH1	2:C:1011:GLY:N	2.63	0.46
3:D:212:ARG:HD3	3:D:342:PRO:HB3	1.97	0.46
3:D:885:ILE:HG12	3:D:937:TYR:CE1	2.51	0.46
5:F:329:TYR:HE1	5:F:333:ILE:HD11	1.81	0.46
2:C:34:VAL:H	2:C:35:PRO:HD2	1.78	0.46
2:C:1014:SER:O	2:C:1018:GLN:HA	2.15	0.46
3:D:1378:TYR:CE2	3:D:1394:VAL:HG22	2.50	0.46
3:D:813:LEU:O	3:D:817:GLU:HG2	2.15	0.46
3:D:1222:GLY:O	3:D:1225:ALA:HB3	2.16	0.46
3:D:1366:LYS:O	3:D:1369:GLU:HB2	2.16	0.46
2:C:52:PHE:CD2	2:C:68:PHE:HB2	2.51	0.46
2:C:841:ASN:ND2	2:C:845:ASN:HB2	2.31	0.46
3:D:1411:GLY:O	3:D:1412:LYS:HB2	2.16	0.46
5:F:261:PRO:O	5:F:265:VAL:HG23	2.15	0.46
5:F:401:GLU:O	5:F:405:LEU:HB2	2.15	0.46
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.98	0.46
1:B:80:LEU:HD23	1:B:83:LYS:HD2	1.98	0.46
1:B:211:LEU:O	1:B:215:VAL:HG13	2.16	0.46
2:C:139:GLN:HG2	2:C:339:LEU:HD21	1.98	0.46
2:C:627:ARG:HA	2:C:638:ASP:HB2	1.97	0.46
2:C:684:PHE:HB3	3:D:633:VAL:HG21	1.97	0.46
2:C:710:ILE:HD11	2:C:758:ARG:CZ	2.46	0.46
2:C:771:GLU:HA	2:C:774:LEU:HB3	1.96	0.46
2:C:926:PHE:C	2:C:928:LYS:H	2.23	0.46
3:D:239:GLY:HA2	3:D:313:MET:HB3	1.98	0.46
3:D:575:GLN:NE2	11:D:1705:HOH:O	2.48	0.46
3:D:701:LEU:O	3:D:747:VAL:HG23	2.15	0.46
3:D:1436:SER:O	3:D:1438:ALA:N	2.49	0.46
5:F:299:TRP:CE3	5:F:303:ARG:HD3	2.51	0.46
5:F:394:ARG:HB3	5:F:395:GLU:H	1.61	0.46
1:A:24:VAL:HA	1:A:195:LEU:O	2.16	0.46
2:C:189:ARG:HD2	2:C:241:LEU:HD22	1.97	0.46
2:C:317:VAL:H	2:C:318:PRO:HD3	1.78	0.46
3:D:115:LEU:HD11	3:D:499:VAL:HG22	1.97	0.46
3:D:1042:ARG:HH12	3:D:1045:MET:HE1	1.81	0.46
3:D:1479:ASP:OD1	3:D:1479:ASP:N	2.49	0.46
1:A:41:ARG:HD2	1:A:177:VAL:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:560:MET:HB3	2:C:564:MET:HE2	1.98	0.46
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.97	0.46
3:D:539:ASP:CG	3:D:598:ARG:HH21	2.23	0.46
3:D:651:GLU:HA	3:D:651:GLU:OE1	2.15	0.46
3:D:786:ILE:O	3:D:787:LEU:C	2.58	0.46
3:D:1112:CYS:HB3	3:D:1201:CYS:HB3	1.58	0.46
3:D:1350:GLU:O	3:D:1352:ILE:N	2.49	0.46
5:F:123:ASP:OD2	5:F:123:ASP:N	2.48	0.46
1:A:25:LEU:HD23	1:A:28:LEU:HD11	1.98	0.45
1:B:212:ASN:O	1:B:215:VAL:HG22	2.16	0.45
2:C:62:GLY:HA2	2:C:103:LYS:HG2	1.98	0.45
2:C:126:SER:HB2	2:C:134:ARG:O	2.16	0.45
2:C:266:ARG:NH1	2:C:271:GLU:O	2.49	0.45
2:C:376:ARG:HH12	5:F:276:ARG:HG2	1.80	0.45
2:C:860:HIS:NE2	2:C:975:TYR:HB2	2.32	0.45
2:C:972:VAL:HG23	2:C:973:VAL:N	2.31	0.45
3:D:95:LEU:HA	3:D:551:ASN:HD21	1.81	0.45
3:D:237:LYS:HB2	3:D:240:GLU:HG3	1.98	0.45
3:D:297:ILE:HG23	3:D:298:VAL:HG23	1.98	0.45
1:A:20:TYR:CD1	1:A:21:GLY:N	2.85	0.45
1:B:58:ILE:HG21	1:B:61:VAL:HG12	1.99	0.45
2:C:385:PHE:HD2	2:C:386:PHE:CD1	2.34	0.45
3:D:8:VAL:CG1	3:D:1434:TRP:CZ2	2.96	0.45
3:D:539:ASP:HB3	3:D:600:LEU:HD22	1.97	0.45
3:D:1135:ARG:O	3:D:1136:LYS:C	2.58	0.45
3:D:1459:LEU:CA	3:D:1464:GLU:HG3	2.44	0.45
3:D:536:ALA:HA	5:F:315:VAL:O	2.16	0.45
3:D:675:ARG:HH12	5:F:423:ASP:HB2	1.80	0.45
3:D:1145:TYR:CD2	3:D:1168:MET:HE2	2.50	0.45
3:D:1194:CYS:SG	3:D:1200:VAL:HA	2.56	0.45
3:D:1350:GLU:O	3:D:1353:GLN:N	2.49	0.45
5:F:104:ARG:HG3	5:F:229:TYR:CZ	2.51	0.45
1:A:79:ILE:CG2	1:A:167:VAL:HG11	2.47	0.45
2:C:54:ILE:HG23	2:C:66:LEU:HB3	1.99	0.45
2:C:144:PRO:HB3	2:C:266:ARG:HB3	1.99	0.45
2:C:428:ARG:HH21	2:C:451:LEU:HD11	1.81	0.45
2:C:751:PRO:HA	2:C:792:VAL:CG1	2.46	0.45
3:D:131:LYS:HB3	3:D:152:LEU:HB2	1.99	0.45
3:D:729:HIS:CD2	3:D:730:PRO:CD	2.99	0.45
3:D:1397:LYS:C	3:D:1398:TRP:CE3	2.90	0.45
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:PRO:O	1:A:201:THR:HB	2.16	0.45
2:C:23:VAL:HG23	2:C:24:GLU:N	2.30	0.45
2:C:560:MET:O	2:C:564:MET:HG3	2.17	0.45
3:D:880:ILE:O	3:D:884:ARG:N	2.49	0.45
3:D:1217:ILE:HD12	3:D:1217:ILE:H	1.82	0.45
3:D:1394:VAL:HB	3:D:1397:LYS:HE2	1.97	0.45
1:B:57:TYR:HD1	1:B:161:ARG:HG3	1.82	0.45
2:C:72:ARG:O	2:C:95:TYR:N	2.40	0.45
2:C:305:PRO:HA	2:C:308:ARG:HD3	1.99	0.45
2:C:627:ARG:HA	2:C:627:ARG:HD3	1.85	0.45
3:D:95:LEU:HB2	3:D:515:GLU:O	2.17	0.45
3:D:270:LEU:HB3	3:D:284:LEU:HD11	1.99	0.45
3:D:368:VAL:HG23	3:D:377:VAL:HG11	1.98	0.45
3:D:643:GLY:O	3:D:726:ILE:HG23	2.17	0.45
3:D:1350:GLU:O	3:D:1351:GLU:C	2.60	0.45
3:D:1478:SER:O	3:D:1480:PHE:N	2.50	0.45
1:A:206:THR:HG22	1:A:208:LEU:N	2.30	0.45
2:C:694:LEU:O	2:C:699:PHE:HB2	2.17	0.45
2:C:1009:SER:O	3:D:624:ASP:O	2.34	0.45
3:D:134:VAL:HG12	3:D:135:LEU:N	2.32	0.45
3:D:659:LYS:HG3	3:D:663:GLU:OE2	2.16	0.45
3:D:662:GLU:OE1	3:D:670:VAL:HG23	2.16	0.45
3:D:959:GLU:HB3	3:D:963:TYR:CE2	2.51	0.45
3:D:1364:HIS:O	3:D:1365:ASP:C	2.60	0.45
1:A:55:SER:HB2	1:A:158:ILE:CG2	2.47	0.45
1:B:100:LEU:O	1:B:114:PHE:HA	2.17	0.45
2:C:846:LYS:CE	3:D:741:ASP:O	2.63	0.45
2:C:872:ASN:OD1	2:C:874:LEU:HG	2.17	0.45
3:D:542:ASP:O	3:D:546:ARG:HG2	2.17	0.45
5:F:107:GLU:HA	5:F:110:MET:HE3	1.98	0.45
2:C:551:GLU:HB3	2:C:906:PHE:CE2	2.52	0.45
3:D:95:LEU:HD21	3:D:517:VAL:CG2	2.46	0.45
3:D:783:ARG:HB3	3:D:784:ASP:H	1.42	0.45
3:D:864:VAL:HG13	3:D:865:THR:N	2.32	0.45
3:D:1208:ASP:O	3:D:1209:LEU:CB	2.60	0.45
3:D:1481:VAL:HG13	4:E:18:ARG:HG3	1.99	0.45
3:D:1484:THR:HG21	4:E:18:ARG:HG2	1.98	0.45
1:A:28:LEU:O	1:A:193:ASP:N	2.50	0.45
1:B:19:GLU:O	1:B:200:TRP:HA	2.17	0.45
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.99	0.45
2:C:668:LEU:HD23	2:C:668:LEU:HA	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:848:VAL:HG12	3:D:632:VAL:HG23	1.99	0.45
3:D:116:LEU:HD21	3:D:465:LEU:HD23	1.99	0.45
3:D:411:THR:O	5:F:178:ARG:HD2	2.17	0.45
3:D:539:ASP:N	3:D:539:ASP:OD1	2.50	0.45
3:D:1023:MET:HA	3:D:1028:ALA:HB3	1.97	0.45
3:D:1079:LYS:C	3:D:1081:GLY:H	2.25	0.45
5:F:79:ASP:O	5:F:80:PRO:C	2.59	0.45
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.97	0.44
1:B:38:ASN:HB2	1:B:39:PRO:HD3	1.98	0.44
2:C:154:ARG:HE	2:C:156:GLY:HA3	1.82	0.44
2:C:265:ARG:H	2:C:265:ARG:HG3	1.64	0.44
2:C:713:ARG:HB2	2:C:713:ARG:NH1	2.32	0.44
3:D:675:ARG:NH2	5:F:420:ASP:O	2.50	0.44
3:D:1305:LEU:HA	3:D:1306:PRO:HD2	1.79	0.44
2:C:435:TYR:HA	3:D:1071:PHE:CE2	2.49	0.44
2:C:860:HIS:HA	2:C:866:PRO:HA	1.98	0.44
2:C:915:LYS:O	2:C:968:LEU:HD22	2.17	0.44
3:D:171:LEU:HD21	3:D:192:ALA:HB1	2.00	0.44
4:E:11:GLY:HA3	11:E:103:HOH:O	2.18	0.44
1:A:70:GLY:CA	1:A:133:GLU:HG2	2.47	0.44
2:C:266:ARG:HD2	2:C:273:GLY:HA3	1.99	0.44
2:C:833:LEU:HA	2:C:837:ASP:OD2	2.17	0.44
3:D:1378:TYR:O	3:D:1420:LEU:HB2	2.17	0.44
1:A:40:LEU:HD23	1:A:43:ILE:HD12	2.00	0.44
2:C:283:ILE:HG22	2:C:284:ARG:HG2	1.98	0.44
2:C:397:GLU:HG3	2:C:631:SER:HB2	1.97	0.44
2:C:971:LYS:HA	2:C:988:VAL:CA	2.43	0.44
3:D:191:LEU:HD12	3:D:195:VAL:HB	1.99	0.44
3:D:523:ASP:O	3:D:526:PRO:HD3	2.17	0.44
3:D:643:GLY:O	3:D:726:ILE:HA	2.18	0.44
5:F:362:SER:C	5:F:364:ARG:H	2.25	0.44
2:C:468:ARG:HE	2:C:487:THR:CG2	2.29	0.44
3:D:1196:THR:HB	3:D:1199:GLY:C	2.42	0.44
3:D:1213:ARG:HB2	3:D:1214:PRO:HD2	1.99	0.44
1:A:225:PHE:CD2	1:B:11:PHE:HE1	2.35	0.44
1:B:23:PHE:CE1	1:B:199:ILE:HD12	2.52	0.44
1:B:167:VAL:CG1	1:B:168:ASP:H	2.23	0.44
2:C:527:GLU:CD	2:C:527:GLU:H	2.25	0.44
2:C:691:SER:O	2:C:692:GLU:C	2.61	0.44
3:D:186:VAL:O	3:D:189:GLN:HB2	2.16	0.44
3:D:659:LYS:O	3:D:662:GLU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:808:THR:O	3:D:809:PRO:C	2.60	0.44
3:D:937:TYR:O	3:D:938:GLY:C	2.60	0.44
3:D:1472:ILE:HG23	3:D:1474:ALA:H	1.83	0.44
1:A:215:VAL:HG13	1:B:222:LEU:HD22	1.99	0.44
1:A:226:SER:O	1:A:227:ASN:HB3	2.18	0.44
2:C:599:GLU:HG3	2:C:600:ASP:H	1.82	0.44
3:D:493:ARG:NH2	3:D:494:LYS:HZ3	2.16	0.44
3:D:787:LEU:HD13	3:D:1023:MET:HG2	2.00	0.44
3:D:1140:ILE:C	3:D:1142:ALA:N	2.73	0.44
3:D:1478:SER:C	3:D:1480:PHE:N	2.76	0.44
2:C:13:ILE:HD12	2:C:14:PRO:CD	2.42	0.44
2:C:292:ARG:HD3	2:C:299:LYS:HB3	1.99	0.44
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.99	0.44
3:D:834:THR:HA	3:D:838:ARG:HE	1.83	0.44
4:E:85:LEU:C	4:E:87:LYS:H	2.26	0.44
2:C:315:ALA:O	2:C:316:GLY:C	2.61	0.44
2:C:605:LYS:O	2:C:611:ILE:HG23	2.18	0.44
2:C:721:ARG:O	2:C:758:ARG:HG3	2.18	0.44
3:D:16:GLU:O	3:D:20:SER:N	2.51	0.44
3:D:152:LEU:HD23	3:D:152:LEU:N	2.25	0.44
3:D:496:LEU:HD11	3:D:500:ARG:HH12	1.83	0.44
3:D:947:ILE:O	3:D:948:THR:HG23	2.17	0.44
2:C:69:LEU:HD13	2:C:97:ARG:HB3	2.00	0.43
2:C:393:GLN:HG3	2:C:406:HIS:HE2	1.82	0.43
3:D:493:ARG:NH1	3:D:1389:LEU:HB3	2.33	0.43
3:D:631:ILE:HG12	3:D:743:ASP:O	2.17	0.43
3:D:739:ASP:OD1	3:D:739:ASP:C	2.61	0.43
3:D:786:ILE:HG21	3:D:1026:SER:O	2.18	0.43
3:D:1081:GLY:C	3:D:1083:ASP:H	2.26	0.43
3:D:1104:GLU:HA	3:D:1461:GLY:HA2	1.99	0.43
5:F:91:VAL:HA	5:F:92:PRO:HD3	1.80	0.43
5:F:132:ARG:HH21	5:F:184:ARG:NE	2.16	0.43
5:F:346:THR:C	5:F:348:SER:H	2.25	0.43
2:C:159:ILE:HG23	2:C:175:GLU:HB2	1.99	0.43
2:C:540:PHE:CE1	2:C:906:PHE:HE1	2.36	0.43
3:D:885:ILE:HG21	3:D:937:TYR:CD1	2.40	0.43
3:D:1105:ILE:HD11	3:D:1374:GLN:CD	2.43	0.43
3:D:1481:VAL:HG13	4:E:18:ARG:HA	1.99	0.43
5:F:79:ASP:N	5:F:80:PRO:CD	2.82	0.43
5:F:379:ARG:HD2	5:F:383:LEU:HB2	2.00	0.43
1:B:44:LEU:HA	1:B:48:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:728:HIS:CG	2:C:729:LEU:N	2.85	0.43
3:D:841:TYR:HB2	3:D:864:VAL:HG22	2.00	0.43
1:A:83:LYS:HE3	1:A:168:ASP:O	2.18	0.43
1:A:87:VAL:HG21	1:A:144:VAL:HG11	2.01	0.43
2:C:713:ARG:HA	2:C:819:VAL:HA	2.00	0.43
3:D:493:ARG:NH1	3:D:1390:LEU:H	2.01	0.43
3:D:653:PHE:O	3:D:654:LYS:C	2.60	0.43
3:D:752:SER:C	3:D:754:PHE:H	2.27	0.43
1:A:158:ILE:H	1:A:159:LYS:HZ3	1.65	0.43
4:E:9:LEU:O	4:E:19:LEU:HD13	2.19	0.43
1:B:112:ARG:NH1	1:B:112:ARG:HB3	2.33	0.43
2:C:537:LYS:O	2:C:539:VAL:N	2.51	0.43
2:C:690:ILE:HD13	2:C:690:ILE:HA	1.72	0.43
3:D:114:THR:HG21	3:D:498:VAL:HG21	2.00	0.43
3:D:752:SER:C	3:D:754:PHE:N	2.76	0.43
3:D:986:ARG:HG3	3:D:990:ASP:OD1	2.18	0.43
3:D:1190:SER:OG	3:D:1191:PRO:CD	2.66	0.43
3:D:1376:MET:HE2	3:D:1420:LEU:O	2.18	0.43
3:D:1400:VAL:HG12	3:D:1404:ASN:ND2	2.32	0.43
5:F:201:LYS:HA	5:F:201:LYS:HD2	1.86	0.43
1:A:51:THR:HG22	1:A:146:ARG:HA	2.01	0.43
1:A:73:GLU:CB	1:A:78:ILE:HG12	2.48	0.43
2:C:52:PHE:HD2	2:C:68:PHE:HB2	1.84	0.43
2:C:141:HIS:HE1	2:C:332:ARG:HH12	1.65	0.43
2:C:274:ARG:HA	2:C:277:ALA:HB3	2.01	0.43
2:C:724:ARG:HE	2:C:738:ASP:CA	2.19	0.43
3:D:836:VAL:N	3:D:837:GLY:CA	2.73	0.43
3:D:1022:VAL:O	3:D:1023:MET:C	2.62	0.43
3:D:1219:GLU:O	3:D:1221:VAL:N	2.49	0.43
1:A:149:GLY:O	1:A:171:PHE:HB2	2.19	0.43
2:C:195:LEU:HB3	2:C:238:LEU:CD2	2.49	0.43
2:C:260:LEU:O	2:C:261:ILE:C	2.62	0.43
2:C:589:ARG:NH2	2:C:596:TYR:CD2	2.87	0.43
2:C:751:PRO:HB2	3:D:680:GLN:HG3	2.00	0.43
2:C:1038:TRP:O	2:C:1039:ALA:C	2.61	0.43
3:D:14:SER:O	3:D:15:PRO:C	2.62	0.43
3:D:566:ILE:O	3:D:566:ILE:HG13	2.16	0.43
3:D:948:THR:O	3:D:949:ILE:HG13	2.19	0.43
3:D:1376:MET:HE3	3:D:1421:LEU:CD1	2.45	0.43
4:E:82:GLU:C	4:E:84:ARG:H	2.25	0.43
