



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:09 PM UTC

PDB ID : 6N60 / pdb_00006n60
Title : Escherichia coli RNA polymerase sigma70-holoenzyme bound to upstream fork promoter DNA and Microcin J25 (MccJ25)
Authors : Braffman, N.; Hauver, J.; Campbell, E.A.; Darst, S.A.
Deposited on : 2018-11-23
Resolution : 3.68 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

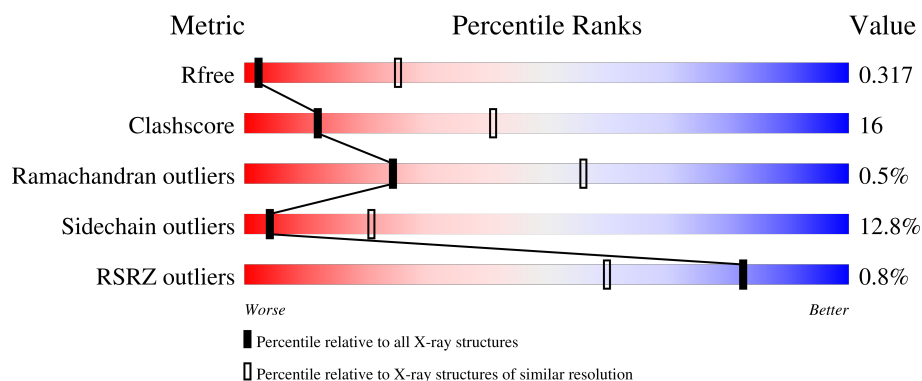
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.68 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	1263 (3.80-3.56)
Clashscore	190562	1305 (3.80-3.56)
Ramachandran outliers	187476	1259 (3.80-3.56)
Sidechain outliers	187428	1256 (3.80-3.56)
RSRZ outliers	180081	1262 (3.80-3.56)

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	239	
1	B	239	
2	C	1342	
3	D	1409	
4	E	91	

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Mol	Chain	Length	Quality of chain
5	F	612	34%15%48%
6	M	21	24%62%10%5%
7	N	29	59%41%
8	T	24	4%50%50%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 27705 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
			1759	1094	312	347	6			
1	B	218	Total	C	N	O	S	0	0	0
			1638	1023	284	325	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLU	-	expression tag	UNP P0A7Z4
A	236	VAL	-	expression tag	UNP P0A7Z4
A	237	LEU	-	expression tag	UNP P0A7Z4
A	238	PHE	-	expression tag	UNP P0A7Z4
A	239	GLN	-	expression tag	UNP P0A7Z4
B	235	GLU	-	expression tag	UNP P0A7Z4
B	236	VAL	-	expression tag	UNP P0A7Z4
B	237	LEU	-	expression tag	UNP P0A7Z4
B	238	PHE	-	expression tag	UNP P0A7Z4
B	239	GLN	-	expression tag	UNP P0A7Z4

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1335	Total	C	N	O	S	0	0	0
			10470	6569	1822	2036	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1236	Total	C	N	O	S	0	0	0
			9578	6015	1711	1806	46			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	VAL	-	expression tag	UNP P0A8T7
D	1408	LEU	-	expression tag	UNP P0A8T7
D	1409	GLU	-	expression tag	UNP P0A8T7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	318	Total	C	N	O	S	0	0	0
			2399	1499	442	446	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	149	ASN	ASP	conflict	UNP Q0P6L9
F	?	-	LEU	deletion	UNP Q0P6L9

- Molecule 6 is a protein called Microcin J25.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	M	21	Total	C	N	O	0	0	0
			144	95	23	26			

- Molecule 7 is a DNA chain called non-template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	N	29	Total	C	N	O	P	0	0	0
			595	284	106	176	29			

- Molecule 8 is a DNA chain called template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	T	24	Total	C	N	O	P	0	0	0
			492	233	94	141	24			

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

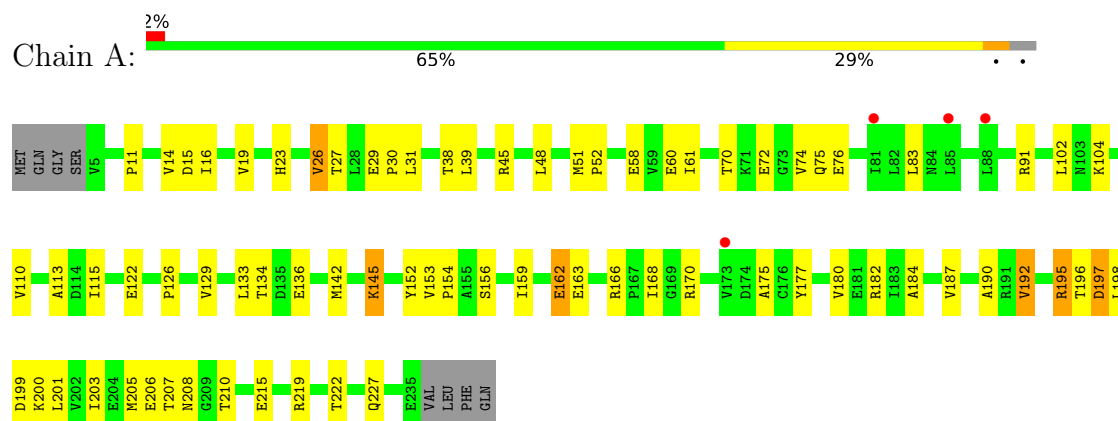
- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

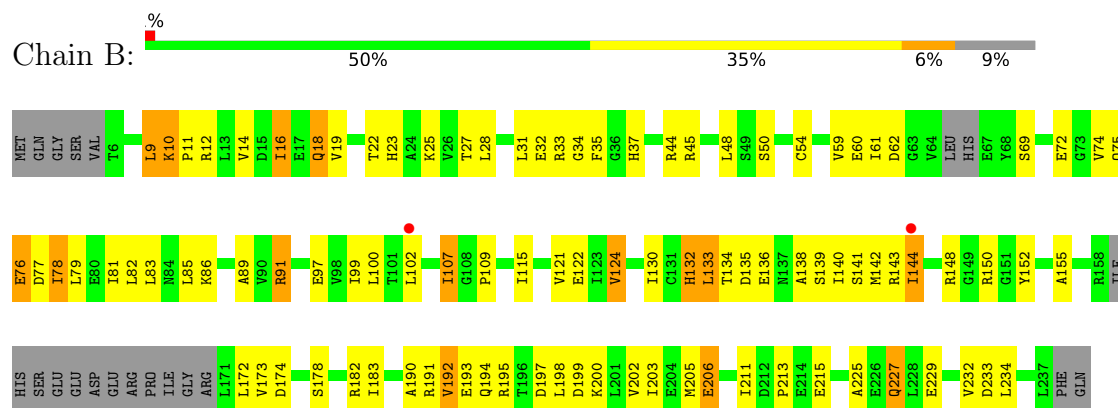
3 Residue-property plots [i](#)

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

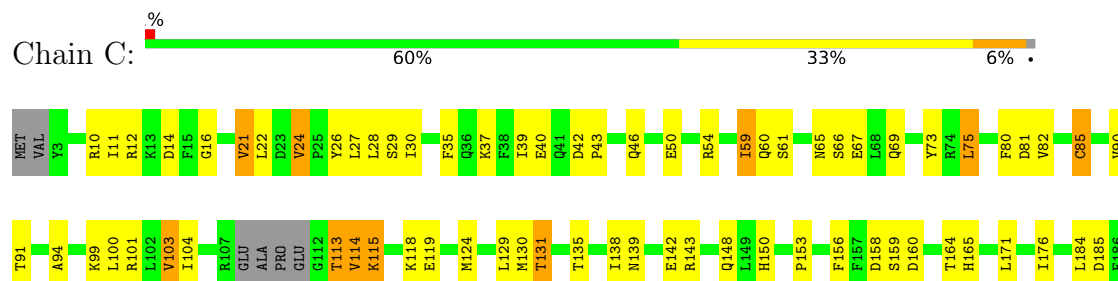
• Molecule 1: DNA-directed RNA polymerase subunit alpha

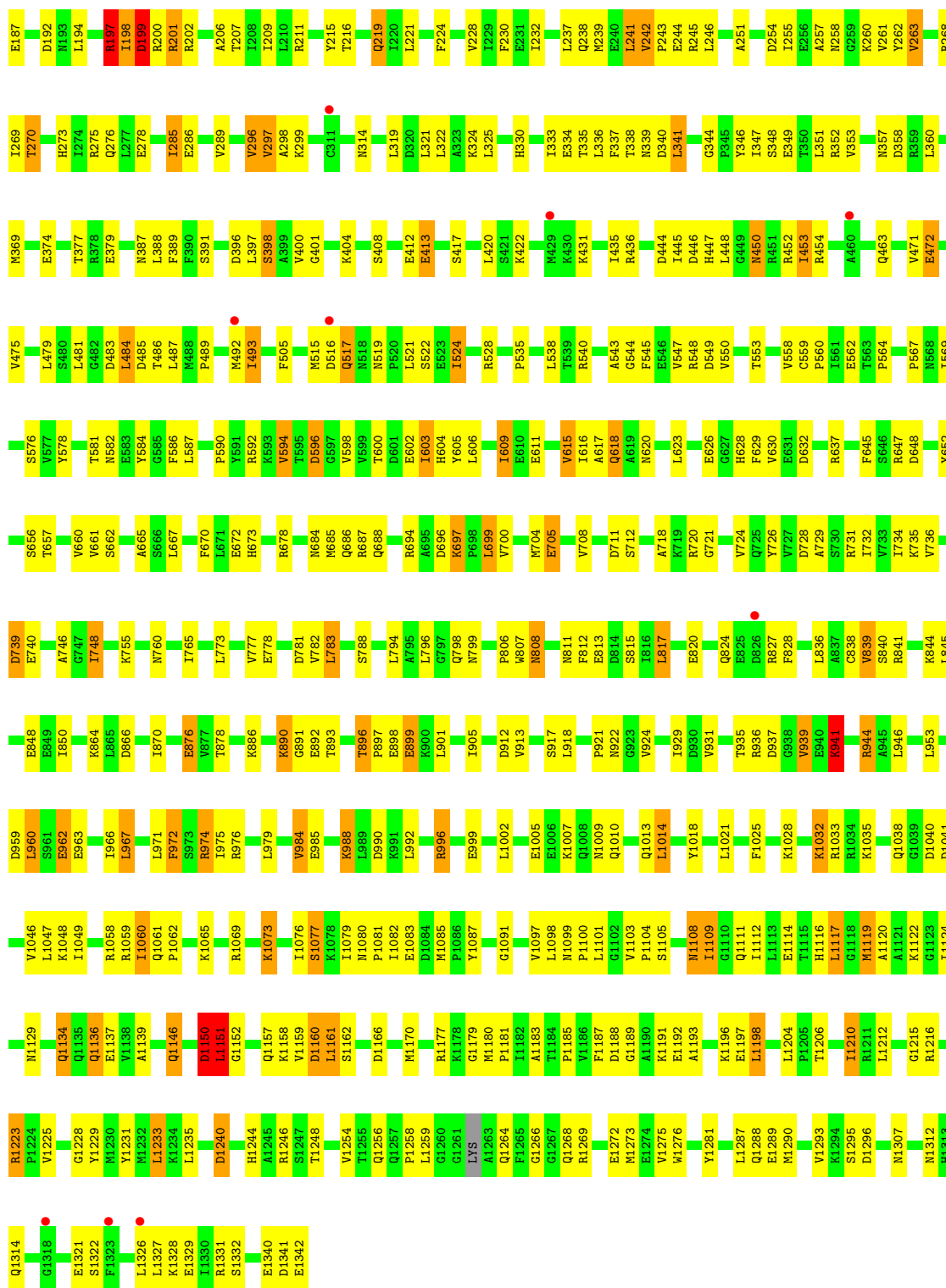


• Molecule 1: DNA-directed RNA polymerase subunit alpha

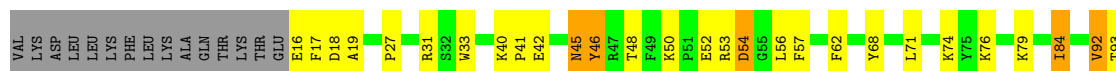


• Molecule 2: DNA-directed RNA polymerase subunit beta

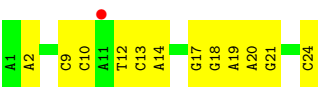




• Molecule 3: DNA-directed RNA polymerase subunit beta'