5:F:222:ARG:HG2	5:F:242:TRP:CE3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:266:ARG:H	2:C:266:ARG:NE	2.16	0.43
2:C:683:ASN:HA	2:C:687:ALA:HB3	2.00	0.43
2:C:997:LEU:HD23	2:C:997:LEU:HA	1.77	0.43
3:D:126:VAL:HG21	3:D:461:ILE:HD11	2.01	0.43
3:D:372:ASP:O	3:D:374:GLU:N	2.52	0.43
3:D:882:PHE:C	3:D:884:ARG:N	2.77	0.43
3:D:1107:VAL:HA	3:D:1200:VAL:O	2.18	0.43
1:A:68:ILE:HA	1:A:69:PRO:HD2	1.83	0.43
2:C:437:ARG:NH2	2:C:487:THR:O	2.52	0.43
2:C:1095:LEU:HD13	3:D:103:TRP:CH2	2.53	0.43
3:D:117:ASP:HB2	3:D:495:ARG:NH1	2.26	0.43
3:D:272:LEU:HG	3:D:282:TYR:CE1	2.52	0.43
3:D:880:ILE:O	3:D:881:LEU:C	2.62	0.43
3:D:953:ASP:HB3	3:D:1019:PRO:HG2	2.01	0.43
3:D:969:ARG:HA	3:D:972:LEU:HD23	2.00	0.43
3:D:1042:ARG:HD3	3:D:1057:VAL:HG11	2.01	0.43
3:D:1398:TRP:HE1	3:D:1417:TRP:CD1	2.37	0.43
5:F:320:PRO:HA	5:F:328:PHE:HA	2.00	0.43
5:F:397:ILE:HA	5:F:400:ILE:HB	1.99	0.43
1:A:49:PRO:HB3	1:A:148:VAL:HG22	2.00	0.42
1:A:177:VAL:HG12	1:A:177:VAL:O	2.19	0.42
1:B:58:ILE:HD13	1:B:59:GLU:N	2.33	0.42
1:B:176:ARG:HB3	1:B:200:TRP:CE3	2.54	0.42
2:C:1008:ARG:HH11	2:C:1011:GLY:N	2.17	0.42
3:D:116:LEU:HB3	3:D:118:LEU:HD12	2.01	0.42
3:D:806:PHE:H	3:D:829:VAL:HG12	1.84	0.42
5:F:95:THR:C	5:F:97:GLU:H	2.26	0.42
5:F:354:LEU:C	5:F:356:LYS:H	2.27	0.42
1:A:58:ILE:HB	1:A:61:VAL:CG2	2.48	0.42
2:C:231:PRO:HA	2:C:234:ALA:HB3	2.01	0.42
2:C:317:VAL:N	2:C:318:PRO:CD	2.82	0.42
2:C:341:THR:HG22	2:C:345:ARG:HE	1.84	0.42
2:C:414:GLY:HA3	2:C:415:PRO:HD3	1.86	0.42
3:D:272:LEU:HB3	3:D:274:ARG:NH1	2.34	0.42
3:D:594:PRO:HB2	3:D:595:GLY:H	1.63	0.42
3:D:1375:MET:HE2	3:D:1424:VAL:HG13	2.01	0.42
1:A:80:LEU:HD23	1:A:83:LYS:HG3	2.01	0.42
2:C:121:MET:HG3	2:C:127:PHE:CE1	2.54	0.42
2:C:360:LEU:HG	2:C:361:MET:H	1.83	0.42
2:C:569:VAL:HA	2:C:570:PRO:HD2	1.87	0.42
2:C:724:ARG:HB2	2:C:741:GLY:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:207:PHE:HB2	3:D:391:ALA:HB3	2.01	0.42
3:D:244:GLU:O	3:D:245:LEU:C	2.62	0.42
3:D:1087:ARG:HB3	3:D:1091:SER:HB2	2.01	0.42
3:D:1341:PRO:O	3:D:1344:VAL:HG12	2.19	0.42
4:E:31:LEU:HD12	4:E:60:ALA:HB2	2.00	0.42
1:A:40:LEU:O	1:A:44:LEU:HB2	2.19	0.42
1:B:216:GLU:OE2	1:B:220:GLU:HB2	2.19	0.42
2:C:575:GLN:HE21	2:C:670:GLN:HA	1.85	0.42
3:D:650:LEU:HB2	3:D:691:LEU:HD22	2.02	0.42
3:D:996:TRP:HA	3:D:999:THR:HB	2.02	0.42
3:D:1486:VAL:HG11	4:E:26:ARG:HB2	2.01	0.42
1:B:104:GLU:HA	1:B:132:LEU:HD22	2.01	0.42
2:C:182:VAL:HG13	2:C:220:GLY:HA3	2.01	0.42
2:C:263:ASP:N	2:C:264:PRO:CD	2.62	0.42
2:C:964:LYS:O	2:C:968:LEU:HG	2.19	0.42
2:C:1037:VAL:O	2:C:1041:GLU:HG3	2.19	0.42
3:D:256:GLU:OE1	3:D:302:GLN:HB3	2.19	0.42
3:D:835:SER:HB2	3:D:838:ARG:HG3	2.02	0.42
3:D:938:GLY:O	3:D:939:PHE:O	2.37	0.42
3:D:1119:SER:HA	3:D:1186:VAL:O	2.20	0.42
3:D:1314:LYS:HB3	3:D:1314:LYS:HE2	1.88	0.42
3:D:1350:GLU:C	3:D:1352:ILE:N	2.75	0.42
4:E:25:LYS:O	4:E:28:GLN:HB2	2.19	0.42
2:C:136:ILE:HB	2:C:336:VAL:HG22	2.02	0.42
3:D:16:GLU:CD	3:D:16:GLU:H	2.27	0.42
3:D:948:THR:HB	3:D:949:ILE:H	1.49	0.42
3:D:1348:LEU:O	3:D:1349:VAL:C	2.62	0.42
3:D:1378:TYR:HD2	3:D:1394:VAL:HA	1.85	0.42
1:A:41:ARG:NH1	1:A:45:LEU:HD11	2.35	0.42
2:C:472:ARG:HA	2:C:483:VAL:HA	2.02	0.42
2:C:1054:THR:HB	2:C:1059:ASP:HB2	2.02	0.42
3:D:46:ASP:CG	3:D:48:ARG:HB2	2.45	0.42
3:D:374:GLU:HG3	3:D:375:GLU:N	2.34	0.42
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.72	0.42
1:B:144:VAL:HG12	1:B:145:ASP:H	1.84	0.42
2:C:139:GLN:O	2:C:333:ILE:HA	2.20	0.42
2:C:173:ASP:HB2	2:C:185:LYS:HB3	2.01	0.42
2:C:589:ARG:HA	2:C:596:TYR:CE1	2.53	0.42
3:D:567:ILE:HG22	3:D:571:LYS:NZ	2.35	0.42
1:A:34:VAL:HA	1:A:179:PHE:HE1	1.84	0.42
1:A:171:PHE:O	1:A:172:SER:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:PHE:CD2	1:B:11:PHE:CE1	3.06	0.42
1:B:37:GLY:HA3	1:B:179:PHE:CE1	2.55	0.42
2:C:15:LEU:HD12	2:C:15:LEU:N	2.30	0.42
2:C:297:GLU:HB3	2:C:298:PHE:H	1.68	0.42
2:C:540:PHE:HE1	2:C:906:PHE:HE1	1.68	0.42
5:F:95:THR:C	5:F:97:GLU:N	2.78	0.42
5:F:125:ASP:HA	5:F:128:ARG:NH2	2.35	0.42
2:C:260:LEU:HD12	2:C:288:ARG:HG2	2.02	0.42
2:C:1052:MET:HE2	2:C:1052:MET:HB2	1.85	0.42
3:D:226:PRO:HA	3:D:330:THR:HG22	2.02	0.42
3:D:714:GLN:HE21	3:D:765:SER:CB	2.32	0.42
5:F:238:TYR:CD2	5:F:238:TYR:C	2.98	0.42
5:F:369:LEU:O	5:F:374:GLY:N	2.50	0.42
1:A:132:LEU:HD11	1:A:138:LEU:HB3	2.02	0.41
2:C:309:TYR:HE1	2:C:319:GLY:HA3	1.85	0.41
2:C:700:TYR:HB3	2:C:833:LEU:HD13	2.01	0.41
2:C:1009:SER:N	3:D:651:GLU:HG3	2.35	0.41
3:D:116:LEU:O	3:D:117:ASP:C	2.62	0.41
3:D:700:VAL:HG13	3:D:718:PRO:HG3	2.01	0.41
3:D:835:SER:O	3:D:836:VAL:HG23	2.20	0.41
3:D:1161:GLU:OE2	3:D:1164:ARG:HG3	2.18	0.41
3:D:1242:HIS:CE1	3:D:1245:GLY:HA3	2.55	0.41
5:F:386:VAL:C	5:F:388:ALA:H	2.27	0.41
5:F:397:ILE:C	5:F:399:GLN:H	2.27	0.41
1:A:37:GLY:HA3	1:A:195:LEU:HD11	2.01	0.41
1:B:38:ASN:O	1:B:42:ARG:HG2	2.21	0.41
2:C:408:ARG:NH2	2:C:455:LEU:HD23	2.35	0.41
2:C:683:ASN:C	2:C:683:ASN:HD22	2.28	0.41
2:C:1107:ASN:HA	2:C:1108:PRO:HD2	1.91	0.41
3:D:463:GLN:NE2	3:D:467:GLU:HG3	2.34	0.41
3:D:662:GLU:OE2	3:D:669:ASN:HA	2.20	0.41
3:D:760:ARG:NH2	4:E:62:THR:OG1	2.53	0.41
3:D:916:TYR:O	3:D:919:PHE:HB3	2.20	0.41
3:D:1046:GLN:HA	3:D:1052:THR:HA	2.01	0.41
3:D:1459:LEU:HD11	3:D:1468:LEU:HD13	2.02	0.41
4:E:30:LEU:HD21	4:E:63:TRP:HB3	2.02	0.41
1:B:12:THR:HB	1:B:24:VAL:HB	2.01	0.41
2:C:121:MET:HG3	2:C:127:PHE:CZ	2.55	0.41
2:C:707:ARG:HD2	2:C:824:ARG:NH1	2.35	0.41
2:C:850:ALA:CA	3:D:632:VAL:HG22	2.48	0.41
2:C:1032:PHE:CD1	2:C:1052:MET:HG2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1040:LEU:HA	2:C:1043:TYR:HB2	2.01	0.41
3:D:539:ASP:HB3	3:D:600:LEU:HB3	2.02	0.41
3:D:1377:LYS:HD2	3:D:1378:TYR:HE2	1.78	0.41
5:F:88:ILE:HD13	5:F:88:ILE:HA	1.70	0.41
5:F:291:ILE:HG23	5:F:304:VAL:HG21	2.02	0.41
1:A:11:PHE:HA	1:A:25:LEU:HD12	2.01	0.41
2:C:1060:ILE:O	2:C:1064:ASN:ND2	2.53	0.41
3:D:539:ASP:CG	3:D:598:ARG:NH2	2.78	0.41
3:D:727:GLN:HB2	3:D:727:GLN:HE21	1.54	0.41
3:D:756:GLN:HE21	3:D:756:GLN:HB3	1.68	0.41
3:D:1225:ALA:HA	3:D:1367:HIS:ND1	2.34	0.41
3:D:1254:GLN:O	3:D:1257:PRO:HG2	2.19	0.41
1:B:64:GLU:HB2	1:B:75:VAL:HG11	2.02	0.41
2:C:284:ARG:HA	2:C:284:ARG:HH11	1.85	0.41
2:C:338:GLU:HG2	2:C:342:ASP:OD2	2.21	0.41
2:C:439:CYS:HB2	2:C:541:SER:H	1.85	0.41
2:C:842:ARG:NH2	2:C:887:GLU:OE2	2.52	0.41
2:C:1059:ASP:OD1	2:C:1062:GLY:CA	2.68	0.41
3:D:108:VAL:HA	3:D:110:SER:N	2.35	0.41
3:D:653:PHE:N	3:D:653:PHE:CD1	2.89	0.41
3:D:1431:THR:HG21	11:D:1713:HOH:O	2.20	0.41
2:C:264:PRO:HB2	2:C:289:THR:HG21	2.02	0.41
2:C:529:VAL:C	2:C:530:GLU:HG3	2.46	0.41
2:C:535:SER:C	2:C:537:LYS:N	2.76	0.41
2:C:839:LEU:HA	2:C:839:LEU:HD23	1.62	0.41
3:D:53:ILE:HG22	3:D:54:LYS:HG3	2.02	0.41
3:D:226:PRO:HG3	3:D:249:TYR:HB2	2.02	0.41
3:D:257:GLY:H	3:D:272:LEU:HD22	1.85	0.41
3:D:304:LEU:O	3:D:305:ALA:HB3	2.21	0.41
3:D:387:LEU:H	3:D:387:LEU:HD12	1.86	0.41
3:D:392:SER:C	3:D:393:ILE:HG13	2.45	0.41
3:D:473:LEU:HD11	3:D:495:ARG:HH21	1.85	0.41
3:D:772:PRO:O	3:D:1209:LEU:HD23	2.21	0.41
3:D:984:THR:HG23	3:D:987:GLU:H	1.86	0.41
3:D:1031:ASN:HB2	3:D:1032:PRO:HD2	2.00	0.41
3:D:1383:ASP:HA	3:D:1384:PRO:HD3	1.90	0.41
4:E:81:PRO:HB2	4:E:84:ARG:HB2	2.02	0.41
5:F:208:SER:HB3	5:F:211:ASP:HB2	2.01	0.41
1:A:101:LEU:HB3	1:A:140:MET:HG2	2.02	0.41
2:C:405:ARG:HB2	2:C:543:ASN:HD21	1.85	0.41
2:C:471:TYR:CE2	2:C:496:ILE:HG21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:949:LYS:HD2	3:D:796:ARG:HH21	1.81	0.41
3:D:211:VAL:HG12	3:D:387:LEU:HA	2.02	0.41
3:D:1364:HIS:ND1	3:D:1366:LYS:HG2	2.35	0.41
2:C:418:LEU:O	2:C:420:ARG:N	2.48	0.41
2:C:776:SER:CA	2:C:780:GLU:HB2	2.44	0.41
3:D:356:PRO:HB2	3:D:359:ALA:HB2	2.02	0.41
2:C:95:TYR:CG	2:C:114:PHE:HB3	2.56	0.41
2:C:276:LYS:C	2:C:278:GLU:H	2.29	0.41
2:C:1056:LYS:HB3	3:D:624:ASP:H	1.86	0.41
2:C:1059:ASP:O	2:C:1060:ILE:C	2.62	0.41
3:D:693:GLU:HA	4:E:48:MET:HE1	2.03	0.41
3:D:731:LEU:HA	3:D:731:LEU:HD23	1.91	0.41
3:D:1066:THR:C	3:D:1068:LEU:N	2.78	0.41
3:D:1161:GLU:O	3:D:1162:GLU:C	2.64	0.41
3:D:1459:LEU:HD22	3:D:1464:GLU:HB2	2.03	0.41
3:D:1495:ILE:O	3:D:1499:ARG:HB2	2.21	0.41
1:A:115:LEU:HA	1:A:116:PRO:HD2	1.84	0.41
2:C:137:VAL:O	2:C:391:LEU:HG	2.21	0.41
2:C:286:SER:OG	2:C:301:GLU:HB2	2.21	0.41
2:C:421:GLU:O	2:C:423:ALA:N	2.49	0.41
2:C:1095:LEU:HD12	3:D:607:LEU:HD12	2.03	0.41
3:D:177:ALA:O	3:D:178:LEU:HB2	2.20	0.41
3:D:1264:GLU:CB	3:D:1266:ARG:HH21	2.33	0.41
2:C:154:ARG:NE	2:C:157:ARG:H	2.18	0.40
2:C:486:MET:HE3	2:C:491:GLU:HA	2.03	0.40
3:D:368:VAL:HB	3:D:377:VAL:HG21	2.02	0.40
3:D:912:LYS:HB3	3:D:912:LYS:HE2	1.73	0.40
3:D:1267:ARG:HD2	3:D:1271:LYS:NZ	2.36	0.40
1:A:23:PHE:CD2	1:A:211:LEU:HD23	2.57	0.40
1:A:63:HIS:CE1	2:C:801:VAL:HG12	2.56	0.40
1:A:158:ILE:H	1:A:159:LYS:NZ	2.18	0.40
1:B:74:ASP:OD2	1:B:75:VAL:N	2.54	0.40
2:C:1040:LEU:HD23	3:D:763:MET:HE1	2.02	0.40
2:C:1059:ASP:OD2	2:C:1080:SER:N	2.54	0.40
3:D:217:LYS:HD2	3:D:339:TRP:CZ2	2.55	0.40
3:D:935:LYS:HB3	3:D:935:LYS:HE2	1.76	0.40
3:D:1271:LYS:HD2	3:D:1334:GLN:OE1	2.21	0.40
3:D:1413:THR:HA	3:D:1414:PRO:HD3	1.79	0.40
3:D:1440:PHE:HE2	3:D:1463:LYS:NZ	2.15	0.40
5:F:88:ILE:HG23	5:F:193:ARG:HG2	2.03	0.40
6:Z:30:UNK:HA	6:Z:31:UNK:HA	1.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ASN:HA	1:B:92:PRO:HD3	1.85	0.40
2:C:224:GLU:HB3	2:C:227:PHE:HB2	2.04	0.40
3:D:410:SER:OG	3:D:411:THR:N	2.55	0.40
3:D:450:TYR:HB2	3:D:452:ILE:HD11	2.03	0.40
3:D:774:SER:HB3	3:D:1362:LYS:O	2.21	0.40
3:D:1103:HIS:CE1	3:D:1463:LYS:HB2	2.56	0.40
3:D:1141:GLU:HA	3:D:1171:VAL:HG11	2.02	0.40
1:A:7:LYS:HE2	1:A:7:LYS:HB3	1.98	0.40
1:A:101:LEU:HD21	1:A:109:VAL:CG1	2.52	0.40
1:A:115:LEU:HD13	1:A:116:PRO:HD2	2.04	0.40
1:B:213:GLN:O	1:B:217:ILE:HG13	2.21	0.40
2:C:271:GLU:O	2:C:273:GLY:N	2.54	0.40
2:C:948:GLU:HB3	2:C:953:VAL:HG23	2.02	0.40
3:D:206:ARG:H	3:D:390:PRO:HB3	1.86	0.40
3:D:879:ARG:HB3	3:D:902:LEU:HD12	2.03	0.40
3:D:906:GLN:HA	3:D:910:SER:OG	2.22	0.40
2:C:807:ARG:HA	2:C:821:GLU:CB	2.51	0.40
3:D:341:GLU:HA	3:D:342:PRO:HD3	1.88	0.40
3:D:1011:PHE:O	3:D:1016:PRO:HA	2.21	0.40
3:D:1037:GLN:HG2	3:D:1042:ARG:HA	2.03	0.40
3:D:1066:THR:HB	3:D:1069:GLU:HB2	2.04	0.40
3:D:1071:PHE:O	3:D:1072:ILE:C	2.64	0.40
3:D:1255:GLY:O	3:D:1258:ARG:N	2.51	0.40
3:D:1365:ASP:HA	3:D:1368:ILE:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	229/315 (73%)	175 (76%)	40 (18%)	14 (6%)	1 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	236/315 (75%)	186 (79%)	45 (19%)	5 (2%)	5	13
2	C	1117/1119 (100%)	877 (78%)	187 (17%)	53 (5%)	2	3
3	D	1502/1524 (99%)	1160 (77%)	260 (17%)	82 (6%)	1	2
4	E	93/99 (94%)	76 (82%)	14 (15%)	3 (3%)	3	7
5	F	349/423 (82%)	286 (82%)	54 (16%)	9 (3%)	4	10
All	All	3526/3795 (93%)	2760 (78%)	600 (17%)	166 (5%)	2	3