R1355	E1276	E1205	I1E	K983	V894	L783	N690	I591	L491	L368	N274	E197	Q94
L1356	G1277	R1206	PRO	L984	C896	L786	N697	Y592	N495	A373	N278	C198	Q98
F1357	E1278	V1209	GLN	E987	A896	T786	M698	N593	G496	P379	R278	E199	R97
A1359	E1281	I1210	SER	E983	Y899	S793	N700	Q594	E497	P379	L282	Q200	R98
Y1363	Y1282	S1211	GLY	Y989	R901	T797	N701	A595	P498	Y382	D289	R202	R99
Q1367	S1283	D1212	GLY	Y999	D902	R798	Q702	L596	I499	Y382	L290	E203	E100
R1372	E1215	E1216	LYS	A1004	S903	R799	T703	A597	I500	T394	E295	E204	R101
ARG	A1216	A1217	ASP	A1005	A904	V801	E704	K599	Q504	V401	E211	L205	E106
ALA	H1218	H1219	LEU	G1006	R906	D802	T707	A600	V506	V401	T208	E204	P110
ALA	D1219	I1220	PRO	E1009	R907	Q805	I708	S602	V507	L412	N209	S210	H113
ALA	I1220	L1221	ALA	Q1010	I908	D806	N708	K603	V507	D413	S210	E211	I114
GLY	R1221	R1222	LEU	Q1010	N910	L807	R709	Y609	L510	E414	S210	E211	W115
ALA	L1223	L1224	LYS	W1019	N910	V808	Q712	K599	T514	V415	L299	T212	F116
PRO	R1224	R1225	ILE	W1020	G912	V809	Q716	A600	C517	R417	E301	R214	L117
ALA	G1225	V1226	ASP	H1023	E913	T810	Q716	T601	P530	E418	D304	K216	K118
ALA	V1226		ALA	THR	A914	E811	Q716	S602	P530	P427	T317	L217	S119
PRO	V1229	V1230	GLN	THR	E925	D812	F719	K631	K531	L422	T316	L218	L120
GLN	T1230	R1231	GLY	MET	P926	D813	N720	A632	E532	R425	T317	K219	S122
THR	R1231	I1232	ASN	PRO	T931	C814	S721	A633	E534	A426	T317	R220	R123
ALA	Y1232	I1233	VAL	VAL	E935	G815	I722	A633	L536	P427	T317	I221	I124
GLU	I1233		LEU	THR	H936	H817	N725	A633	K531	H430	N320	L223	L127
ASP	E1236	E1237	ILE	GLU	I937	E818	A730	A633	E532	H430	N320	L224	L127
ALA	Q1238	Q1239	PRO	VAL	GLY	R842	R731	A633	R431	L432	K321	F227	R133
ALA	D1239	V1240	THR	PHE	GLY	A845	G732	I641	E534	L432	K321	V228	E136
LEU	Y1241	R1242	ARG	VAL	GLY	E946	A733	I646	R535	Q435	K325	Q229	R137
ALA	E1317		ALA	PHE	THR	V948	A735	F647	S539	E438	M330	N232	Y140
GLU	S1318		GLN	THR	THR	L849	I737	E648	H545	I442	K334	K233	F141
LEU	I1319		THR	ASP	ALA	K850	Q738	R649	V550	Q448	K334	P234	E142
ASN	I1320		THR	ASP	ALA	A854	R739	R650	B551	Q448	F338	E235	S143
ALA	A1323		ILE	ILE	SER	L857	L740	A657	T553	A459	R339	W236	Y144
GLY	S1324		GLY	ASP	ALA	V858	R744	E658	T553	A459	R339	V241	V145
GLY	Q1326		LYS	PRO	ALA	T862	G745	A661	E554	L343	L343	V244	I147
SER	E1327		ALA	PRO	GLU	H865	L746	A662	Y555	L343	L343	L245	Q158
ASP	T1328		VAL	THR	S948	Q867	N747	E663	A559	R346	R346	P246	T161
ASN	R1329		GLN	THR	Q951	Q867	I754	E666	N560	Q465	V347	L249	E162
ASN	I1256		LEU	ARG	Q951	Q867	I754	E666	L563	V468	D348	L252	Q164
GLU	R1257		THR	THR	L960	Q867	I754	E666	L563	V468	Y349	L252	Q164
GLU	R1258		ASP	THR	L960	Q867	I754	E666	L563	V468	Y349	L252	Q164
	L1261		GLY	ASP	V863	N875	P758	L672	V564	T473	R352	L255	D167
	R1262		VAL	GLY	V863	N875	P758	L672	V564	T473	R352	L255	D167
	K1263		GLN	LEU	V863	N875	P758	L672	V564	T473	R352	L255	D167
	T1265		ILE	THR	K972	V882	A761	E677	S568	E476	T356	D256	D174
			SER	GLY	K972	V882	A761	E677	S568	E476	T356	D256	D174
			SER	LEU	V875	V885	R764	E677	S568	E476	T356	D256	D174
			SER	SER	1975	V							



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	172.91Å 172.91Å 387.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.55 – 3.68 49.55 – 3.68	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.55-3.68) 98.3 (49.55-3.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.67Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.263 , 0.306 0.275 , 0.317	Depositor DCC
R_{free} test set	1971 reflections (3.05%)	wwPDB-VP
Wilson B-factor (Å ²)	175.9	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 122.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27705	wwPDB-VP
Average B, all atoms (Å ²)	182.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.14	0/1780	0.41	0/2415
1	B	0.17	0/1655	0.46	2/2247 (0.1%)
2	C	0.18	0/10634	0.42	2/14353 (0.0%)
3	D	0.15	0/9724	0.41	0/13134
4	E	0.12	0/629	0.35	0/847
5	F	0.17	0/2428	0.51	4/3280 (0.1%)
6	M	0.43	0/149	0.98	2/202 (1.0%)
7	N	0.28	0/666	0.44	0/1026
8	T	0.25	0/552	0.41	0/849
All	All	0.17	0/28217	0.43	10/38353 (0.0%)

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
1	B	0	1
2	C	0	5
3	D	0	3
5	F	0	1
6	M	0	1
All	All	0	11

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	517	GLN	N-CA-C	10.33	125.04	110.68
5	F	583	THR	CA-C-N	7.20	135.30	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	583	THR	C-N-CA	7.20	135.30	121.54
1	B	9	LEU	CA-C-N	5.65	131.87	121.70
1	B	9	LEU	C-N-CA	5.65	131.87	121.70
2	C	517	GLN	N-CA-CB	-5.63	103.36	110.45
6	M	18	SER	CA-C-N	5.33	131.30	121.70
6	M	18	SER	C-N-CA	5.33	131.30	121.70
5	F	584	ARG	CA-C-N	-5.06	112.81	122.53
5	F	584	ARG	C-N-CA	-5.06	112.81	122.53

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	14	VAL	Peptide
2	C	1150	ASP	Peptide
2	C	197	ARG	Peptide
2	C	198	ILE	Peptide
2	C	939	VAL	Peptide
2	C	941	LYS	Peptide
3	D	1166	GLY	Peptide
3	D	1168	GLU	Peptide
3	D	935	PHE	Peptide
5	F	584	ARG	Mainchain
6	M	16	PRO	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1759	0	1759	48	0
1	B	1638	0	1629	73	0
2	C	10470	0	10445	347	0
3	D	9578	0	9710	340	0
4	E	627	0	634	21	0
5	F	2399	0	2324	77	0
6	M	144	0	131	16	0
7	N	595	0	329	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	T	492	0	269	10	0
9	D	1	0	0	0	0
10	D	2	0	0	0	0
All	All	27705	0	27230	853	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 16.

All (853) 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:1006:GLY:N	3:D:1009:GLU:OE2	1.92	1.01
5:F:414:LYS:HB2	5:F:434:TRP:HE1	1.30	0.94
5:F:600:HIS:HE2	5:F:602:SER:HG	1.05	0.94
3:D:208:THR:O	3:D:214:ARG:NH1	2.01	0.92
1:B:76:GLU:OE2	1:B:132:HIS:ND1	2.05	0.88
2:C:99:LYS:NZ	2:C:119:GLU:OE2	2.09	0.84
2:C:953:LEU:HD11	2:C:1033:ARG:HG3	1.59	0.84
2:C:1192:GLU:OE1	3:D:764:ARG:NH1	2.11	0.83
2:C:1105:SER:HA	3:D:736:GLN:HE22	1.43	0.83
3:D:816:THR:HB	3:D:889:ASP:HB2	1.59	0.83
4:E:15:ASN:ND2	4:E:18:ASP:OD1	2.10	0.83
3:D:1263:LYS:HE3	3:D:1315:ALA:HB1	1.63	0.80
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.64	0.80
3:D:1158:GLU:OE2	3:D:1222:ARG:NH1	2.15	0.80
3:D:960:LEU:HB3	3:D:963:VAL:HG11	1.65	0.78
3:D:842:ARG:HH22	3:D:1250:ASP:HB2	1.49	0.77
5:F:474:MET:HG3	5:F:478:PRO:HB3	1.67	0.77
2:C:516:ASP:OD1	2:C:522:SER:OG	2.03	0.77
2:C:337:PHE:HD1	2:C:338:THR:H	1.32	0.77
7:N:13:DA:H61	8:T:12:DT:H3	1.29	0.77
3:D:1275:LEU:HB3	3:D:1278:GLU:HB2	1.65	0.77
2:C:941:LYS:HG3	2:C:946:LEU:HG	1.67	0.76
3:D:42:GLU:OE2	5:F:451:ARG:NE	2.18	0.75
5:F:584:ARG:H	5:F:587:ILE:HD13	1.50	0.75
2:C:1223:ARG:NH2	3:D:719:PHE:O	2.19	0.74
2:C:700:VAL:O	2:C:1069:ARG:NH2	2.20	0.74
5:F:572:THR:HG23	5:F:575:GLU:HB2	1.68	0.73
2:C:1312:ASN:HD21	2:C:1314:GLN:HE21	1.34	0.73
2:C:1005:GLU:HG2	2:C:1007:LYS:H	1.54	0.72
2:C:39:ILE:HD11	2:C:75:LEU:HG	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:452:ARG:NH1	2:C:584:TYR:O	2.21	0.72
1:A:197:ASP:OD1	1:A:197:ASP:N	2.23	0.72
2:C:1146:GLN:NE2	2:C:1150:ASP:OD1	2.23	0.72
2:C:199:ASP:O	2:C:201:ARG:N	2.22	0.71
2:C:686:GLN:HG2	2:C:796:LEU:HD22	1.73	0.71
1:B:9:LEU:HA	1:B:10:LYS:HB3	1.72	0.71
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.72	0.71
3:D:140:TYR:OH	3:D:312:ARG:NH1	2.24	0.71
1:A:159:ILE:HG13	1:A:162:GLU:HB2	1.73	0.70
3:D:1239:ASP:OD1	3:D:1242:ARG:NH2	2.24	0.70
2:C:21:VAL:HG11	2:C:592:ARG:HD2	1.73	0.70
2:C:242:VAL:HG13	2:C:244:GLU:H	1.54	0.70
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.72	0.70
2:C:905:ILE:HG12	5:F:595:LEU:HD22	1.74	0.69
2:C:528:ARG:NH2	2:C:576:SER:O	2.25	0.69
2:C:1246:ARG:HD2	2:C:1266:GLY:H	1.58	0.69
2:C:924:VAL:HG12	2:C:1058:ARG:HH22	1.57	0.68
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.75	0.68
2:C:26:TYR:O	2:C:29:SER:OG	2.11	0.68
2:C:976:ARG:NH1	2:C:990:ASP:OD1	2.26	0.68
3:D:478:LEU:HG	4:E:47:THR:HG22	1.75	0.68
1:B:75:GLN:HG2	1:B:132:HIS:HE1	1.57	0.68
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.74	0.68
3:D:746:LEU:HD13	3:D:754:ILE:HD11	1.74	0.67
2:C:100:LEU:HD12	2:C:489:PRO:HB3	1.74	0.67
1:B:182:ARG:NH1	3:D:534:GLU:OE1	2.27	0.67
1:B:182:ARG:NH1	3:D:581:MET:SD	2.67	0.67
3:D:325:LYS:HD3	5:F:508:GLU:HG2	1.77	0.67
1:A:195:ARG:HG2	1:A:198:LEU:HG	1.75	0.67
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.75	0.67
3:D:576:ARG:NH1	3:D:593:ASN:O	2.27	0.67
2:C:962:GLU:O	2:C:966:ILE:HG12	1.95	0.67
4:E:40:PRO:O	4:E:52:ARG:NH2	2.28	0.67
1:B:109:PRO:HA	1:B:132:HIS:HA	1.76	0.67
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.59	0.67
2:C:202:ARG:HD3	2:C:369:MET:HG2	1.75	0.67
3:D:1206:ARG:NH2	3:D:1223:LEU:O	2.28	0.67
2:C:1073:LYS:HG2	3:D:462:ASP:HB2	1.75	0.66
3:D:205:LEU:O	3:D:214:ARG:NH2	2.28	0.66
5:F:414:LYS:HB2	5:F:434:TRP:NE1	2.09	0.66
2:C:42:ASP:OD2	2:C:46:GLN:HB3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1161:GLY:HA3	3:D:1178:THR:O	1.96	0.66
3:D:223:LEU:O	3:D:227:PHE:HB2	1.96	0.66
3:D:926:PRO:HG2	3:D:1248:ILE:HD11	1.77	0.66
5:F:441:ARG:NH2	7:N:21:DG:OP2	2.29	0.66
2:C:239:MET:HB3	2:C:285:ILE:HD12	1.77	0.66
2:C:808:ASN:H	3:D:633:ALA:HB2	1.61	0.66
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.78	0.65
3:D:850:LYS:HD3	3:D:854:ALA:HB3	1.78	0.65
3:D:1144:LEU:HD11	3:D:1236:GLU:HB3	1.77	0.65
1:A:45:ARG:NH1	1:B:34:GLY:O	2.30	0.65
2:C:812:PHE:O	3:D:504:GLN:NE2	2.29	0.65
1:B:190:ALA:HB2	1:B:200:LYS:HB2	1.78	0.65
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.61	0.65
3:D:736:GLN:HG3	6:M:1:GLY:HA3	1.77	0.65
6:M:8:GLU:N	6:M:18:SER:O	2.21	0.65
2:C:864:LYS:NZ	2:C:876:GLU:O	2.26	0.65
3:D:613:GLY:O	3:D:617:THR:OG1	2.13	0.64
3:D:362:ARG:H	3:D:365:GLN:HE21	1.43	0.64
3:D:612:LEU:HB3	3:D:616:PRO:HG3	1.79	0.64
2:C:199:ASP:C	2:C:201:ARG:H	2.05	0.64
2:C:739:ASP:OD1	2:C:739:ASP:N	2.26	0.64
3:D:818:GLU:HB3	3:D:887:SER:HB2	1.80	0.64
3:D:220:ARG:O	3:D:224:LEU:HG	1.98	0.64
3:D:664:ILE:HD12	3:D:682:VAL:HG22	1.80	0.64
3:D:1284:ARG:NH1	3:D:1317:GLU:OE2	2.31	0.64
3:D:1357:ILE:HG22	3:D:1359:ALA:H	1.63	0.64
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.79	0.64
2:C:811:ASN:O	2:C:1099:ASN:ND2	2.31	0.63
2:C:1065:LYS:HD3	2:C:1235:LEU:HD12	1.80	0.63
3:D:200:GLN:O	3:D:204:GLU:HG2	1.98	0.63
3:D:1230:THR:HB	3:D:1257:VAL:HG11	1.80	0.63
2:C:268:ARG:HH22	2:C:270:THR:HG23	1.64	0.63
3:D:1286:LYS:O	3:D:1290:ARG:HB2	1.98	0.63
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.26	0.63
3:D:210:SER:O	3:D:213:LYS:N	2.31	0.62
1:B:195:ARG:HB3	1:B:198:LEU:CD2	2.30	0.62
2:C:959:ASP:O	2:C:963:GLU:HG2	1.98	0.62
3:D:54:ASP:N	3:D:54:ASP:OD1	2.32	0.62
3:D:517:CYS:HA	3:D:716:GLN:HE22	1.63	0.62
2:C:27:LEU:O	2:C:528:ARG:NH1	2.32	0.62
2:C:598:VAL:HG22	2:C:628:HIS:HE1	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.79	0.62
2:C:841:ARG:HA	2:C:1046:VAL:HA	1.80	0.62
3:D:846:GLU:HG2	3:D:881:LYS:HB3	1.80	0.62
3:D:1232:TYR:HD1	3:D:1233:ILE:HD12	1.62	0.62
5:F:483:LEU:HD13	5:F:483:LEU:H	1.64	0.62
2:C:517:GLN:HG2	2:C:517:GLN:O	2.00	0.62
3:D:418:GLU:HG3	4:E:45:LYS:H	1.65	0.62
2:C:1119:MET:HE1	2:C:1210:ILE:HD11	1.82	0.61
4:E:50:ALA:O	4:E:54:ILE:HG12	1.99	0.61
2:C:516:ASP:O	2:C:522:SER:OG	2.19	0.61
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.83	0.61
3:D:19:ALA:HB2	3:D:1343:GLU:HG3	1.81	0.61
5:F:449:THR:OG1	5:F:503:GLU:OE2	2.16	0.61
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.81	0.61
3:D:1167:LYS:HZ3	3:D:1170:LYS:HD2	1.65	0.61
5:F:426:LYS:HD3	7:N:27:DA:H3'	1.82	0.61
1:B:91:ARG:HG3	1:B:122:GLU:HB3	1.82	0.61
1:A:75:GLN:HG3	1:A:76:GLU:OE2	2.01	0.61
2:C:1160:ASP:OD1	2:C:1161:LEU:N	2.34	0.61
3:D:678:ARG:O	3:D:682:VAL:HG23	2.01	0.61
2:C:113:THR:O	2:C:115:LYS:N	2.34	0.60
3:D:1162:ILE:HG23	3:D:1178:THR:HB	1.83	0.60
5:F:383:ASN:HB2	5:F:412:LEU:HD21	1.82	0.60
2:C:936:ARG:HH21	2:C:939:VAL:HG21	1.66	0.60
3:D:893:GLY:O	3:D:1258:ARG:NH1	2.31	0.60
3:D:1155:ILE:HD11	3:D:1211:SER:HB3	1.83	0.60
4:E:25:ARG:NH1	4:E:65:ASP:OD1	2.34	0.60
5:F:420:GLU:OE1	5:F:423:ARG:NH2	2.33	0.60
2:C:104:ILE:O	2:C:115:LYS:HA	2.01	0.60
3:D:741:ALA:O	3:D:762:ASN:ND2	2.34	0.60
3:D:746:LEU:HD23	3:D:758:PRO:HG3	1.83	0.60
2:C:732:ILE:HG21	2:C:783:LEU:HD12	1.84	0.60
3:D:1323:ALA:HB1	3:D:1328:THR:HG23	1.82	0.60
3:D:739:GLN:HG3	6:M:10:PHE:HE2	1.67	0.60
3:D:1172:LYS:HA	3:D:1191:PRO:HA	1.81	0.60
8:T:13:DC:H2''	8:T:14:DA:C8	2.36	0.60
2:C:1212:LEU:HD22	2:C:1225:VAL:HG21	1.83	0.60
3:D:1005:LYS:HD2	3:D:1009:GLU:HG3	1.82	0.60
2:C:941:LYS:H	2:C:941:LYS:HD3	1.67	0.59
2:C:1009:ASN:O	2:C:1013:GLN:HG2	2.02	0.59
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:454:VAL:HA	5:F:457:ILE:HD12	1.84	0.59
2:C:67:GLU:HB3	2:C:103:VAL:HG22	1.83	0.59
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.82	0.59
2:C:734:ILE:HD11	2:C:783:LEU:HD11	1.84	0.59
2:C:971:LEU:HD22	2:C:1018:TYR:HD2	1.67	0.58
3:D:1363:TYR:O	3:D:1367:GLN:N	2.29	0.58
2:C:337:PHE:HD1	2:C:338:THR:N	2.01	0.58
2:C:578:TYR:HE2	2:C:656:SER:HB3	1.68	0.58
3:D:317:THR:OG1	3:D:320:ASN:O	2.22	0.58
5:F:119:ILE:HG23	5:F:375:ALA:HB1	1.84	0.58
1:A:51:MET:HE3	1:A:52:PRO:HD2	1.85	0.58
1:B:195:ARG:HB3	1:B:198:LEU:HD21	1.85	0.58
3:D:809:VAL:HB	3:D:912:GLY:H	1.69	0.58
2:C:138:ILE:HG22	2:C:139:ASN:HD22	1.67	0.58
2:C:211:ARG:NH1	2:C:357:ASN:O	2.37	0.58
2:C:389:PHE:HB3	2:C:420:LEU:HD12	1.85	0.58
1:B:191:ARG:NH2	3:D:413:ASP:OD2	2.37	0.58
2:C:185:ASP:HB2	2:C:197:ARG:HG3	1.86	0.58
2:C:431:LYS:O	2:C:435:ILE:HG12	2.03	0.58
3:D:709:ARG:O	3:D:709:ARG:NE	2.37	0.58
2:C:870:ILE:HG21	2:C:931:VAL:HG11	1.87	0.57
3:D:264:ASP:OD1	3:D:264:ASP:N	2.34	0.57
5:F:106:GLY:HA2	5:F:385:ARG:HH12	1.69	0.57
8:T:20:DA:H1'	8:T:21:DG:H5'	1.86	0.57
1:A:26:VAL:HG22	1:A:203:ILE:HB	1.85	0.57
2:C:840:SER:HB3	2:C:1048:LYS:HG2	1.85	0.57
2:C:1122:LYS:HG2	2:C:1229:TYR:CZ	2.39	0.57
2:C:1119:MET:HG3	2:C:1204:LEU:HD13	1.86	0.57
3:D:278:ARG:HD2	3:D:295:GLU:OE2	2.04	0.57
3:D:490:ILE:HG22	3:D:500:ILE:HG13	1.85	0.57
2:C:685:MET:HA	2:C:688:GLN:HE21	1.70	0.57
3:D:68:TYR:HA	3:D:92:VAL:HG23	1.87	0.57
5:F:105:MET:HE1	5:F:385:ARG:HG2	1.87	0.57
2:C:836:LEU:HD21	2:C:921:PRO:HD3	1.85	0.57
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.87	0.57
3:D:813:ASP:OD1	3:D:814:CYS:N	2.38	0.57
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.87	0.57
3:D:657:ALA:O	3:D:661:VAL:HG13	2.04	0.57
2:C:820:GLU:HA	2:C:1079:ILE:HD11	1.86	0.56
3:D:432:LEU:HD21	3:D:489:ASN:HB3	1.86	0.56
6:M:5:HIS:O	6:M:5:HIS:ND1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ASP:O	1:B:81:ILE:HG12	2.05	0.56
3:D:975:ILE:HD13	3:D:980:THR:HG21	1.86	0.56
2:C:598:VAL:HG22	2:C:628:HIS:CE1	2.41	0.56
3:D:57:PHE:HD2	3:D:98:ARG:HH22	1.52	0.56
2:C:299:LYS:HE3	2:C:334:GLU:HG3	1.88	0.56
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.53	0.56
3:D:161:THR:HG22	3:D:164:GLN:HG3	1.85	0.56
1:B:190:ALA:N	1:B:198:LEU:O	2.27	0.56
2:C:1120:ALA:HB1	2:C:1198:LEU:HD12	1.87	0.56
3:D:382:TYR:HE1	3:D:401:VAL:HG21	1.71	0.56
3:D:917:VAL:HG12	3:D:921:GLN:HE21	1.70	0.56
7:N:22:DT:H2''	7:N:23:DT:H5''	1.87	0.56
1:A:72:GLU:OE2	2:C:726:TYR:OH	2.23	0.56
1:B:18:GLN:HA	1:B:18:GLN:HE21	1.70	0.56
2:C:224:PHE:CD2	2:C:347:ILE:HG13	2.41	0.56
2:C:238:GLN:HG2	2:C:286:GLU:HG2	1.88	0.56
3:D:127:LEU:HD11	3:D:194:LEU:HD21	1.87	0.56
8:T:9:DC:H1'	8:T:10:DC:H5'	1.87	0.56