All (166) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	GLN
2	C	42	VAL
2	C	263	ASP
2	C	272	ALA
2	C	738	ASP
2	C	739	GLU
2	C	1115	LEU
3	D	137	PRO
3	D	587	ARG
3	D	593	ASN
3	D	594	PRO
3	D	809	PRO
3	D	939	PHE
3	D	940	THR
3	D	1128	VAL
3	D	1386	ASP
3	D	1391	GLU
3	D	1437	ALA
3	D	1441	GLN
3	D	1482	ARG
4	E	82	GLU
1	A	14	ARG
1	A	105	GLY
1	A	153	ALA
1	A	158	ILE
1	A	159	LYS
1	B	233	VAL
2	C	60	GLY
2	C	80	GLN
2	C	105	THR

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Mol	Chain	Res	Type
2	C	223	ASP
2	C	262	ALA
2	C	316	GLY
2	C	369	PRO
2	C	419	THR
2	C	1016	ILE
3	D	110	SER
3	D	178	LEU
3	D	192	ALA
3	D	196	VAL
3	D	409	VAL
3	D	525	ARG
3	D	549	ASN
3	D	595	GLY
3	D	822	ALA
3	D	823	LEU
3	D	830	ALA
3	D	918	ALA
3	D	949	ILE
3	D	1209	LEU
3	D	1220	ALA
3	D	1266	ARG
3	D	1297	GLU
3	D	1341	PRO
3	D	1412	LYS
3	D	1444	THR
5	F	141	VAL
5	F	153	PRO
1	A	38	ASN
1	B	125	PRO
1	B	158	ILE
2	C	208	ALA
2	C	288	ARG
2	C	422	ARG
2	C	541	SER
2	C	626	ARG
2	C	728	HIS
2	C	876	VAL
2	C	908	GLY
2	C	1042	ALA
2	C	1108	PRO
2	C	1113	GLU