1:B:155:ALA:HB1	1:B:172:LEU:HB3	1.88	0.56
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.32	0.56
5:F:588:ARG:O	5:F:588:ARG:NE	2.37	0.56
6:M:7:PRO:HA	6:M:19:PHE:H	1.69	0.56
3:D:905:ARG:H	3:D:905:ARG:HD2	1.71	0.56
3:D:1173:ARG:HB2	3:D:1192:LYS:HB3	1.88	0.56
5:F:588:ARG:HH21	5:F:592:ALA:HB2	1.71	0.56
2:C:1119:MET:HE3	2:C:1204:LEU:HD22	1.88	0.55
3:D:527:LEU:HB2	3:D:550:VAL:HG12	1.88	0.55
5:F:482:GLU:O	5:F:485:GLU:HG3	2.06	0.55
2:C:142:GLU:OE2	2:C:515:MET:SD	2.64	0.55
2:C:1272:GLU:OE2	3:D:798:ARG:NH2	2.38	0.55
3:D:232:ASN:HD22	3:D:232:ASN:N	2.05	0.55
3:D:1265:THR:N	3:D:1305:ASP:OD2	2.38	0.55
3:D:491:LEU:HD11	3:D:610:ARG:HH12	1.70	0.55
3:D:972:LYS:HD3	3:D:1004:ALA:HA	1.88	0.55
8:T:19:DA:H2''	8:T:20:DA:H5'	1.88	0.55
3:D:394:ILE:HG23	5:F:536:THR:HG22	1.89	0.55
3:D:1348:LYS:O	3:D:1352:ILE:HG12	2.07	0.55
1:A:113:ALA:HB2	1:A:126:PRO:HB3	1.89	0.55
3:D:810:THR:O	3:D:1363:TYR:OH	2.24	0.55
2:C:1069:ARG:HG2	2:C:1233:LEU:HD21	1.87	0.55
3:D:722:ILE:HA	3:D:725:MET:HE3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:786:THR:HG23	6:M:7:PRO:HD3	1.88	0.55
5:F:379:MET:O	5:F:383:ASN:ND2	2.39	0.55
3:D:1238:GLN:O	3:D:1242:ARG:HB2	2.07	0.55
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.87	0.55
2:C:960:LEU:HB3	2:C:1025:PHE:HE2	1.72	0.55
2:C:1160:ASP:OD1	2:C:1162:SER:N	2.40	0.55
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.89	0.54
2:C:1062:PRO:HA	2:C:1076:ILE:HG22	1.89	0.54
3:D:268:LEU:HD21	3:D:324:LEU:HD13	1.89	0.54
2:C:562:GLU:OE2	2:C:662:SER:OG	2.15	0.54
2:C:616:ILE:HG13	2:C:652:TYR:HB2	1.88	0.54
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.89	0.54
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.88	0.54
5:F:606:VAL:O	5:F:609:SER:OG	2.20	0.54
2:C:731:ARG:NH2	2:C:962:GLU:OE2	2.40	0.54
2:C:890:LYS:NZ	2:C:891:GLY:O	2.41	0.54
2:C:898:GLU:OE1	2:C:898:GLU:N	2.40	0.54
2:C:1258:PRO:HD2	3:D:346:ARG:HB2	1.89	0.54
2:C:1289:GLU:OE2	3:D:473:THR:HG22	2.06	0.54
3:D:147:ILE:HG13	3:D:177:ASP:HB3	1.89	0.54
5:F:600:HIS:NE2	5:F:602:SER:OG	2.25	0.54
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.89	0.54
6:M:7:PRO:HA	6:M:19:PHE:N	2.22	0.54
1:B:192:VAL:HB	1:B:195:ARG:HG2	1.90	0.54
2:C:158:ASP:OD1	2:C:159:SER:N	2.40	0.54
2:C:734:ILE:HD12	2:C:777:VAL:HG21	1.90	0.54
3:D:214:ARG:O	3:D:218:THR:HG22	2.08	0.54
3:D:412:LEU:HA	3:D:415:VAL:HG22	1.90	0.54
1:B:60:GLU:O	1:B:142:MET:HB2	2.08	0.54
2:C:748:ILE:HD11	2:C:966:ILE:HG22	1.89	0.54
2:C:960:LEU:HB3	2:C:1025:PHE:CE2	2.43	0.54
2:C:1060:ILE:HD11	2:C:1076:ILE:HG12	1.90	0.54
2:C:1105:SER:HA	3:D:736:GLN:NE2	2.19	0.54
3:D:739:GLN:HG3	6:M:10:PHE:CE2	2.42	0.54
5:F:561:MET:HA	5:F:567:MET:HE1	1.90	0.53
2:C:40:GLU:O	2:C:73:TYR:OH	2.25	0.53
2:C:721:GLY:N	2:C:740:GLU:OE1	2.41	0.53
3:D:1328:THR:HG22	3:D:1332:LEU:HD23	1.89	0.53
2:C:142:GLU:OE2	2:C:515:MET:HE1	2.09	0.53
1:B:99:ILE:HA	1:B:144:ILE:O	2.09	0.53
2:C:176:ILE:HD12	2:C:184:LEU:HD23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:268:ARG:NH2	2:C:270:THR:HG23	2.24	0.53
2:C:670:PHE:HZ	2:C:1117:LEU:HD13	1.74	0.53
2:C:412:GLU:HB3	2:C:413:GLU:OE2	2.09	0.53
2:C:349:GLU:O	2:C:353:VAL:HG23	2.09	0.53
2:C:971:LEU:HG	2:C:1014:LEU:HD23	1.90	0.53
3:D:473:THR:HG23	3:D:476:ALA:H	1.72	0.53
1:B:100:LEU:HD11	1:B:121:VAL:HG21	1.90	0.53
3:D:555:TYR:HB3	3:D:563:LEU:HD21	1.90	0.53
3:D:648:GLU:OE1	3:D:648:GLU:N	2.42	0.53
2:C:489:PRO:O	2:C:493:ILE:HG22	2.08	0.53
3:D:50:LYS:HB3	3:D:71:LEU:HD11	1.91	0.53
5:F:530:LEU:HD23	5:F:530:LEU:H	1.73	0.53
7:N:1:DG:H2"	7:N:2:DA:C8	2.43	0.53
1:A:74:VAL:HG22	1:A:76:GLU:H	1.74	0.53
3:D:658:GLU:O	3:D:661:VAL:HG22	2.09	0.53
5:F:492:ASP:OD1	5:F:492:ASP:N	2.42	0.53
1:B:9:LEU:HA	1:B:10:LYS:CB	2.37	0.52
1:B:82:LEU:HD22	1:B:173:VAL:HG22	1.90	0.52
2:C:1100:PRO:O	2:C:1104:PRO:HD3	2.09	0.52
1:B:193:GLU:HG3	1:B:194:GLN:HG3	1.91	0.52
2:C:408:SER:O	2:C:431:LYS:NZ	2.42	0.52
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.90	0.52
3:D:559:ALA:O	3:D:560:ASN:ND2	2.42	0.52
3:D:700:ASN:O	3:D:704:GLU:HB2	2.09	0.52
4:E:39:VAL:HG22	4:E:40:PRO:HD2	1.90	0.52
6:M:8:GLU:HB2	6:M:18:SER:HB2	1.91	0.52
2:C:199:ASP:C	2:C:201:ARG:N	2.68	0.52
2:C:1119:MET:HE3	2:C:1204:LEU:HB3	1.92	0.52
3:D:478:LEU:HB3	4:E:20:VAL:HG13	1.92	0.52
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.92	0.52
2:C:118:LYS:NZ	2:C:485:ASP:OD1	2.40	0.52
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.45	0.52
2:C:521:LEU:HB2	2:C:794:LEU:HD21	1.92	0.52
2:C:798:GLN:HB2	2:C:828:PHE:HE1	1.74	0.52
3:D:845:ALA:HB3	3:D:881:LYS:HG2	1.91	0.52
5:F:411:GLY:O	5:F:434:TRP:HD1	1.92	0.52
5:F:412:LEU:HD13	5:F:435:ILE:HD11	1.92	0.52
1:A:227:GLN:NE2	1:B:9:LEU:O	2.43	0.52
2:C:148:GLN:NE2	2:C:535:PRO:O	2.42	0.52
3:D:747:MET:SD	3:D:747:MET:N	2.83	0.52
3:D:793:SER:O	3:D:797:THR:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:14:ASP:HA	2:C:1183:ALA:HB3	1.91	0.52
2:C:975:ILE:HG13	2:C:1014:LEU:HD22	1.91	0.52
3:D:744:ARG:HG3	3:D:759:ILE:HB	1.91	0.52
1:B:136:GLU:C	1:B:138:ALA:H	2.17	0.52
3:D:847:ASP:OD1	3:D:847:ASP:N	2.42	0.52
3:D:233:LYS:HB3	3:D:235:GLU:OE2	2.09	0.52
3:D:334:LYS:HA	3:D:339:ARG:HD2	1.92	0.52
1:B:16:ILE:HG23	1:B:25:LYS:O	2.09	0.52
5:F:583:THR:HG22	5:F:584:ARG:HB2	1.92	0.52
1:B:28:LEU:HG	1:B:31:LEU:HD21	1.92	0.51
2:C:1085:MET:HE2	2:C:1085:MET:HA	1.92	0.51
3:D:93:THR:HG22	3:D:94:GLN:H	1.75	0.51
3:D:495:ASN:HD22	3:D:497:GLU:HB2	1.74	0.51
3:D:812:ASP:O	3:D:896:ALA:N	2.42	0.51
3:D:1198:VAL:HG23	3:D:1204:VAL:HG11	1.92	0.51
5:F:586:ARG:NH1	5:F:589:GLN:OE1	2.43	0.51
1:A:154:PRO:HB2	2:C:1059:ARG:NH2	2.25	0.51
8:T:12:DT:H2"	8:T:13:DC:C6	2.45	0.51
1:B:81:ILE:O	1:B:85:LEU:HG	2.09	0.51
1:B:152:TYR:HB2	3:D:535:ARG:HH21	1.75	0.51
2:C:230:PHE:HD2	2:C:335:THR:HG21	1.76	0.51
3:D:1019:ASN:OD1	3:D:1020:TRP:N	2.44	0.51
5:F:562:ARG:HG2	5:F:591:GLU:OE2	2.10	0.51
2:C:27:LEU:HD12	2:C:711:ASP:HB2	1.92	0.51
2:C:728:ASP:OD1	2:C:729:ALA:N	2.44	0.51
1:A:58:GLU:HB2	1:A:145:LYS:HD2	1.91	0.51
2:C:263:VAL:HG22	2:C:273:HIS:CD2	2.45	0.51
3:D:356:THR:OG1	3:D:357:VAL:N	2.44	0.51
2:C:321:LEU:HD23	2:C:324:LYS:HD2	1.92	0.51
2:C:1105:SER:HB2	3:D:731:ARG:HG3	1.92	0.51
3:D:430:HIS:CD2	3:D:432:LEU:HB2	2.45	0.51
3:D:733:SER:O	3:D:737:ILE:HG12	2.11	0.51
3:D:1162:ILE:O	3:D:1178:THR:OG1	2.18	0.51
1:B:102:LEU:O	1:B:141:SER:HA	2.11	0.51
2:C:322:LEU:HD23	2:C:325:LEU:HD21	1.91	0.51
1:A:14:VAL:HG22	1:A:15:ASP:H	1.75	0.51
1:A:60:GLU:HB2	1:A:170:ARG:HG2	1.93	0.51
2:C:1276:TRP:CZ2	3:D:801:VAL:HG21	2.44	0.51
3:D:123:ARG:HD2	3:D:1337:VAL:HG21	1.93	0.51
3:D:518:VAL:HG11	3:D:707:ILE:HD13	1.91	0.51
3:D:813:ASP:OD1	3:D:815:GLY:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1325:PHE:CD2	3:D:1326:GLN:HG3	2.46	0.51
1:B:11:PRO:HG3	1:B:31:LEU:HD13	1.92	0.51
3:D:322:ARG:HG2	3:D:323:PRO:HD2	1.93	0.51
3:D:848:VAL:HG11	3:D:858:VAL:HG23	1.93	0.51
2:C:548:ARG:NH2	2:C:567:PRO:O	2.44	0.50
3:D:42:GLU:N	3:D:42:GLU:OE1	2.44	0.50
3:D:1173:ARG:CB	3:D:1192:LYS:HB3	2.41	0.50
3:D:317:THR:OG1	3:D:322:ARG:O	2.18	0.50
5:F:584:ARG:N	5:F:587:ILE:HD13	2.24	0.50
2:C:12:ARG:O	2:C:1157:GLN:NE2	2.45	0.50
2:C:890:LYS:HG3	2:C:891:GLY:N	2.26	0.50
2:C:941:LYS:HD3	2:C:941:LYS:N	2.25	0.50
2:C:1329:GLU:O	2:C:1332:SER:OG	2.29	0.50
3:D:62:PHE:O	3:D:101:ARG:HD2	2.10	0.50
1:A:23:HIS:HB2	1:A:205:MET:O	2.12	0.50
1:B:44:ARG:HA	1:B:183:ILE:HD13	1.92	0.50
2:C:198:ILE:O	2:C:199:ASP:O	2.29	0.50
2:C:798:GLN:HE22	2:C:827:ARG:HB2	1.77	0.50
3:D:507:VAL:HG11	3:D:598:LYS:HB2	1.92	0.50
3:D:110:PRO:HD2	3:D:183:GLU:HG2	1.94	0.50
3:D:1318:SER:OG	3:D:1342:ASP:OD2	2.10	0.50
5:F:380:VAL:HG13	5:F:412:LEU:HD23	1.93	0.50
1:A:11:PRO:HD2	1:B:227:GLN:NE2	2.26	0.50
2:C:450:ASN:N	2:C:450:ASN:OD1	2.45	0.50
2:C:487:LEU:HD23	2:C:487:LEU:H	1.75	0.50
7:N:8:DC:H2"	7:N:9:DC:C6	2.47	0.50
2:C:543:ALA:O	2:C:548:ARG:NH1	2.44	0.50
5:F:489:MET:HB3	5:F:493:LYS:HG3	1.94	0.49
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.93	0.49
1:A:196:THR:OG1	1:A:197:ASP:OD1	2.27	0.49
2:C:206:ALA:O	2:C:209:ILE:HG22	2.12	0.49
3:D:282:LEU:HD21	5:F:410:ILE:HG12	1.93	0.49
1:A:31:LEU:HD21	1:A:39:LEU:HD12	1.94	0.49
2:C:255:ILE:HD12	2:C:263:VAL:HG23	1.94	0.49
2:C:257:ALA:HB3	2:C:262:TYR:HE1	1.77	0.49
2:C:1101:LEU:HB3	3:D:731:ARG:HD3	1.95	0.49
3:D:45:ASN:HB3	3:D:48:THR:O	2.12	0.49
1:A:215:GLU:OE2	1:A:219:ARG:NH2	2.45	0.49
1:B:182:ARG:HD3	1:B:206:GLU:OE2	2.11	0.49
2:C:735:LYS:HA	2:C:748:ILE:HG22	1.93	0.49
2:C:1340:GLU:HB2	3:D:19:ALA:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:291:ILE:HD13	5:F:409:ASN:HB3	1.94	0.49
3:D:909:ILE:HD11	3:D:913:GLU:HB3	1.94	0.49
2:C:996:ARG:HD2	2:C:999:GLU:OE2	2.13	0.49
5:F:452:ILE:HG13	5:F:457:ILE:HD11	1.95	0.49
1:B:225:ALA:O	1:B:229:GLU:N	2.46	0.49
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.93	0.49
2:C:684:ASN:OD1	2:C:687:ARG:NH1	2.46	0.49
3:D:362:ARG:N	3:D:365:GLN:HE21	2.11	0.49
2:C:603:ILE:HD13	2:C:603:ILE:H	1.77	0.49
3:D:1284:ARG:HH12	3:D:1317:GLU:HG3	1.77	0.49
3:D:1295:ASN:OD1	3:D:1296:GLY:N	2.46	0.49
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.27	0.49
1:A:48:LEU:HA	1:A:180:VAL:HG21	1.94	0.49
2:C:251:ALA:H	2:C:268:ARG:HA	1.77	0.49
2:C:678:ARG:NH2	6:M:21:GLY:O	2.46	0.49
2:C:901:LEU:O	2:C:905:ILE:HG13	2.13	0.49
3:D:352:ARG:HE	3:D:465:GLN:NE2	2.10	0.49
3:D:978:ARG:CZ	3:D:999:TYR:HB3	2.42	0.49
6:M:11:VAL:HG11	6:M:17:ILE:CD1	2.42	0.49
2:C:632:ASP:N	2:C:632:ASP:OD1	2.39	0.48
3:D:40:LYS:HB3	3:D:42:GLU:OE1	2.13	0.48
1:B:60:GLU:N	1:B:143:ARG:O	2.46	0.48
2:C:187:GLU:OE2	2:C:197:ARG:NH2	2.46	0.48
1:B:191:ARG:NH1	3:D:413:ASP:OD1	2.41	0.48
3:D:744:ARG:HG2	3:D:761:ALA:O	2.13	0.48
3:D:805:GLN:HE22	3:D:1348:LYS:HD2	1.78	0.48
4:E:32:VAL:O	4:E:34:GLY:N	2.42	0.48
2:C:24:VAL:HG21	2:C:704:MET:HE1	1.95	0.48
2:C:446:ASP:OD2	2:C:547:VAL:HA	2.14	0.48
2:C:447:HIS:CE1	2:C:553:THR:HG21	2.49	0.48
2:C:1116:HIS:CE1	3:D:641:ILE:HB	2.48	0.48
3:D:364:HIS:O	3:D:364:HIS:ND1	2.47	0.48
1:B:19:VAL:HB	1:B:23:HIS:HB3	1.95	0.48
2:C:813:GLU:HA	3:D:504:GLN:NE2	2.28	0.48
1:B:33:ARG:HH11	2:C:1081:PRO:HG3	1.78	0.48
2:C:1120:ALA:O	2:C:1124:ILE:HG12	2.14	0.48
2:C:16:GLY:HA3	2:C:1188:ASP:OD2	2.14	0.48
2:C:617:ALA:N	2:C:652:TYR:O	2.40	0.48
3:D:527:LEU:HD21	3:D:536:LEU:HG	1.95	0.48
3:D:745:GLY:O	3:D:758:PRO:HB3	2.13	0.48
3:D:1191:PRO:HB2	3:D:1194:ARG:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:216:THR:OG1	2:C:219:GLN:OE1	2.29	0.48
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.96	0.48
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.48	0.48
2:C:1259:LEU:HB2	3:D:346:ARG:HD2	1.95	0.48
2:C:1342:GLU:OXT	3:D:18:ASP:OD2	2.32	0.48
2:C:1069:ARG:HD3	2:C:1231:TYR:HD2	1.79	0.48
2:C:341:LEU:H	2:C:341:LEU:HG	1.36	0.48
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.96	0.48
6:M:2:GLY:O	6:M:20:TYR:HA	2.14	0.47
2:C:606:LEU:HD23	2:C:611:GLU:HA	1.96	0.47
3:D:850:LYS:HE2	3:D:875:ASN:ND2	2.29	0.47
2:C:138:ILE:HD13	2:C:143:ARG:HD3	1.94	0.47
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.95	0.47
3:D:487:THR:HG21	4:E:4:VAL:HG23	1.96	0.47
7:N:27:DA:H2''	7:N:28:DA:H5'	1.96	0.47
1:A:27:THR:HA	1:A:201:LEU:O	2.15	0.47
1:B:152:TYR:HB2	3:D:535:ARG:NH2	2.29	0.47
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.15	0.47
2:C:1273:MET:HA	2:C:1276:TRP:CE3	2.50	0.47
3:D:217:LEU:O	3:D:221:ILE:HG22	2.14	0.47
3:D:802:ASP:OD2	3:D:1325:PHE:CD2	2.67	0.47
5:F:444:ALA:HB1	5:F:457:ILE:HD13	1.97	0.47
7:N:9:DC:H2''	7:N:10:DC:C6	2.48	0.47
1:B:182:ARG:HB3	1:B:206:GLU:HG3	1.96	0.47
2:C:12:ARG:HG2	2:C:1183:ALA:HB2	1.97	0.47
2:C:198:ILE:HD13	2:C:388:LEU:HD13	1.96	0.47
2:C:207:THR:HG21	2:C:351:LEU:HG	1.96	0.47
2:C:398:SER:O	2:C:401:GLY:N	2.48	0.47
2:C:746:ALA:HB2	2:C:974:ARG:NE	2.29	0.47
3:D:27:PRO:HB3	3:D:241:VAL:HG23	1.97	0.47
3:D:807:LEU:HD12	3:D:808:VAL:N	2.29	0.47
5:F:124:GLU:OE2	5:F:422:ARG:NH2	2.46	0.47
1:A:192:VAL:HB	1:A:198:LEU:HD12	1.95	0.47
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.96	0.47
3:D:1216:ALA:HB1	3:D:1218:HIS:CD2	2.50	0.47
1:A:222:THR:HA	1:B:232:VAL:HB	1.95	0.47
2:C:521:LEU:HD23	2:C:708:VAL:HG11	1.96	0.47
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.80	0.47
2:C:1032:LYS:HA	2:C:1035:LYS:HD3	1.97	0.47
2:C:1160:ASP:CG	2:C:1161:LEU:N	2.73	0.47
3:D:551:ARG:HA	3:D:568:SER:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1215:GLU:HB2	3:D:1220:ILE:HD11	1.96	0.47
3:D:1216:ALA:O	3:D:1220:ILE:HG12	2.15	0.47
3:D:1261:LEU:HD13	3:D:1304:ARG:CZ	2.45	0.47
5:F:429:THR:OG1	7:N:27:DA:H2'	2.14	0.47
1:B:86:LYS:HD3	1:B:174:ASP:HB2	1.96	0.47
2:C:357:ASN:ND2	2:C:358:ASP:OD1	2.48	0.47
2:C:817:LEU:HD21	2:C:1080:ASN:HD22	1.79	0.47
3:D:641:ILE:HD12	3:D:764:ARG:HH11	1.80	0.47
3:D:708:ASN:OD1	3:D:708:ASN:N	2.48	0.47
4:E:44:ASP:OD2	4:E:52:ARG:NH1	2.48	0.47
5:F:465:ARG:HG2	5:F:468:ARG:HH22	1.80	0.47
2:C:807:TRP:HB2	2:C:1097:VAL:HG11	1.97	0.47
2:C:841:ARG:CZ	3:D:256:ASP:HB3	2.44	0.47
2:C:1010:GLN:O	2:C:1014:LEU:HD12	2.15	0.47
3:D:198:CYS:O	3:D:202:ARG:HG3	2.15	0.47
3:D:360:TYR:OH	3:D:442:ILE:HD11	2.14	0.47
3:D:647:PRO:O	3:D:650:LYS:HB3	2.15	0.47
4:E:31:GLN:HB2	4:E:46:THR:HG21	1.96	0.47
5:F:96:ASP:OD2	5:F:99:ARG:HB2	2.15	0.47
2:C:1065:LYS:HE3	3:D:463:GLY:HA3	1.95	0.47
3:D:53:ARG:HA	3:D:54:ASP:HA	1.50	0.47
3:D:144:TYR:CD2	3:D:180:MET:HB2	2.50	0.47
3:D:349:TYR:HE1	3:D:379:PRO:HG2	1.80	0.47
2:C:582:ASN:HB3	2:C:586:PHE:H	1.80	0.46
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.48	0.46
3:D:127:LEU:HD21	3:D:234:PRO:HB3	1.97	0.46
5:F:466:ILE:HD11	5:F:487:MET:HE3	1.97	0.46
2:C:618:GLN:HG3	3:D:770:LEU:HD21	1.96	0.46
2:C:936:ARG:HG2	2:C:937:ASP:H	1.79	0.46
3:D:857:LEU:HD22	3:D:875:ASN:ND2	2.30	0.46
3:D:1241:TYR:HB3	3:D:1246:VAL:HG23	1.97	0.46
5:F:573:LEU:HD23	5:F:574:GLU:H	1.80	0.46
6:M:18:SER:HA	6:M:19:PHE:CB	2.46	0.46
1:A:91:ARG:HB2	1:A:210:THR:HG23	1.97	0.46
1:B:34:GLY:N	1:B:199:ASP:OD2	2.48	0.46
3:D:1218:HIS:CD2	3:D:1218:HIS:H	2.32	0.46
1:A:104:LYS:HG2	1:A:110:VAL:HG22	1.97	0.46
3:D:246:PRO:HD2	3:D:249:LEU:HD12	1.98	0.46
3:D:301:GLU:OE2	5:F:97:PRO:HG3	2.15	0.46
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.97	0.46
3:D:430:HIS:HA	3:D:921:GLN:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LEU:HB3	1:A:142:MET:HG2	1.98	0.46
1:B:192:VAL:HG12	1:B:193:GLU:H	1.81	0.46
3:D:735:ALA:O	3:D:739:GLN:HG2	2.15	0.46
3:D:1252:HIS:O	3:D:1255:VAL:HG12	2.15	0.46
2:C:1256:GLN:HG2	2:C:1321:GLU:HG2	1.98	0.46
3:D:137:ARG:HG2	3:D:142:GLU:HB2	1.98	0.46
3:D:1179:PRO:HD3	3:D:1184:ASP:OD1	2.16	0.46
5:F:105:MET:HE2	5:F:105:MET:HB2	1.80	0.46
2:C:836:LEU:HD23	2:C:918:LEU:HD11	1.97	0.46
3:D:113:HIS:HB3	3:D:116:PHE:HD1	1.81	0.46
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.48	0.46
3:D:1271:SER:HB3	3:D:1298:VAL:O	2.15	0.46
2:C:59:ILE:HD12	2:C:472:GLU:HG2	1.98	0.46
2:C:609:ILE:H	2:C:609:ILE:HG13	1.31	0.46
3:D:1226:VAL:O	3:D:1230:THR:HG22	2.16	0.46
1:A:156:SER:H	2:C:1059:ARG:NH2	2.13	0.46
1:B:133:LEU:HD11	1:B:140:ILE:HG21	1.97	0.46
2:C:289:VAL:HG22	2:C:319:LEU:HG	1.97	0.46
2:C:348:SER:O	2:C:352:ARG:HG3	2.16	0.46
2:C:984:VAL:HG23	2:C:985:GLU:HG3	1.98	0.46
2:C:1137:GLU:HG3	2:C:1139:ALA:H	1.81	0.46
2:C:245:ARG:HG2	2:C:337:PHE:CE2	2.51	0.45
2:C:396:ASP:OD2	2:C:398:SER:HB3	2.16	0.45
2:C:517:GLN:OE1	2:C:760:ASN:N	2.44	0.45
2:C:781:ASP:OD1	2:C:782:VAL:N	2.49	0.45
2:C:815:SER:HB2	2:C:1077:SER:OG	2.15	0.45
2:C:1103:VAL:HG11	2:C:1112:ILE:HD11	1.99	0.45
3:D:133:ARG:HD2	3:D:133:ARG:HA	1.75	0.45
3:D:662:ALA:O	3:D:666:GLU:HG3	2.16	0.45
1:B:50:SER:HA	1:B:150:ARG:O	2.16	0.45
2:C:629:PHE:HB2	2:C:647:ARG:HG3	1.98	0.45
2:C:836:LEU:HB3	2:C:918:LEU:HD21	1.98	0.45
4:E:44:ASP:OD1	4:E:44:ASP:N	2.50	0.45
2:C:796:LEU:HD12	2:C:796:LEU:H	1.80	0.45
2:C:941:LYS:HG3	2:C:946:LEU:CG	2.41	0.45
1:B:76:GLU:HB2	1:B:81:ILE:HD11	1.98	0.45
2:C:564:PRO:HA	2:C:684:ASN:HD21	1.81	0.45
3:D:262:THR:HG22	5:F:504:PRO:HB2	1.98	0.45
3:D:514:THR:HG21	3:D:596:LEU:HD23	1.98	0.45
5:F:359:LYS:HD2	5:F:359:LYS:HA	1.79	0.45
2:C:600:THR:HG22	2:C:602:GLU:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1272:GLU:HG2	2:C:1276:TRP:NE1	2.32	0.45
3:D:770:LEU:H	3:D:770:LEU:HD22	1.82	0.45
4:E:35:LYS:NZ	4:E:71:GLU:OE2	2.35	0.45
7:N:21:DG:H2'	7:N:22:DT:H71	1.98	0.45
1:A:208:ASN:ND2	1:A:210:THR:OG1	2.50	0.45
2:C:596:ASP:OD1	2:C:596:ASP:N	2.50	0.45
2:C:1060:ILE:HG12	2:C:1061:GLN:N	2.31	0.45
3:D:530:PRO:HB3	3:D:577:ALA:O	2.17	0.45
3:D:554:GLU:OE1	3:D:570:LYS:NZ	2.50	0.45
2:C:890:LYS:NZ	2:C:891:GLY:H	2.15	0.45
2:C:1150:ASP:O	2:C:1151:LEU:HB2	2.16	0.45
2:C:661:VAL:HB	2:C:665:ALA:HB3	1.99	0.45
3:D:709:ARG:H	3:D:709:ARG:HE	1.65	0.45
3:D:1325:PHE:HD2	3:D:1326:GLN:HG3	1.81	0.45
4:E:25:ARG:NH2	4:E:68:GLU:OE1	2.50	0.45
2:C:251:ALA:HB2	2:C:269:ILE:HD12	1.99	0.45
2:C:984:VAL:HA	2:C:985:GLU:HA	1.66	0.45
3:D:600:ALA:O	3:D:603:LYS:HG2	2.17	0.45
3:D:914:ALA:HB2	3:D:1359:ALA:HB1	1.98	0.45
3:D:1220:ILE:HD12	3:D:1224:ARG:NH2	2.31	0.45
1:B:211:ILE:HD11	1:B:215:GLU:HB3	1.99	0.44
2:C:135:THR:HG21	2:C:515:MET:SD	2.57	0.44
3:D:963:VAL:HB	3:D:980:THR:HG23	1.99	0.44
2:C:35:PHE:O	2:C:39:ILE:HG22	2.18	0.44
2:C:298:ALA:HB2	2:C:336:LEU:HD21	1.99	0.44
2:C:590:PRO:HG3	2:C:605:TYR:CE2	2.53	0.44
3:D:197:GLU:O	3:D:201:LEU:HG	2.17	0.44
3:D:232:ASN:HD22	3:D:232:ASN:H	1.64	0.44
3:D:1271:SER:O	3:D:1271:SER:OG	2.36	0.44
2:C:798:GLN:HB2	2:C:828:PHE:CE1	2.52	0.44
3:D:661:VAL:O	3:D:664:ILE:HG12	2.16	0.44
3:D:1332:LEU:HD13	3:D:1332:LEU:HA	1.78	0.44
5:F:462:LYS:NZ	8:T:2:DA:OP2	2.37	0.44
3:D:141:PHE:HD1	3:D:180:MET:HE3	1.83	0.44
3:D:289:ASP:HA	3:D:292:VAL:HG22	2.00	0.44
3:D:664:ILE:CD1	3:D:682:VAL:HG22	2.47	0.44
4:E:66:VAL:HG22	4:E:69:ARG:HH21	1.83	0.44
2:C:1240:ASP:OD1	2:C:1240:ASP:N	2.39	0.44
3:D:1268:ASN:HD22	3:D:1269:ALA:N	2.16	0.44
5:F:432:THR:HG21	7:N:28:DA:C5	2.53	0.44
1:A:134:THR:O	1:A:134:THR:OG1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:37:LYS:HA	2:C:37:LYS:HD3	1.75	0.44
2:C:150:HIS:CD2	2:C:454:ARG:HE	2.35	0.44
2:C:1134:GLN:H	2:C:1134:GLN:HG3	1.64	0.44
3:D:907:HIS:CD2	3:D:908:ILE:H	2.35	0.44
5:F:402:LEU:HA	5:F:405:ILE:HG12	2.00	0.44
7:N:26:DT:C2	7:N:27:DA:C8	3.05	0.44
1:A:152:TYR:CD1	2:C:824:GLN:HG2	2.53	0.44
2:C:113:THR:C	2:C:115:LYS:H	2.25	0.44
3:D:412:LEU:O	3:D:416:ILE:HB	2.18	0.44
1:B:69:SER:H	1:B:78:ILE:HD11	1.83	0.44
2:C:544:GLY:O	2:C:548:ARG:HD2	2.18	0.44
2:C:545:PHE:CE2	2:C:549:ASP:HB2	2.53	0.44
2:C:848:GLU:OE1	2:C:886:LYS:NZ	2.50	0.44
2:C:1134:GLN:O	2:C:1136:GLN:HG2	2.18	0.44
3:D:16:GLU:HG3	3:D:17:PHE:HD1	1.82	0.44
3:D:786:THR:CG2	6:M:7:PRO:HD3	2.48	0.44
3:D:1146:GLU:OE2	3:D:1310:THR:HG22	2.18	0.44
8:T:17:DG:H2"	8:T:18:DG:C8	2.53	0.44
1:B:31:LEU:HB2	1:B:199:ASP:O	2.18	0.44
1:B:115:ILE:HD11	1:B:130:ILE:HD11	2.00	0.44
6:M:4:GLY:HA2	6:M:19:PHE:C	2.42	0.44
2:C:453:ILE:HD12	2:C:587:LEU:HD21	2.00	0.43
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.58	0.43
2:C:1244:HIS:CD2	2:C:1264:GLN:HB2	2.53	0.43
5:F:483:LEU:HD13	5:F:483:LEU:N	2.31	0.43
1:A:152:TYR:CG	2:C:824:GLN:HG2	2.53	0.43
2:C:230:PHE:O	2:C:333:ILE:HB	2.18	0.43
2:C:487:LEU:HD12	2:C:492:MET:HE2	2.00	0.43
1:A:182:ARG:H	1:A:206:GLU:HB3	1.82	0.43
1:A:190:ALA:H	1:A:199:ASP:HA	1.84	0.43
1:B:48:LEU:HD22	3:D:539:SER:HB3	2.00	0.43
3:D:1226:VAL:O	3:D:1229:VAL:HG12	2.18	0.43
1:B:79:LEU:HA	1:B:82:LEU:HD12	2.00	0.43
2:C:962:GLU:HG2	2:C:963:GLU:N	2.33	0.43
2:C:1129:ASN:OD1	2:C:1177:ARG:NH2	2.52	0.43
3:D:56:LEU:HD12	3:D:56:LEU:H	1.83	0.43
3:D:482:ALA:O	3:D:488:ASN:ND2	2.49	0.43
1:B:100:LEU:HD21	1:B:121:VAL:HG11	2.00	0.43
2:C:400:VAL:HG21	2:C:452:ARG:CZ	2.48	0.43
2:C:471:VAL:O	2:C:475:VAL:HG23	2.19	0.43