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Mol	Chain	Res	Type
3	D	82	LYS
3	D	119	SER
3	D	230	TRP
3	D	287	GLY
3	D	483	HIS
3	D	603	LEU
3	D	652	LEU
3	D	835	SER
3	D	1166	LEU
3	D	1245	GLY
3	D	1269	LYS
3	D	1348	LEU
3	D	1389	LEU
3	D	1390	LEU
3	D	1442	ASN
5	F	255	ALA
1	A	59	GLU
1	A	160	ASP
2	C	31	GLN
2	C	261	ILE
2	C	482	GLU
2	C	638	ASP
2	C	735	ARG
2	C	880	MET
2	C	1079	PRO
3	D	117	ASP
3	D	248	PRO
3	D	255	GLU
3	D	316	GLN
3	D	373	PRO
3	D	437	VAL
3	D	509	PRO
3	D	601	ARG
3	D	654	LYS
3	D	801	GLY
3	D	836	VAL
3	D	1040	GLY
3	D	1238	MET
3	D	1248	GLY
3	D	1349	VAL
5	F	394	ARG
1	A	227	ASN

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Mol	Chain	Res	Type
2	C	36	PRO
2	C	37	GLU
2	C	99	GLN
2	C	111	ASP
2	C	195	LEU
2	C	820	ARG
2	C	835	VAL
2	C	907	ASP
2	C	945	ARG
3	D	245	LEU
3	D	303	PRO
3	D	440	VAL
3	D	485	SER
3	D	869	MET
3	D	883	ALA
3	D	1365	ASP
3	D	1408	ILE
4	E	86	GLN
5	F	389	PHE
5	F	395	GLU
1	A	4	SER
1	A	228	PRO
1	B	49	PRO
2	C	289	THR
2	C	570	PRO
2	C	784	ASP
2	C	796	GLU
2	C	808	ARG
3	D	227	LEU
3	D	305	ALA
3	D	1023	MET
3	D	1072	ILE
3	D	1125	PRO
3	D	1410	GLU
4	E	39	VAL
5	F	80	PRO
5	F	152	ASP
1	A	17	GLY
2	C	427	VAL
3	D	328	GLY
3	D	457	GLY
3	D	530	VAL

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Mol	Chain	Res	Type
3	D	1067	VAL
1	A	157	GLY
2	C	318	PRO
2	C	924	VAL
2	C	1020	PRO
2	C	226	VAL
1	B	120	VAL
2	C	155	PRO
3	D	612	GLY
5	F	314	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/273 (74%)	159 (79%)	43 (21%)	1	3
1	B	206/273 (76%)	179 (87%)	27 (13%)	4	9
2	C	941/941 (100%)	802 (85%)	139 (15%)	3	7
3	D	1264/1279 (99%)	1082 (86%)	182 (14%)	3	7
4	E	83/87 (95%)	73 (88%)	10 (12%)	5	12
5	F	306/370 (83%)	280 (92%)	26 (8%)	10	24
All	All	3002/3223 (93%)	2575 (86%)	427 (14%)	3	7

All (427) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	12	THR
1	A	15	THR
1	A	19	GLU
1	A	24	VAL
1	A	25	LEU
1	A	26	GLU
1	A	34	VAL

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Mol	Chain	Res	Type
1	A	43	ILE
1	A	44	LEU
1	A	45	LEU
1	A	61	VAL
1	A	62	LEU
1	A	86	VAL
1	A	87	VAL
1	A	88	ARG
1	A	90	LEU
1	A	94	LEU
1	A	96	THR
1	A	100	LEU
1	A	112	ARG
1	A	115	LEU
1	A	127	LEU
1	A	131	THR
1	A	132	LEU
1	A	134	GLU
1	A	138	LEU
1	A	142	VAL
1	A	148	VAL
1	A	154	GLU
1	A	158	ILE
1	A	159	LYS
1	A	167	VAL
1	A	170	VAL
1	A	182	GLU
1	A	184	THR
1	A	196	THR
1	A	197	LEU
1	A	200	TRP
1	A	202	ASP
1	A	205	VAL
1	A	221	HIS
1	A	224	TYR
1	B	5	LYS
1	B	10	VAL
1	B	22	GLU
1	B	30	ARG
1	B	40	LEU
1	B	42	ARG
1	B	54	THR

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Mol	Chain	Res	Type
1	B	58	ILE
1	B	60	ASP
1	B	61	VAL
1	B	64	GLU
1	B	73	GLU
1	B	87	VAL
1	B	100	LEU
1	B	104	GLU
1	B	138	LEU
1	B	140	MET
1	B	165	ILE
1	B	176	ARG
1	B	180	GLN
1	B	181	VAL
1	B	183	ASP
1	B	184	THR
1	B	197	LEU
1	B	208	LEU
1	B	215	VAL
1	B	233	VAL
2	C	1	MET
2	C	2	GLU
2	C	3	ILE
2	C	8	ARG
2	C	15	LEU
2	C	21	ILE
2	C	39	ARG
2	C	54	ILE
2	C	73	LEU
2	C	81	ASP
2	C	99	GLN
2	C	101	ILE
2	C	103	LYS
2	C	113	VAL
2	C	122	THR
2	C	138	SER
2	C	143	SER
2	C	154	ARG
2	C	157	ARG
2	C	159	ILE
2	C	165	LEU
2	C	181	VAL