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:200:GLN:HE21	3:D:200:GLN:HB2	1.63	0.43
3:D:1166:GLY:O	3:D:1173:ARG:HG2	2.18	0.43
3:D:1262:ARG:O	3:D:1282:TYR:N	2.33	0.43
5:F:400:GLN:O	5:F:404:LEU:HG	2.19	0.43
5:F:487:MET:HE2	5:F:487:MET:HA	2.00	0.43
2:C:273:HIS:HA	2:C:276:GLN:HB3	1.99	0.43
2:C:524:ILE:HD11	2:C:712:SER:HB2	2.00	0.43
2:C:799:ASN:OD1	2:C:799:ASN:N	2.52	0.43
2:C:1158:LYS:HD3	2:C:1158:LYS:HA	1.83	0.43
3:D:770:LEU:O	3:D:774:ILE:HG13	2.19	0.43
5:F:559:LEU:HD12	5:F:559:LEU:HA	1.88	0.43
1:A:153:VAL:HB	1:A:175:ALA:HB3	1.98	0.43
1:B:107:ILE:HG23	1:B:135:ASP:HA	2.01	0.43
2:C:156:PHE:CE2	2:C:158:ASP:HB2	2.54	0.43
2:C:594:VAL:HA	2:C:598:VAL:O	2.18	0.43
2:C:1295:SER:OG	3:D:346:ARG:O	2.23	0.43
3:D:1265:THR:HG23	3:D:1305:ASP:OD2	2.19	0.43
5:F:111:LEU:HD22	5:F:116:GLU:HG2	1.99	0.43
5:F:479:THR:OG1	5:F:480:PRO:HD2	2.18	0.43
1:B:197:ASP:C	1:B:198:LEU:HD22	2.44	0.43
2:C:80:PHE:HB2	2:C:85:CYS:SG	2.58	0.43
2:C:192:ASP:OD1	2:C:436:ARG:NH2	2.52	0.43
2:C:996:ARG:HD2	2:C:999:GLU:CD	2.44	0.43
3:D:343:LEU:HD11	3:D:1324:SER:HB2	2.01	0.43
3:D:865:HIS:CE1	3:D:867:GLN:HB2	2.54	0.43
3:D:981:GLU:OE2	3:D:983:LYS:HE2	2.19	0.43
7:N:9:DC:H2''	7:N:10:DC:C5	2.54	0.43
2:C:216:THR:H	2:C:219:GLN:NE2	2.16	0.43
2:C:1166:ASP:O	2:C:1170:MET:HG2	2.19	0.43
1:B:205:MET:HE3	1:B:213:PRO:HB3	2.01	0.43
2:C:1101:LEU:HD12	3:D:505:ASP:OD1	2.19	0.43
3:D:266:ASN:O	3:D:270:ARG:HB2	2.19	0.43
3:D:510:LEU:HD22	3:D:601:ILE:HD11	1.99	0.43
3:D:555:TYR:HB2	3:D:585:LYS:O	2.18	0.43
3:D:813:ASP:HA	3:D:895:CYS:HB2	2.01	0.43
3:D:889:ASP:OD1	3:D:1286:LYS:NZ	2.41	0.43
3:D:1162:ILE:O	3:D:1178:THR:CB	2.66	0.43
3:D:1203:ARG:HH12	3:D:1205:GLU:HG2	1.84	0.43
3:D:1211:SER:OG	3:D:1212:ASP:N	2.52	0.43
5:F:575:GLU:O	5:F:579:GLN:HG2	2.19	0.43
2:C:42:ASP:HA	2:C:43:PRO:HD3	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:484:LEU:HD12	2:C:485:ASP:H	1.84	0.42
2:C:967:LEU:HD23	2:C:1021:LEU:HD13	2.01	0.42
2:C:1108:ASN:O	2:C:1111:GLN:HG2	2.18	0.42
2:C:1276:TRP:CE2	3:D:801:VAL:HG21	2.54	0.42
3:D:364:HIS:HB3	3:D:487:THR:HG23	2.01	0.42
3:D:499:ILE:HD12	3:D:499:ILE:HA	1.87	0.42
4:E:66:VAL:HG22	4:E:69:ARG:NH2	2.34	0.42
5:F:387:VAL:HG11	5:F:409:ASN:OD1	2.19	0.42
1:B:62:ASP:HB2	1:B:141:SER:O	2.19	0.42
3:D:422:LEU:O	3:D:468:VAL:HA	2.19	0.42
3:D:708:ASN:HB3	3:D:712:GLN:O	2.19	0.42
3:D:858:VAL:HG12	3:D:862:THR:OG1	2.20	0.42
3:D:902:ASP:OD1	3:D:903:LEU:N	2.52	0.42
3:D:1263:LYS:HA	3:D:1281:GLU:HA	2.00	0.42
3:D:1313:SER:O	3:D:1316:THR:OG1	2.34	0.42
1:B:206:GLU:OE1	3:D:531:LYS:NZ	2.52	0.42
2:C:699:LEU:HB2	2:C:799:ASN:HD22	1.83	0.42
2:C:996:ARG:HA	2:C:996:ARG:HD3	1.77	0.42
3:D:641:ILE:HG23	3:D:764:ARG:NH1	2.34	0.42
5:F:532:LEU:O	5:F:536:THR:HG23	2.19	0.42
2:C:142:GLU:OE2	2:C:515:MET:CE	2.67	0.42
2:C:1159:VAL:HA	2:C:1160:ASP:HA	1.82	0.42
3:D:41:PRO:HG3	3:D:274:ASN:OD1	2.20	0.42
1:B:233:ASP:OD1	1:B:234:LEU:N	2.53	0.42
2:C:560:PRO:O	3:D:780:ARG:NH2	2.52	0.42
2:C:985:GLU:HB3	2:C:988:LYS:HG2	2.02	0.42
2:C:1087:TYR:HE1	2:C:1215:GLY:HA2	1.84	0.42
3:D:19:ALA:HB2	3:D:1343:GLU:HA	2.01	0.42
3:D:142:GLU:HG2	5:F:100:MET:HE1	2.01	0.42
3:D:432:LEU:HD13	3:D:499:ILE:HG21	2.02	0.42
3:D:925:GLU:HB3	3:D:926:PRO:HD3	2.02	0.42
1:B:32:GLU:HB2	1:B:35:PHE:CD1	2.54	0.42
2:C:81:ASP:O	2:C:85:CYS:HB2	2.19	0.42
2:C:705:GLU:CD	2:C:705:GLU:H	2.27	0.42
2:C:1281:TYR:HE1	3:D:489:ASN:HD21	1.67	0.42
2:C:1288:GLN:HE21	3:D:1355:ARG:HA	1.85	0.42
3:D:46:TYR:CD2	5:F:500:ILE:HG12	2.54	0.42
3:D:161:THR:HG23	3:D:163:GLU:H	1.85	0.42
3:D:801:VAL:O	3:D:805:GLN:HB3	2.19	0.42
3:D:885:VAL:HG22	3:D:899:TYR:HA	2.00	0.42
1:A:11:PRO:HD2	1:B:227:GLN:HE22	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ARG:O	1:A:168:ILE:N	2.53	0.42
3:D:1179:PRO:HD3	3:D:1184:ASP:HB3	2.00	0.42
1:B:178:SER:H	3:D:535:ARG:HH22	1.68	0.42
2:C:50:GLU:O	2:C:54:ARG:HG3	2.20	0.42
2:C:215:TYR:HE2	2:C:422:LYS:HD2	1.83	0.42
2:C:806:PRO:O	3:D:633:ALA:HA	2.19	0.42
2:C:937:ASP:C	2:C:939:VAL:H	2.28	0.42
3:D:910:ASN:HB3	4:E:15:ASN:OD1	2.20	0.42
5:F:484:ALA:HB1	5:F:491:GLU:HB2	2.02	0.42
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.35	0.42
2:C:387:ASN:HA	2:C:391:SER:HB2	2.01	0.42
2:C:972:PHE:HD1	2:C:972:PHE:HA	1.71	0.42
2:C:1152:GLY:N	2:C:1197:GLU:OE2	2.51	0.42
1:B:135:ASP:O	1:B:136:GLU:HB2	2.20	0.42
2:C:242:VAL:HG12	2:C:245:ARG:HG3	2.02	0.42
2:C:886:LYS:H	2:C:917:SER:HB3	1.85	0.42
2:C:1101:LEU:O	3:D:731:ARG:HG2	2.20	0.42
3:D:814:CYS:HB2	3:D:889:ASP:HB3	2.02	0.42
3:D:848:VAL:HB	3:D:858:VAL:H	1.85	0.42
3:D:1167:LYS:HE3	3:D:1167:LYS:HB3	1.91	0.42
5:F:478:PRO:HB2	5:F:483:LEU:HD12	2.02	0.42
8:T:13:DC:H2''	8:T:14:DA:N7	2.35	0.42
2:C:897:PRO:HB3	5:F:564:GLY:H	1.85	0.41
2:C:1179:GLY:O	2:C:1181:PRO:HD3	2.20	0.41
3:D:57:PHE:CZ	3:D:252:LEU:HB2	2.55	0.41
3:D:198:CYS:HB2	3:D:224:LEU:HD13	2.02	0.41
3:D:722:ILE:HG12	3:D:737:ILE:HD12	2.02	0.41
4:E:58:LEU:HD12	4:E:59:ILE:HG12	2.02	0.41
5:F:515:GLU:HA	5:F:516:ASP:HA	1.60	0.41
8:T:24:DC:C6	8:T:24:DC:H5'	2.55	0.41
1:B:27:THR:HG22	1:B:202:VAL:HG22	2.00	0.41
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	2.02	0.41
2:C:1307:ASN:HB3	2:C:1312:ASN:O	2.21	0.41
3:D:362:ARG:H	3:D:365:GLN:NE2	2.15	0.41
3:D:1263:LYS:HE2	3:D:1281:GLU:HB3	2.02	0.41
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.56	0.41
1:B:195:ARG:HB3	1:B:198:LEU:HD23	2.02	0.41
3:D:97:VAL:HG13	3:D:100:GLU:OE2	2.20	0.41
3:D:347:VAL:HG12	3:D:348:ASP:O	2.20	0.41
3:D:612:LEU:HB3	3:D:616:PRO:CG	2.49	0.41
6:M:11:VAL:HG11	6:M:17:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:8:DC:H2"	7:N:9:DC:C5	2.55	0.41
1:A:58:GLU:OE1	1:A:145:LYS:NZ	2.50	0.41
1:A:222:THR:HG23	1:B:232:VAL:HG23	2.02	0.41
2:C:194:LEU:HD12	2:C:194:LEU:HA	1.88	0.41
2:C:444:ASP:OD1	2:C:444:ASP:N	2.53	0.41
2:C:866:ASP:OD2	2:C:944:ARG:HD2	2.20	0.41
2:C:1122:LYS:HG2	2:C:1229:TYR:CE1	2.56	0.41
2:C:1290:MET:HE2	2:C:1290:MET:HB2	1.98	0.41
3:D:45:ASN:O	3:D:46:TYR:HD1	2.03	0.41
3:D:217:LEU:O	3:D:218:THR:C	2.63	0.41
3:D:598:LYS:O	3:D:601:ILE:HG22	2.21	0.41
2:C:130:MET:HG2	2:C:131:THR:O	2.20	0.41
2:C:726:TYR:CZ	2:C:728:ASP:HB2	2.56	0.41
2:C:896:THR:OG1	2:C:899:GLU:OE2	2.34	0.41
2:C:1028:LYS:HB3	2:C:1028:LYS:HE2	1.84	0.41
3:D:232:ASN:HA	3:D:236:TRP:HZ3	1.85	0.41
3:D:527:LEU:HD23	3:D:532:GLU:HG2	2.02	0.41
3:D:807:LEU:HD11	3:D:894:VAL:HG23	2.02	0.41
2:C:404:LYS:HD2	2:C:404:LYS:HA	1.94	0.41
2:C:935:THR:O	2:C:1040:ASP:N	2.53	0.41
3:D:278:ARG:NH2	5:F:446:GLN:OE1	2.54	0.41
3:D:365:GLN:HA	3:D:438:GLU:H	1.86	0.41
3:D:609:TYR:HB2	3:D:617:THR:HG21	2.03	0.41
3:D:677:GLU:O	3:D:681:LYS:HD3	2.20	0.41
5:F:131:GLN:O	5:F:135:ALA:HB2	2.20	0.41
5:F:436:ARG:HH11	5:F:436:ARG:HB3	1.85	0.41
1:A:156:SER:H	2:C:1059:ARG:HH22	1.69	0.41
2:C:1331:ARG:HD3	3:D:33:TRP:CE2	2.56	0.41
3:D:325:LYS:HE2	3:D:330:MET:SD	2.61	0.41
3:D:425:ARG:NH1	3:D:459:ALA:HA	2.35	0.41
3:D:1282:TYR:O	3:D:1286:LYS:HB2	2.20	0.41
1:A:219:ARG:HA	1:A:222:THR:HB	2.02	0.41
2:C:257:ALA:HB3	2:C:262:TYR:CE1	2.55	0.41
2:C:260:LYS:HG2	2:C:261:VAL:H	1.86	0.41
2:C:483:ASP:HB2	2:C:486:THR:HG22	2.03	0.41
3:D:123:ARG:HD3	3:D:123:ARG:HA	1.89	0.41
5:F:402:LEU:O	5:F:405:ILE:HG12	2.21	0.41
5:F:547:VAL:HG13	5:F:598:LEU:HD22	2.03	0.41
1:B:59:VAL:HG22	1:B:144:ILE:HG13	2.01	0.41
1:B:225:ALA:O	1:B:229:GLU:HG2	2.20	0.41
2:C:657:THR:OG1	2:C:1187:PHE:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:813:GLU:HA	3:D:504:GLN:HE22	1.85	0.41
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.53	0.41
3:D:417:ARG:NH2	4:E:43:ASN:O	2.53	0.41
3:D:553:THR:HG22	3:D:567:THR:HB	2.03	0.41
3:D:798:ARG:O	3:D:801:VAL:HG22	2.21	0.41
3:D:1174:ARG:HE	3:D:1189:MET:HE2	1.86	0.41
3:D:1326:GLN:HG3	3:D:1326:GLN:H	1.45	0.41
5:F:100:MET:HE2	5:F:100:MET:HB3	1.68	0.41
1:A:83:LEU:HD23	2:C:694:ARG:NH1	2.36	0.41
2:C:246:LEU:HB3	2:C:269:ILE:HG21	2.03	0.41
2:C:615:VAL:HG21	2:C:645:PHE:HD2	1.86	0.41
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.86	0.41
2:C:1268:GLN:O	2:C:1269:ARG:C	2.64	0.41
3:D:697:MET:HG3	3:D:698:MET:N	2.35	0.41
2:C:242:VAL:HG22	2:C:243:PRO:HD2	2.03	0.40
2:C:275:ARG:HH11	2:C:275:ARG:HB2	1.86	0.40
2:C:696:ASP:O	2:C:697:LYS:HB3	2.21	0.40
3:D:292:VAL:O	3:D:296:LYS:HG3	2.20	0.40
3:D:682:VAL:HG12	3:D:686:TRP:HD1	1.85	0.40
3:D:1170:LYS:C	3:D:1172:LYS:H	2.29	0.40
4:E:15:ASN:O	4:E:17:PHE:N	2.54	0.40
5:F:395:THR:OG1	5:F:396:ASN:N	2.54	0.40
2:C:14:ASP:H	2:C:1157:GLN:CD	2.30	0.40
2:C:153:PRO:HB2	2:C:401:GLY:HA3	2.02	0.40
2:C:1328:LYS:HD3	2:C:1328:LYS:HA	1.85	0.40
3:D:1330:ARG:HA	3:D:1333:THR:OG1	2.22	0.40
1:B:89:ALA:HB3	1:B:124:VAL:HG12	2.04	0.40
2:C:820:GLU:N	2:C:1080:ASN:O	2.55	0.40
2:C:1296:ASP:OD2	2:C:1322:SER:OG	2.28	0.40
3:D:367:GLY:HA3	3:D:448:GLN:HB2	2.02	0.40
3:D:518:VAL:CG1	3:D:707:ILE:HD13	2.51	0.40
3:D:526:VAL:C	3:D:527:LEU:HD12	2.46	0.40
3:D:984:LEU:CB	3:D:993:GLU:HB2	2.52	0.40
3:D:1333:THR:O	3:D:1337:VAL:HG13	2.22	0.40
2:C:296:VAL:HG12	2:C:297:VAL:H	1.86	0.40
2:C:1159:VAL:HG23	2:C:1160:ASP:HB2	2.03	0.40
3:D:118:LYS:NZ	3:D:136:GLU:OE2	2.47	0.40
3:D:325:LYS:HE3	3:D:330:MET:HA	2.04	0.40
3:D:338:PHE:HD1	3:D:338:PHE:HA	1.70	0.40
5:F:503:GLU:CD	5:F:504:PRO:HD2	2.47	0.40
3:D:84:ILE:H	3:D:84:ILE:HD13	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:124:ILE:H	3:D:124:ILE:HG13	1.61	0.40
3:D:615:LYS:H	3:D:615:LYS:HG3	1.61	0.40
3:D:857:LEU:HG	3:D:858:VAL:HG22	2.04	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	229/239 (96%)	204 (89%)	23 (10%)	2 (1%)	14	45
1	B	212/239 (89%)	189 (89%)	23 (11%)	0	100	100
2	C	1329/1342 (99%)	1243 (94%)	77 (6%)	9 (1%)	18	50
3	D	1230/1409 (87%)	1166 (95%)	62 (5%)	2 (0%)	43	71
4	E	77/91 (85%)	73 (95%)	3 (4%)	1 (1%)	9	38
5	F	312/612 (51%)	293 (94%)	18 (6%)	1 (0%)	36	65
6	M	19/21 (90%)	13 (68%)	4 (21%)	2 (10%)	0	5
All	All	3408/3953 (86%)	3181 (93%)	210 (6%)	17 (0%)	24	56

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	199	ASP
2	C	200	ARG
2	C	1151	LEU
1	A	177	TYR
2	C	340	ASP
3	D	1326	GLN
6	M	17	ILE
4	E	16	ARG

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Mol	Chain	Res	Type
5	F	134	VAL
6	M	16	PRO
1	A	163	GLU
2	C	114	VAL
2	C	339	ASN
2	C	398	SER
2	C	1150	ASP
2	C	1341	ASP
3	D	1167	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/206 (92%)	174 (92%)	16 (8%)	10	34
1	B	176/206 (85%)	150 (85%)	26 (15%)	3	16
2	C	1138/1157 (98%)	983 (86%)	155 (14%)	3	19
3	D	1022/1170 (87%)	896 (88%)	126 (12%)	4	21
4	E	67/75 (89%)	59 (88%)	8 (12%)	5	23
5	F	232/539 (43%)	202 (87%)	30 (13%)	4	20
6	M	13/14 (93%)	10 (77%)	3 (23%)	1	6
All	All	2838/3367 (84%)	2474 (87%)	364 (13%)	4	21

All (364) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	19	VAL
1	A	26	VAL
1	A	61	ILE
1	A	115	ILE
1	A	122	GLU
1	A	129	VAL
1	A	133	LEU

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Mol	Chain	Res	Type
1	A	136	GLU
1	A	145	LYS
1	A	162	GLU
1	A	187	VAL
1	A	192	VAL
1	A	195	ARG
1	A	197	ASP
1	A	207	THR
1	B	10	LYS
1	B	12	ARG
1	B	16	ILE
1	B	18	GLN
1	B	22	THR
1	B	54	CYS
1	B	61	ILE
1	B	72	GLU
1	B	74	VAL
1	B	76	GLU
1	B	78	ILE
1	B	83	LEU
1	B	91	ARG
1	B	97	GLU
1	B	107	ILE
1	B	124	VAL
1	B	132	HIS
1	B	133	LEU
1	B	134	THR
1	B	139	SER
1	B	144	ILE
1	B	148	ARG
1	B	192	VAL
1	B	203	ILE
1	B	206	GLU
1	B	227	GLN
2	C	11	ILE
2	C	21	VAL
2	C	22	LEU
2	C	24	VAL
2	C	28	LEU
2	C	30	ILE
2	C	59	ILE
2	C	60	GLN