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Mol	Chain	Res	Type
2	C	184	MET
2	C	186	VAL
2	C	189	ARG
2	C	193	LEU
2	C	206	THR
2	C	209	ARG
2	C	214	TYR
2	C	216	GLU
2	C	232	GLU
2	C	239	PHE
2	C	242	LEU
2	C	250	ARG
2	C	265	ARG
2	C	266	ARG
2	C	289	THR
2	C	290	LEU
2	C	297	GLU
2	C	304	LEU
2	C	307	LEU
2	C	308	ARG
2	C	317	VAL
2	C	321	GLU
2	C	325	ILE
2	C	335	THR
2	C	353	ARG
2	C	358	ARG
2	C	361	MET
2	C	367	LEU
2	C	371	LYS
2	C	372	LEU
2	C	379	GLU
2	C	387	SER
2	C	391	LEU
2	C	393	GLN
2	C	394	PHE
2	C	398	THR
2	C	402	SER
2	C	421	GLU
2	C	441	VAL
2	C	443	THR
2	C	448	ASN
2	C	455	LEU

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Mol	Chain	Res	Type
2	C	474	VAL
2	C	483	VAL
2	C	489	THR
2	C	491	GLU
2	C	503	LEU
2	C	514	VAL
2	C	522	VAL
2	C	539	VAL
2	C	542	VAL
2	C	554	ASP
2	C	571	LEU
2	C	584	GLU
2	C	587	VAL
2	C	600	ASP
2	C	610	ARG
2	C	616	GLU
2	C	625	LEU
2	C	637	LEU
2	C	640	ARG
2	C	644	VAL
2	C	645	VAL
2	C	649	VAL
2	C	657	ASP
2	C	661	SER
2	C	672	VAL
2	C	673	LEU
2	C	674	VAL
2	C	676	ILE
2	C	680	ASP
2	C	683	ASN
2	C	689	VAL
2	C	690	ILE
2	C	698	ASP
2	C	699	PHE
2	C	714	ASP
2	C	715	THR
2	C	717	LEU
2	C	720	GLU
2	C	722	ILE
2	C	723	THR
2	C	729	LEU
2	C	739	GLU

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Mol	Chain	Res	Type
2	C	740	GLU
2	C	749	VAL
2	C	750	LYS
2	C	799	ILE
2	C	807	ARG
2	C	822	VAL
2	C	829	GLN
2	C	838	LYS
2	C	848	VAL
2	C	855	VAL
2	C	856	GLU
2	C	869	VAL
2	C	871	LEU
2	C	881	ASN
2	C	890	LEU
2	C	911	GLU
2	C	913	GLU
2	C	937	ASP
2	C	969	GLN
2	C	973	VAL
2	C	981	GLU
2	C	999	HIS
2	C	1000	MET
2	C	1008	ARG
2	C	1015	LEU
2	C	1016	ILE
2	C	1043	TYR
2	C	1055	LEU
2	C	1060	ILE
2	C	1061	GLU
2	C	1078	GLU
2	C	1081	VAL
2	C	1113	GLU
3	D	12	LEU
3	D	17	LYS
3	D	32	ILE
3	D	38	LYS
3	D	40	GLU
3	D	48	ARG
3	D	85	VAL
3	D	97	THR
3	D	108	VAL

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Mol	Chain	Res	Type
3	D	130	SER
3	D	142	LEU
3	D	152	LEU
3	D	153	LEU
3	D	178	LEU
3	D	184	GLU
3	D	185	VAL
3	D	190	GLU
3	D	191	LEU
3	D	213	VAL
3	D	241	ILE
3	D	251	PHE
3	D	252	ARG
3	D	260	GLU
3	D	271	VAL
3	D	317	VAL
3	D	323	GLU
3	D	333	LEU
3	D	341	GLU
3	D	346	ARG
3	D	371	ILE
3	D	375	GLU
3	D	376	GLU
3	D	380	GLU
3	D	389	GLU
3	D	396	VAL
3	D	399	ARG
3	D	411	THR
3	D	431	VAL
3	D	434	ARG
3	D	452	ILE
3	D	463	GLN
3	D	478	LEU
3	D	493	ARG
3	D	500	ARG
3	D	502	PHE
3	D	510	GLU
3	D	523	ASP
3	D	524	LEU
3	D	530	VAL
3	D	539	ASP
3	D	560	GLN

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Mol	Chain	Res	Type
3	D	564	GLU
3	D	565	ILE
3	D	566	ILE
3	D	593	ASN
3	D	624	ASP
3	D	632	VAL
3	D	636	GLN
3	D	648	MET
3	D	650	LEU
3	D	666	ILE
3	D	670	VAL
3	D	676	MET
3	D	680	GLN
3	D	686	GLU
3	D	692	GLU
3	D	695	ILE
3	D	703	ASN
3	D	708	LEU
3	D	711	LEU
3	D	713	ILE
3	D	728	LEU
3	D	756	GLN
3	D	762	GLN
3	D	771	SER
3	D	780	LYS
3	D	782	SER
3	D	805	GLU
3	D	818	ARG
3	D	827	ILE
3	D	834	THR
3	D	836	VAL
3	D	842	VAL
3	D	853	VAL
3	D	860	LEU
3	D	864	VAL
3	D	873	LEU
3	D	876	SER
3	D	894	LYS
3	D	903	ASP
3	D	907	GLU
3	D	915	VAL
3	D	920	LEU

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Mol	Chain	Res	Type
3	D	921	ARG
3	D	922	LEU
3	D	947	ILE
3	D	948	THR
3	D	952	ASP
3	D	964	LEU
3	D	971	LEU
3	D	972	LEU
3	D	983	LEU
3	D	994	GLN
3	D	1020	LEU
3	D	1029	ARG
3	D	1035	ILE
3	D	1041	LEU
3	D	1055	VAL
3	D	1086	LEU
3	D	1096	ARG
3	D	1116	ASN
3	D	1119	SER
3	D	1120	VAL
3	D	1124	GLN
3	D	1128	VAL
3	D	1133	ARG
3	D	1149	LEU
3	D	1155	VAL
3	D	1161	GLU
3	D	1162	GLU
3	D	1164	ARG
3	D	1170	ASP
3	D	1188	VAL
3	D	1192	LEU
3	D	1200	VAL
3	D	1202	GLN
3	D	1204	CYS
3	D	1208	ASP
3	D	1213	ARG
3	D	1216	SER
3	D	1221	VAL
3	D	1229	ILE
3	D	1234	THR
3	D	1238	MET
3	D	1253	THR

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Mol	Chain	Res	Type
3	D	1259	VAL
3	D	1274	ILE
3	D	1276	GLU
3	D	1277	ILE
3	D	1281	VAL
3	D	1286	THR
3	D	1287	GLU
3	D	1288	GLU
3	D	1297	GLU
3	D	1301	LYS
3	D	1305	LEU
3	D	1307	LYS
3	D	1313	VAL
3	D	1314	LYS
3	D	1319	VAL
3	D	1331	ASP
3	D	1342	GLU
3	D	1344	VAL
3	D	1346	ARG
3	D	1348	LEU
3	D	1350	GLU
3	D	1352	ILE
3	D	1359	GLN
3	D	1362	LYS
3	D	1363	LEU
3	D	1368	ILE
3	D	1370	ILE
3	D	1376	MET
3	D	1380	GLU
3	D	1381	VAL
3	D	1388	ARG
3	D	1390	LEU
3	D	1396	GLU
3	D	1415	VAL
3	D	1422	MET
3	D	1424	VAL
3	D	1430	SER
3	D	1431	THR
3	D	1460	ILE
3	D	1467	ILE
3	D	1468	LEU
3	D	1472	ILE

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Mol	Chain	Res	Type
3	D	1479	ASP
3	D	1482	ARG
3	D	1486	VAL
3	D	1487	VAL
3	D	1496	GLU
4	E	19	LEU
4	E	23	VAL
4	E	31	LEU
4	E	37	ASN
4	E	39	VAL
4	E	43	GLU
4	E	66	LYS
4	E	68	LEU
4	E	69	LEU
4	E	80	VAL
5	F	81	VAL
5	F	88	ILE
5	F	106	VAL
5	F	123	ASP
5	F	127	ILE
5	F	141	VAL
5	F	150	THR
5	F	179	GLU
5	F	205	ARG
5	F	208	SER
5	F	228	GLU
5	F	237	THR
5	F	249	ARG
5	F	256	ARG
5	F	260	ILE
5	F	264	MET
5	F	290	GLU
5	F	291	ILE
5	F	304	VAL
5	F	307	THR
5	F	319	THR
5	F	336	GLU
5	F	358	LEU
5	F	361	LEU
5	F	382	THR
5	F	394	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	HIS
1	A	81	ASN
1	A	91	ASN
1	A	128	HIS
1	A	156	HIS
1	A	180	GLN
1	A	213	GLN
1	B	213	GLN
1	B	229	GLN
2	C	22	GLN
2	C	45	GLN
2	C	179	ASN
2	C	393	GLN
2	C	406	HIS
2	C	538	GLN
2	C	543	ASN
2	C	552	HIS
2	C	575	GLN
2	C	639	GLN
2	C	663	ASN
2	C	683	ASN
2	C	829	GLN
2	C	843	HIS
2	C	845	ASN
2	C	881	ASN
2	C	884	GLN
2	C	889	HIS
2	C	920	GLN
2	C	1100	GLN
3	D	33	ASN
3	D	125	GLN
3	D	294	HIS
3	D	302	GLN
3	D	442	ASN
3	D	507	ASN
3	D	529	GLN
3	D	560	GLN
3	D	617	ASN
3	D	636	GLN
3	D	680	GLN
3	D	703	ASN
3	D	714	GLN

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Mol	Chain	Res	Type
3	D	727	GLN
3	D	729	HIS
3	D	737	ASN
3	D	906	GLN
3	D	917	GLN
3	D	1034	GLN
3	D	1075	HIS
3	D	1172	HIS
3	D	1242	HIS
3	D	1333	HIS
3	D	1353	GLN
3	D	1359	GLN
3	D	1374	GLN
3	D	1442	ASN
4	E	33	HIS
4	E	37	ASN
5	F	175	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 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PO4	A	401	-	4,4,4	1.05	0	6,6,6	0.43	0
10	G4P	D	1605	8	36,38,38	1.49	2 (5%)	56,61,61	1.61	8 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	G4P	D	1605	8	-	6/27/43/43	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	1605	G4P	O6-C6	6.99	1.36	1.23
10	D	1605	G4P	PC-O3C	2.04	1.61	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	1605	G4P	C5-C4-N3	-5.75	119.23	128.39
10	D	1605	G4P	C2-N3-C4	5.59	121.92	112.30
10	D	1605	G4P	N9-C4-N3	3.55	133.05	125.95
10	D	1605	G4P	C2-N1-C6	-2.50	120.58	125.11
10	D	1605	G4P	N9-C8-N7	-2.34	109.07	113.40
10	D	1605	G4P	C6-C5-N7	2.27	134.42	130.29
10	D	1605	G4P	C4-C5-N7	-2.08	107.38	110.67
10	D	1605	G4P	C5-C6-N1	2.04	118.45	113.25

There are no chirality outliers.

All (6) torsion outliers are listed below:

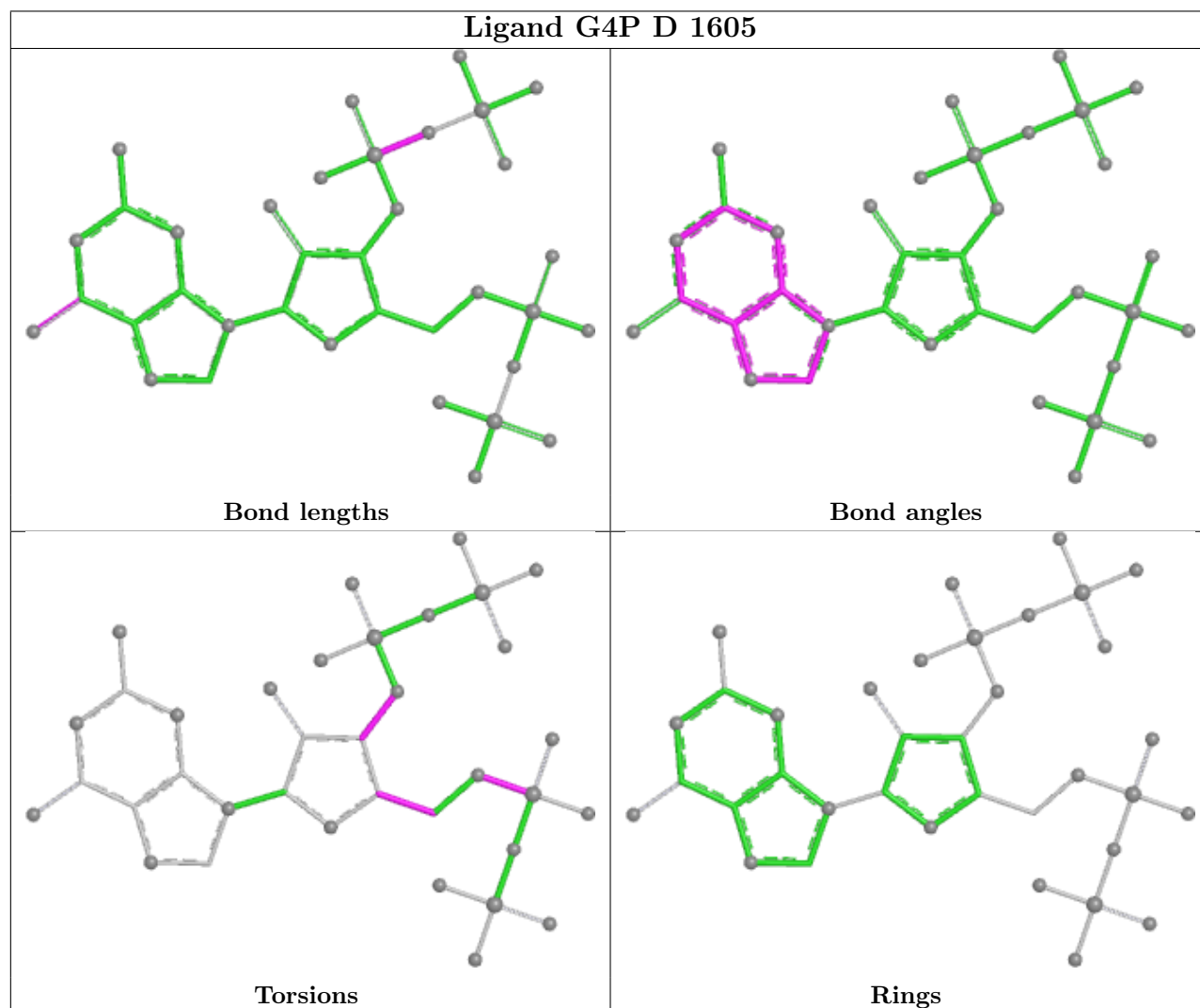
Mol	Chain	Res	Type	Atoms
10	D	1605	G4P	C5'-O5'-PA-O3A
10	D	1605	G4P	C5'-O5'-PA-O1A
10	D	1605	G4P	C5'-O5'-PA-O2A
10	D	1605	G4P	O4'-C4'-C5'-O5'
10	D	1605	G4P	C4'-C3'-O3'-PC
10	D	1605	G4P	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	1605	G4P	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	231/315 (73%)	0.63	21 (9%)	15 13	51, 78, 162, 212	1 (0%)
1	B	238/315 (75%)	1.68	72 (30%)	1 1	70, 149, 236, 260	0
2	C	1119/1119 (100%)	1.09	217 (19%)	3 3	49, 97, 222, 263	2 (0%)
3	D	1504/1524 (98%)	1.11	338 (22%)	2 2	49, 95, 245, 296	4 (0%)
4	E	95/99 (95%)	0.83	16 (16%)	4 4	58, 104, 192, 203	0
5	F	351/423 (82%)	1.66	121 (34%)	1 1	68, 124, 245, 277	2 (0%)
6	Z	0/48	-	-	-	-	-
All	All	3538/3843 (92%)	1.16	785 (22%)	2 2	49, 102, 232, 296	9 (0%)

All (785) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ASP	12.8
3	D	428	LYS	12.2
1	A	4	SER	11.1
1	B	158	ILE	11.0
5	F	144	ILE	10.3
3	D	328	GLY	10.0
1	A	1	MET	9.8
3	D	418	GLY	9.2
3	D	326	GLU	9.1
5	F	147	LEU	8.8
1	B	157	GLY	8.7
1	B	96	THR	8.7
1	B	238	GLU	8.6
3	D	235	ALA	8.5
1	A	2	LEU	8.5
3	D	1247	ALA	8.4
5	F	236	SER	8.2
3	D	616	GLN	8.1

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Mol	Chain	Res	Type	RSRZ
1	A	5	LYS	8.1
3	D	417	PRO	7.9
5	F	148	LYS	7.7
3	D	236	TYR	7.7
2	C	269	LEU	7.6
3	D	1089	ALA	7.5
3	D	613	ARG	7.4
1	B	62	LEU	7.4
2	C	275	TYR	7.4
3	D	375	GLU	7.4
2	C	254	VAL	7.4
1	B	98	THR	7.4
1	B	160	ASP	7.2
2	C	221	LEU	7.2
3	D	895	VAL	7.1
3	D	229	ALA	7.0
3	D	595	GLY	6.9
3	D	227	LEU	6.9
2	C	42	VAL	6.7
2	C	360	LEU	6.7
3	D	230	TRP	6.6
3	D	420	VAL	6.5
1	B	97	VAL	6.5
1	B	162	ILE	6.4
1	A	6	LEU	6.3
3	D	1249	ALA	6.3
1	B	93	SER	6.3
2	C	763	GLY	6.2
1	B	2	LEU	6.1
2	C	1031	ARG	6.0
3	D	228	ALA	6.0
3	D	1245	GLY	6.0
5	F	355	GLU	6.0
3	D	394	LEU	6.0
5	F	321	ILE	6.0
3	D	324	ALA	5.9
5	F	237	THR	5.9
2	C	272	ALA	5.9
3	D	1246	VAL	5.8
2	C	39	ARG	5.8
2	C	268	ASP	5.7
2	C	773	LEU	5.6

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Mol	Chain	Res	Type	RSRZ
2	C	762	LYS	5.6
5	F	324	GLU	5.4
5	F	73	PRO	5.4
1	A	188	GLN	5.4
1	B	141	GLU	5.4
2	C	214	TYR	5.3
3	D	245	LEU	5.3
3	D	425	GLY	5.3
5	F	391	GLY	5.3
1	B	155	LYS	5.3
3	D	1250	ALA	5.2
5	F	383	LEU	5.2
3	D	241	ILE	5.1
3	D	73	CYS	5.1
3	D	416	ALA	5.1
2	C	293	PHE	5.1
1	B	236	PRO	5.1
2	C	165	LEU	5.1
2	C	1027	PHE	5.1
2	C	267	TYR	5.1
3	D	1241	PHE	5.0
2	C	261	ILE	5.0
3	D	594	PRO	5.0
3	D	391	ALA	5.0
2	C	729	LEU	5.0
5	F	423	ASP	4.9
5	F	143	HIS	4.9
3	D	432	TYR	4.8
2	C	34	VAL	4.8
3	D	1408	ILE	4.8
3	D	76	CYS	4.8
3	D	1243	THR	4.8
3	D	1248	GLY	4.8
2	C	217	LEU	4.8
3	D	1244	GLY	4.7
3	D	108	VAL	4.7
5	F	354	LEU	4.7
2	C	228	ALA	4.7
2	C	1002	GLU	4.7
3	D	237	LYS	4.7
2	C	420	ARG	4.7
2	C	418	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
3	D	331	VAL	4.6
3	D	353	VAL	4.6
3	D	364	GLY	4.5
5	F	202	TYR	4.5
3	D	330	THR	4.5
2	C	419	THR	4.5
3	D	430	ASP	4.5
3	D	205	TYR	4.5
5	F	96	LEU	4.5
5	F	203	THR	4.5
3	D	371	ILE	4.4
2	C	194	VAL	4.4
3	D	1090	ASP	4.4
1	A	186	LEU	4.4
1	B	57	TYR	4.4
5	F	408	LEU	4.4
2	C	153	ALA	4.4
5	F	142	ARG	4.4
3	D	1198	TYR	4.4
3	D	900	ILE	4.4
5	F	139	ALA	4.3
2	C	422	ARG	4.3
3	D	921	ARG	4.3
2	C	287	GLY	4.3
3	D	1440	PHE	4.3
5	F	240	THR	4.3
2	C	108	ILE	4.3
3	D	102	ILE	4.3
1	B	115	LEU	4.3
3	D	77	GLY	4.3
3	D	427	VAL	4.3
5	F	75	ILE	4.3
3	D	60	CYS	4.3
3	D	1197	ARG	4.3
2	C	262	ALA	4.3
3	D	381	ALA	4.3
5	F	103	ALA	4.3
5	F	146	GLY	4.3
3	D	225	LEU	4.2
5	F	141	VAL	4.2
2	C	258	TYR	4.2
2	C	208	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
3	D	614	PHE	4.2
3	D	223	LEU	4.2
2	C	370	ALA	4.2
4	E	2	ALA	4.2
3	D	329	GLU	4.2
3	D	355	VAL	4.2
3	D	240	GLU	4.1
1	B	159	LYS	4.1
4	E	85	LEU	4.1
2	C	152	PRO	4.1
2	C	361	MET	4.1
2	C	40	GLU	4.1
2	C	421	GLU	4.1
3	D	1399	ASP	4.1
2	C	523	ILE	4.1
3	D	75	ARG	4.1
2	C	774	LEU	4.1
3	D	812	ALA	4.0
1	B	58	ILE	4.0
5	F	349	LEU	4.0
3	D	439	LEU	4.0
3	D	168	THR	4.0
3	D	901	GLN	4.0
3	D	810	GLU	4.0
1	B	143	ARG	4.0
3	D	242	LEU	4.0
3	D	261	LEU	4.0
1	B	1	MET	4.0
2	C	242	LEU	4.0
3	D	144	GLY	4.0
3	D	402	PRO	3.9
2	C	814	GLU	3.9
3	D	327	GLU	3.9
5	F	198	ILE	3.9
5	F	418	LEU	3.9
3	D	147	VAL	3.9
3	D	400	VAL	3.9
3	D	109	PRO	3.9
3	D	615	ARG	3.9
2	C	113	VAL	3.9
3	D	345	TYR	3.8
3	D	1091	SER	3.8

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Mol	Chain	Res	Type	RSRZ
2	C	197	LEU	3.8
3	D	419	ASP	3.8
3	D	79	GLU	3.8
3	D	72	VAL	3.8
3	D	179	VAL	3.8
2	C	67	ASP	3.8
5	F	329	TYR	3.8
2	C	218	VAL	3.8
5	F	244	ARG	3.8
3	D	808	THR	3.8
2	C	118	ILE	3.8
1	B	109	VAL	3.8
2	C	167	LYS	3.8
2	C	176	VAL	3.8
3	D	1128	VAL	3.8
1	B	95	GLN	3.7
5	F	358	LEU	3.7
2	C	315	ALA	3.7
2	C	344	PHE	3.7
3	D	78	VAL	3.7
2	C	719	PRO	3.7
2	C	768	THR	3.7
3	D	56	TYR	3.7
3	D	378	ILE	3.7
5	F	390	PHE	3.7
5	F	74	LYS	3.7
2	C	1028	GLY	3.7
1	B	144	VAL	3.7
2	C	196	LEU	3.7
3	D	1237	THR	3.7
3	D	806	PHE	3.7
2	C	811	PRO	3.7
5	F	278	LEU	3.6
2	C	33	ASP	3.6
5	F	234	LYS	3.6
3	D	138	LYS	3.6
3	D	617	ASN	3.6
3	D	360	ARG	3.6
3	D	1388	ARG	3.6
5	F	394	ARG	3.6
3	D	269	PHE	3.6
5	F	389	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
2	C	290	LEU	3.6
5	F	151	LEU	3.6
5	F	376	ILE	3.6
1	B	156	HIS	3.6
2	C	512	ARG	3.6
1	A	231	ALA	3.6
2	C	423	ALA	3.6
5	F	199	ALA	3.6
5	F	313	GLU	3.6
3	D	292	VAL	3.5
1	B	100	LEU	3.5
2	C	211	LEU	3.5
2	C	253	ALA	3.5
3	D	59	ALA	3.5
3	D	387	LEU	3.5
3	D	170	PRO	3.5
5	F	201	LYS	3.5
5	F	325	LYS	3.5
1	A	230	ALA	3.5
3	D	1113	GLY	3.5
3	D	373	PRO	3.5
2	C	115	LEU	3.5
5	F	371	LEU	3.5
2	C	209	ARG	3.5
1	A	7	LYS	3.4
5	F	356	LYS	3.4
2	C	769	PRO	3.4
1	B	132	LEU	3.4
3	D	311	LEU	3.4
2	C	239	PHE	3.4
1	B	61	VAL	3.4
2	C	171	TRP	3.4
5	F	77	THR	3.4
2	C	66	LEU	3.4
3	D	310	LEU	3.4
5	F	392	VAL	3.4
3	D	429	SER	3.4
5	F	150	THR	3.4
2	C	898	GLY	3.4
3	D	107	ASP	3.4
2	C	257	VAL	3.4
3	D	354	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
2	C	204	GLN	3.4
3	D	320	ALA	3.4
5	F	344	ALA	3.4
3	D	350	HIS	3.4
3	D	829	VAL	3.4
5	F	209	PHE	3.4
5	F	386	VAL	3.4
3	D	141	ILE	3.3
2	C	716	LYS	3.3
3	D	180	LYS	3.3
2	C	241	LEU	3.3
2	C	388	ARG	3.3
3	D	318	ARG	3.3
3	D	376	GLU	3.3
1	B	117	VAL	3.3
2	C	302	VAL	3.3
2	C	373	VAL	3.3
3	D	385	VAL	3.3
5	F	368	VAL	3.3
2	C	279	GLU	3.3
3	D	486	ARG	3.3
2	C	277	ALA	3.3
2	C	195	LEU	3.3
3	D	282	TYR	3.3
5	F	145	PRO	3.3
3	D	101	HIS	3.3
3	D	457	GLY	3.3
2	C	816	LYS	3.3
2	C	924	VAL	3.3
2	C	284	ARG	3.3
5	F	412	GLU	3.3
1	B	99	LEU	3.2
2	C	417	GLY	3.2
5	F	332	PHE	3.2
3	D	968	ASP	3.2
3	D	67	ARG	3.2
5	F	415	THR	3.2
3	D	169	TYR	3.2
3	D	434	ARG	3.2
3	D	183	GLU	3.2
3	D	1391	GLU	3.2
1	B	131	THR	3.2

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Mol	Chain	Res	Type	RSRZ
3	D	281	THR	3.2
3	D	222	GLY	3.2
3	D	358	GLY	3.2
3	D	401	TYR	3.2
2	C	114	PHE	3.2
5	F	421	PHE	3.2
1	B	6	LEU	3.2
2	C	731	GLU	3.2
5	F	194	LEU	3.2
3	D	297	ILE	3.2
2	C	256	TYR	3.2
3	D	1503	VAL	3.2
5	F	205	ARG	3.1
2	C	348	LEU	3.1
1	B	130	ALA	3.1
3	D	487	ALA	3.1
2	C	283	ILE	3.1
3	D	393	ILE	3.1
3	D	407	VAL	3.1
3	D	415	VAL	3.1
2	C	26	TYR	3.1
2	C	717	LEU	3.1
2	C	2	GLU	3.1
5	F	319	THR	3.1
3	D	379	ALA	3.1
3	D	883	ALA	3.1
2	C	186	VAL	3.1
3	D	1130	ARG	3.1
3	D	333	LEU	3.1
3	D	896	ALA	3.1
1	B	111	ALA	3.1
3	D	103	TRP	3.1
3	D	104	PHE	3.1
2	C	225	SER	3.1
3	D	404	GLU	3.0
2	C	155	PRO	3.0
2	C	38	LYS	3.0
3	D	830	ALA	3.0
3	D	1409	ALA	3.0
1	B	170	VAL	3.0
2	C	68	PHE	3.0
3	D	619	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
3	D	1389	LEU	3.0
4	E	3	GLU	3.0
1	B	165	ILE	3.0
2	C	266	ARG	3.0
3	D	182	GLY	3.0
3	D	312	ARG	3.0
1	B	118	ALA	3.0
2	C	29	ALA	3.0
3	D	319	ALA	3.0
2	C	317	VAL	3.0
2	C	813	VAL	3.0
3	D	233	LYS	3.0
5	F	152	ASP	3.0
5	F	400	ILE	3.0
3	D	221	ALA	3.0
5	F	357	ALA	3.0
2	C	227	PHE	3.0
3	D	298	VAL	3.0
3	D	361	VAL	3.0
5	F	359	SER	3.0
5	F	413	SER	3.0
1	B	161	ARG	3.0
5	F	91	VAL	3.0
2	C	123	GLU	2.9
5	F	149	GLU	2.9
4	E	4	PRO	2.9
5	F	382	THR	2.9
3	D	271	VAL	2.9
2	C	637	LEU	2.9
3	D	314	PRO	2.9
3	D	612	GLY	2.9
3	D	918	ALA	2.9
2	C	207	LEU	2.9
2	C	260	LEU	2.9
2	C	59	LYS	2.9
1	A	189	ARG	2.9
1	B	163	ASN	2.9
5	F	322	GLY	2.9
2	C	289	THR	2.9
2	C	48	PHE	2.9
2	C	351	LEU	2.9
3	D	175	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
3	D	283	PHE	2.9
3	D	998	GLU	2.9
5	F	241	TRP	2.9
2	C	220	GLY	2.9
3	D	383	GLY	2.9
1	B	235	ALA	2.9
1	B	89	PHE	2.9
3	D	251	PHE	2.9
2	C	35	PRO	2.8
1	A	158	ILE	2.8
1	B	101	LEU	2.8
2	C	443	THR	2.8
5	F	102	LEU	2.8
1	B	65	PHE	2.8
2	C	226	VAL	2.8
2	C	369	PRO	2.8
3	D	349	PRO	2.8
2	C	738	ASP	2.8
1	B	127	LEU	2.8
3	D	253	ALA	2.8
3	D	1505	ALA	2.8
1	B	56	VAL	2.8
1	B	87	VAL	2.8
3	D	315	ARG	2.8
5	F	140	ARG	2.8
2	C	899	GLN	2.8
5	F	245	GLN	2.8
3	D	367	ILE	2.8
3	D	894	LYS	2.8
3	D	897	TRP	2.8
1	A	157	GLY	2.8
1	B	90	LEU	2.8
2	C	100	LEU	2.8
2	C	131	GLY	2.8
5	F	283	GLY	2.8
2	C	96	ALA	2.8
3	D	163	TYR	2.8
3	D	216	VAL	2.8
5	F	195	VAL	2.8
3	D	390	PRO	2.8
1	B	122	ILE	2.8
4	E	51	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	1	MET	2.8
3	D	294	HIS	2.8
3	D	1502	ALA	2.8
3	D	804	LEU	2.7
5	F	197	SER	2.7
3	D	1129	THR	2.7
3	D	1251	ASP	2.7
4	E	96	GLU	2.7
3	D	882	PHE	2.7
3	D	1393	GLN	2.7
5	F	260	ILE	2.7
1	B	4	SER	2.7
2	C	322	VAL	2.7
3	D	399	ARG	2.7
3	D	441	ARG	2.7
3	D	622	ARG	2.7
4	E	91	ARG	2.7
5	F	232	ARG	2.7
2	C	316	GLY	2.7
3	D	224	ARG	2.7
3	D	467	GLU	2.7
5	F	414	ARG	2.7
3	D	268	ALA	2.7
3	D	336	PHE	2.7
2	C	281	LEU	2.7
2	C	356	ARG	2.7
3	D	61	GLY	2.7
2	C	663	ASN	2.7
3	D	184	GLU	2.7
5	F	248	ASN	2.7
3	D	1381	VAL	2.7
5	F	307	THR	2.7
5	F	417	LYS	2.7
2	C	172	ILE	2.6
2	C	783	ARG	2.6
5	F	186	HIS	2.6
4	E	95	GLY	2.6
2	C	303	PHE	2.6
3	D	577	ALA	2.6
1	B	60	ASP	2.6
3	D	270	LEU	2.6
3	D	1242	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
3	D	426	LYS	2.6
3	D	392	SER	2.6
5	F	78	SER	2.6
3	D	1413	THR	2.6
1	B	145	ASP	2.6
3	D	200	ASP	2.6
3	D	142	LEU	2.6
1	A	185	ARG	2.6
1	B	88	ARG	2.6
3	D	571	LYS	2.6
2	C	43	GLY	2.6
2	C	1001	VAL	2.6
2	C	311	PHE	2.6
2	C	312	ALA	2.6
3	D	208	PRO	2.6
3	D	197	SER	2.6
3	D	289	THR	2.6
3	D	316	GLN	2.6
3	D	596	SER	2.6
2	C	98	LEU	2.6
3	D	899	LEU	2.6
2	C	145	GLY	2.6
2	C	416	GLY	2.6
3	D	238	PRO	2.6
3	D	446	VAL	2.6
5	F	388	ALA	2.6
3	D	1305	LEU	2.5
5	F	163	LEU	2.5
3	D	249	TYR	2.5
3	D	332	TYR	2.5
3	D	234	GLU	2.5
3	D	975	GLU	2.5
2	C	282	GLY	2.5
2	C	767	PRO	2.5
3	D	248	PRO	2.5
3	D	66	GLN	2.5
3	D	405	ASP	2.5
5	F	323	ASP	2.5
2	C	464	LEU	2.5
3	D	304	LEU	2.5
3	D	652	LEU	2.5
5	F	154	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	463	GLU	2.5
5	F	80	PRO	2.5
3	D	317	VAL	2.5
3	D	363	ALA	2.5
3	D	1307	LYS	2.5
5	F	403	LYS	2.5
2	C	815	LEU	2.5
3	D	971	LEU	2.5
3	D	1086	LEU	2.5
2	C	766	GLU	2.5
2	C	629	TYR	2.5
3	D	665	GLY	2.5
3	D	226	PRO	2.5
3	D	484	PRO	2.5
2	C	182	VAL	2.5
3	D	195	VAL	2.5
1	A	11	PHE	2.5
2	C	349	ALA	2.5
3	D	611	GLN	2.5
3	D	845	ASN	2.5
4	E	50	THR	2.5
5	F	269	ASN	2.5
3	D	58	CYS	2.5
5	F	370	LYS	2.5
2	C	389	SER	2.5
5	F	326	ASP	2.5
2	C	244	PRO	2.5
3	D	63	TYR	2.5
3	D	213	VAL	2.5
1	B	232	ALA	2.5
3	D	1240	THR	2.4
2	C	308	ARG	2.4
2	C	307	LEU	2.4
2	C	730	SER	2.4
2	C	765	SER	2.4
2	C	263	ASP	2.4
5	F	263	HIS	2.4
1	B	125	PRO	2.4
1	B	53	VAL	2.4
1	A	23	PHE	2.4
1	A	225	PHE	2.4
5	F	275	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
5	F	274	THR	2.4
2	C	30	LEU	2.4
5	F	94	LEU	2.4
2	C	37	GLU	2.4
3	D	80	VAL	2.4
3	D	444	VAL	2.4
3	D	821	VAL	2.4
5	F	235	PHE	2.4
2	C	168	ARG	2.4
2	C	715	THR	2.4
3	D	171	LEU	2.4
3	D	264	LEU	2.4
2	C	75	GLU	2.4
3	D	1417	TRP	2.4
2	C	86	LYS	2.4
2	C	166	PRO	2.4
3	D	322	VAL	2.4
3	D	445	ARG	2.4
5	F	233	PHE	2.4
5	F	282	LEU	2.4
3	D	592	THR	2.4
2	C	764	GLU	2.4
2	C	1080	SER	2.4
1	B	3	ASP	2.4
5	F	153	PRO	2.4
1	B	142	VAL	2.4
1	B	167	VAL	2.4
3	D	105	VAL	2.4
3	D	145	VAL	2.4
2	C	78	PHE	2.4
1	A	224	TYR	2.3
2	C	238	LEU	2.3
3	D	161	LEU	2.3
3	D	1252	ILE	2.3
5	F	291	ILE	2.3
1	B	64	GLU	2.3
3	D	325	GLU	2.3
3	D	494	LYS	2.3
3	D	193	PRO	2.3
2	C	807	ARG	2.3
3	D	1441	GLN	2.3
2	C	193	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	1407	LEU	2.3
5	F	369	LEU	2.3
2	C	158	TYR	2.3
3	D	1088	THR	2.3
1	B	139	ASN	2.3
3	D	265	GLU	2.3
3	D	408	GLU	2.3
3	D	220	ARG	2.3
3	D	636	GLN	2.3
5	F	222	ARG	2.3
1	A	8	ALA	2.3
1	B	80	LEU	2.3
3	D	403	PHE	2.3
5	F	366	ALA	2.3
3	D	1000	THR	2.3
5	F	288	TYR	2.3
2	C	188	LYS	2.3
3	D	497	GLU	2.3
2	C	631	SER	2.3
5	F	76	SER	2.3
3	D	986	ARG	2.3
3	D	335	LEU	2.3
2	C	101	ILE	2.3
2	C	314	THR	2.3
2	C	341	THR	2.3
2	C	781	LYS	2.3
3	D	62	LYS	2.3
3	D	1084	THR	2.3
5	F	393	THR	2.3
2	C	445	GLU	2.3
3	D	69	GLU	2.3
1	B	14	ARG	2.3
2	C	318	PRO	2.3
3	D	1239	ARG	2.3
4	E	94	PRO	2.3
5	F	312	GLN	2.3
2	C	414	GLY	2.3
3	D	70	GLY	2.3
3	D	231	VAL	2.3
3	D	886	VAL	2.3
3	D	902	LEU	2.3
3	D	1400	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	207	PHE	2.3
1	B	129	ILE	2.2
2	C	255	ALA	2.2
1	B	102	LYS	2.2
3	D	262	LYS	2.2
5	F	385	GLU	2.2
4	E	93	TYR	2.2
3	D	1087	ARG	2.2
3	D	110	SER	2.2
2	C	927	GLY	2.2
2	C	355	VAL	2.2
3	D	68	PHE	2.2
3	D	359	ALA	2.2
2	C	511	GLU	2.2
3	D	4	GLU	2.2
3	D	263	GLU	2.2
3	D	1308	GLU	2.2
2	C	925	TYR	2.2
2	C	231	PRO	2.2
3	D	1268	PRO	2.2
3	D	938	GLY	2.2
3	D	1439	SER	2.2
2	C	64	LEU	2.2
2	C	276	LYS	2.2
3	D	482	LYS	2.2
2	C	722	ILE	2.2
3	D	129	PHE	2.2
3	D	827	ILE	2.2
5	F	381	HIS	2.2
3	D	898	GLU	2.2
5	F	290	GLU	2.2
3	D	832	ARG	2.2
2	C	77	PRO	2.2
2	C	107	LEU	2.2
3	D	366	LYS	2.2
3	D	424	GLY	2.2
3	D	1092	GLY	2.2
1	B	233	VAL	2.2
3	D	578	VAL	2.2
4	E	89	MET	2.2
2	C	127	PHE	2.2
2	C	162	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	1495	ILE	2.2
3	D	491	LYS	2.2
3	D	1390	LEU	2.2
5	F	308	LEU	2.2
5	F	315	VAL	2.2
3	D	982	PHE	2.2
2	C	1074	GLU	2.1
3	D	244	GLU	2.1
3	D	382	GLU	2.1
2	C	345	ARG	2.1
3	D	944	THR	2.1
4	E	84	ARG	2.1
2	C	170	PRO	2.1
1	B	107	LYS	2.1
3	D	1318	TYR	2.1
4	E	87	LYS	2.1
3	D	337	LEU	2.1
3	D	421	LEU	2.1
3	D	309	GLY	2.1
1	B	13	VAL	2.1
1	B	128	HIS	2.1
2	C	199	VAL	2.1
3	D	1402	ALA	2.1
3	D	374	GLU	2.1
3	D	173	PRO	2.1
3	D	1093	TYR	2.1
5	F	93	LEU	2.1
3	D	287	GLY	2.1
2	C	117	HIS	2.1
3	D	844	ALA	2.1
2	C	1119	ARG	2.1
3	D	150	ARG	2.1
3	D	198	ARG	2.1
3	D	273	ARG	2.1
2	C	36	PRO	2.1
2	C	53	PRO	2.1
3	D	593	ASN	2.1
2	C	71	TYR	2.1
3	D	215	TYR	2.1
2	C	427	VAL	2.1
3	D	293	VAL	2.1
3	D	435	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	191	ASP	2.1
1	B	126	ASP	2.1
2	C	868	ASP	2.1
3	D	136	ASP	2.1
2	C	32	ALA	2.1
2	C	49	ARG	2.1
2	C	770	GLU	2.1
2	C	923	GLU	2.1
3	D	57	GLU	2.1
3	D	232	GLU	2.1
2	C	299	LYS	2.1
5	F	360	LYS	2.1
3	D	1306	PRO	2.1
1	B	140	MET	2.1
3	D	994	GLN	2.1
4	E	86	GLN	2.1
3	D	291	LEU	2.1
5	F	361	LEU	2.1
1	B	135	GLY	2.1
3	D	386	HIS	2.1
5	F	337	HIS	2.1
2	C	425	PHE	2.1
3	D	181	ASP	2.0
1	B	164	ALA	2.0
5	F	272	SER	2.0
2	C	248	PRO	2.0
3	D	191	LEU	2.0
3	D	272	LEU	2.0
3	D	823	LEU	2.0
3	D	973	GLN	2.0
2	C	337	GLY	2.0
2	C	664	GLY	2.0
2	C	65	VAL	2.0
2	C	90	TYR	2.0
3	D	836	VAL	2.0
2	C	805	ARG	2.0
2	C	490	GLU	2.0
2	C	531	PHE	2.0
3	D	903	ASP	2.0
4	E	52	GLU	2.0
3	D	149	LYS	2.0
3	D	1265	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
5	F	200	LYS	2.0
3	D	1398	TRP	2.0
1	B	166	PRO	2.0
3	D	285	PRO	2.0
3	D	826	PRO	2.0
2	C	390	GLN	2.0
5	F	277	GLN	2.0
2	C	60	GLY	2.0
2	C	230	ARG	2.0
3	D	431	VAL	2.0
3	D	488	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

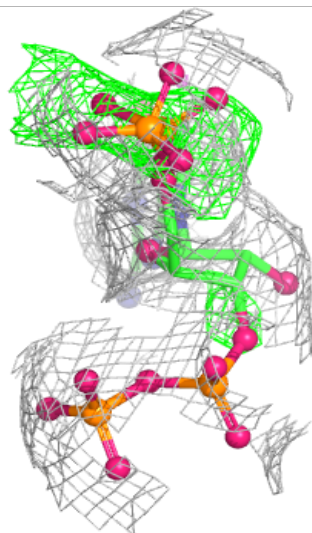
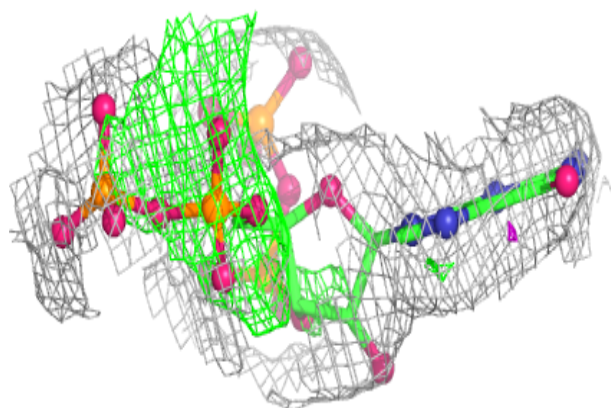
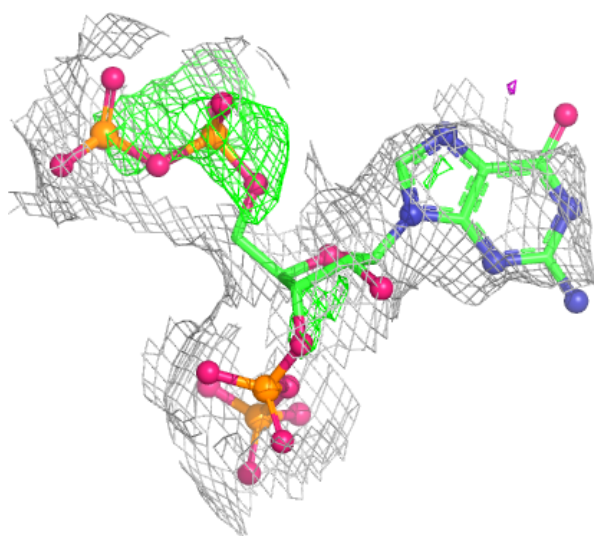
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	MG	C	1201	1/1	0.65	0.36	131,131,131,131	0
8	MG	D	1601	1/1	0.81	0.39	133,133,133,133	0
10	G4P	D	1605	36/36	0.90	0.20	183,197,222,224	0
8	MG	D	1606	1/1	0.94	0.07	155,155,155,155	0
8	MG	D	1604	1/1	0.94	0.14	86,86,86,86	0
9	ZN	D	1602	1/1	0.96	0.20	225,225,225,225	0
9	ZN	D	1603	1/1	0.98	0.07	168,168,168,168	0
7	PO4	A	401	5/5	0.98	0.15	143,144,148,149	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around G4P D 1605:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.