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Mol	Chain	Res	Type
2	C	65	ASN
2	C	66	SER
2	C	75	LEU
2	C	82	VAL
2	C	85	CYS
2	C	90	VAL
2	C	91	THR
2	C	103	VAL
2	C	113	THR
2	C	114	VAL
2	C	115	LYS
2	C	124	MET
2	C	131	THR
2	C	160	ASP
2	C	164	THR
2	C	165	HIS
2	C	171	LEU
2	C	197	ARG
2	C	199	ASP
2	C	201	ARG
2	C	219	GLN
2	C	228	VAL
2	C	232	ILE
2	C	237	LEU
2	C	241	LEU
2	C	242	VAL
2	C	254	ASP
2	C	258	ASN
2	C	263	VAL
2	C	270	THR
2	C	278	GLU
2	C	285	ILE
2	C	296	VAL
2	C	297	VAL
2	C	330	HIS
2	C	341	LEU
2	C	360	LEU
2	C	374	GLU
2	C	377	THR
2	C	379	GLU
2	C	397	LEU
2	C	413	GLU

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Mol	Chain	Res	Type
2	C	417	SER
2	C	445	ILE
2	C	448	LEU
2	C	450	ASN
2	C	453	ILE
2	C	472	GLU
2	C	481	LEU
2	C	484	LEU
2	C	493	ILE
2	C	524	ILE
2	C	538	LEU
2	C	540	ARG
2	C	550	VAL
2	C	558	VAL
2	C	569	ILE
2	C	581	THR
2	C	594	VAL
2	C	596	ASP
2	C	603	ILE
2	C	604	HIS
2	C	609	ILE
2	C	615	VAL
2	C	618	GLN
2	C	620	ASN
2	C	623	LEU
2	C	626	GLU
2	C	630	VAL
2	C	637	ARG
2	C	648	ASP
2	C	660	VAL
2	C	667	LEU
2	C	672	GLU
2	C	697	LYS
2	C	699	LEU
2	C	705	GLU
2	C	724	VAL
2	C	739	ASP
2	C	748	ILE
2	C	765	ILE
2	C	773	LEU
2	C	778	GLU
2	C	783	LEU

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Mol	Chain	Res	Type
2	C	788	SER
2	C	808	ASN
2	C	817	LEU
2	C	839	VAL
2	C	844	LYS
2	C	845	LEU
2	C	876	GLU
2	C	878	THR
2	C	890	LYS
2	C	892	GLU
2	C	893	THR
2	C	896	THR
2	C	899	GLU
2	C	912	ASP
2	C	913	VAL
2	C	922	ASN
2	C	929	ILE
2	C	941	LYS
2	C	944	ARG
2	C	960	LEU
2	C	962	GLU
2	C	967	LEU
2	C	972	PHE
2	C	974	ARG
2	C	979	LEU
2	C	984	VAL
2	C	988	LYS
2	C	992	LEU
2	C	996	ARG
2	C	1002	LEU
2	C	1014	LEU
2	C	1032	LYS
2	C	1038	GLN
2	C	1041	ASP
2	C	1047	LEU
2	C	1060	ILE
2	C	1073	LYS
2	C	1077	SER
2	C	1082	ILE
2	C	1083	GLU
2	C	1098	LEU
2	C	1108	ASN

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Mol	Chain	Res	Type
2	C	1109	ILE
2	C	1114	GLU
2	C	1117	LEU
2	C	1119	MET
2	C	1134	GLN
2	C	1136	GLN
2	C	1146	GLN
2	C	1151	LEU
2	C	1160	ASP
2	C	1161	LEU
2	C	1180	MET
2	C	1198	LEU
2	C	1210	ILE
2	C	1223	ARG
2	C	1233	LEU
2	C	1240	ASP
2	C	1248	THR
2	C	1254	VAL
2	C	1293	VAL
2	C	1326	LEU
2	C	1327	LEU
3	D	45	ASN
3	D	46	TYR
3	D	52	GLU
3	D	54	ASP
3	D	74	LYS
3	D	76	LYS
3	D	79	LYS
3	D	84	ILE
3	D	92	VAL
3	D	97	VAL
3	D	99	ARG
3	D	145	VAL
3	D	158	GLN
3	D	161	THR
3	D	167	ASP
3	D	174	ASP
3	D	177	ASP
3	D	201	LEU
3	D	211	GLU
3	D	216	LYS
3	D	223	LEU

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Mol	Chain	Res	Type
3	D	224	LEU
3	D	229	GLN
3	D	232	ASN
3	D	244	VAL
3	D	252	LEU
3	D	255	LEU
3	D	264	ASP
3	D	299	LEU
3	D	316	ILE
3	D	317	THR
3	D	324	LEU
3	D	338	PHE
3	D	394	ILE
3	D	416	ILE
3	D	435	GLN
3	D	474	LEU
3	D	497	GLU
3	D	506	VAL
3	D	510	LEU
3	D	514	THR
3	D	518	VAL
3	D	536	LEU
3	D	545	HIS
3	D	564	VAL
3	D	591	ILE
3	D	594	GLN
3	D	641	ILE
3	D	646	ILE
3	D	650	LYS
3	D	663	GLU
3	D	672	LEU
3	D	678	ARG
3	D	680	ASN
3	D	697	MET
3	D	702	GLN
3	D	705	THR
3	D	707	ILE
3	D	708	ASN
3	D	709	ARG
3	D	712	GLN
3	D	720	ASN
3	D	740	LEU

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Mol	Chain	Res	Type
3	D	746	LEU
3	D	747	MET
3	D	764	ARG
3	D	770	LEU
3	D	780	ARG
3	D	783	LEU
3	D	805	GLN
3	D	807	LEU
3	D	808	VAL
3	D	817	HIS
3	D	847	ASP
3	D	850	LYS
3	D	858	VAL
3	D	862	THR
3	D	867	GLN
3	D	882	VAL
3	D	894	VAL
3	D	895	CYS
3	D	901	ARG
3	D	907	HIS
3	D	908	ILE
3	D	925	GLU
3	D	931	THR
3	D	951	GLN
3	D	960	LEU
3	D	963	VAL
3	D	972	LYS
3	D	987	GLU
3	D	1009	GLU
3	D	1010	GLN
3	D	1138	LEU
3	D	1140	ARG
3	D	1155	ILE
3	D	1162	ILE
3	D	1163	VAL
3	D	1164	SER
3	D	1170	LYS
3	D	1178	THR
3	D	1186	TYR
3	D	1202	GLU
3	D	1209	VAL
3	D	1211	SER

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Mol	Chain	Res	Type
3	D	1215	GLU
3	D	1218	HIS
3	D	1221	LEU
3	D	1223	LEU
3	D	1233	ILE
3	D	1242	ARG
3	D	1276	GLU
3	D	1287	ILE
3	D	1289	ASN
3	D	1290	ARG
3	D	1291	GLU
3	D	1293	GLU
3	D	1310	THR
3	D	1316	THR
3	D	1326	GLN
3	D	1329	THR
3	D	1332	LEU
3	D	1333	THR
3	D	1343	GLU
3	D	1344	LEU
3	D	1349	GLU
4	E	3	ARG
4	E	4	VAL
4	E	16	ARG
4	E	28	ARG
4	E	39	VAL
4	E	44	ASP
4	E	47	THR
4	E	58	LEU
5	F	98	VAL
5	F	100	MET
5	F	108	VAL
5	F	395	THR
5	F	400	GLN
5	F	423	ARG
5	F	427	PHE
5	F	436	ARG
5	F	449	THR
5	F	452	ILE
5	F	469	GLN
5	F	470	MET
5	F	471	LEU

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Mol	Chain	Res	Type
5	F	483	LEU
5	F	488	LEU
5	F	492	ASP
5	F	494	ILE
5	F	500	ILE
5	F	540	LEU
5	F	547	VAL
5	F	568	ASN
5	F	572	THR
5	F	573	LEU
5	F	575	GLU
5	F	578	LYS
5	F	584	ARG
5	F	586	ARG
5	F	588	ARG
5	F	600	HIS
5	F	606	VAL
6	M	13	ILE
6	M	15	THR
6	M	17	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	GLN
1	B	18	GLN
1	B	75	GLN
1	B	84	ASN
1	B	147	GLN
1	B	227	GLN
2	C	69	GLN
2	C	139	ASN
2	C	258	ASN
2	C	276	GLN
2	C	314	ASN
2	C	357	ASN
2	C	490	GLN
2	C	513	GLN
2	C	580	GLN
2	C	620	ASN
2	C	628	HIS
2	C	677	ASN

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Mol	Chain	Res	Type
2	C	688	GLN
2	C	922	ASN
2	C	1017	GLN
2	C	1038	GLN
2	C	1061	GLN
2	C	1080	ASN
2	C	1111	GLN
2	C	1116	HIS
2	C	1134	GLN
2	C	1237	HIS
2	C	1288	GLN
2	C	1313	HIS
2	C	1314	GLN
3	D	196	GLN
3	D	200	GLN
3	D	232	ASN
3	D	365	GLN
3	D	435	GLN
3	D	465	GLN
3	D	495	ASN
3	D	560	ASN
3	D	702	GLN
3	D	716	GLN
3	D	736	GLN
3	D	805	GLN
3	D	907	HIS
3	D	929	GLN
3	D	1218	HIS
3	D	1227	HIS
3	D	1244	GLN
3	D	1252	HIS
3	D	1268	ASN
5	F	396	ASN
5	F	545	HIS
5	F	579	GLN

5.3.3 RNA ⓘ

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	231/239 (96%)	-0.30	4 (1%) 69 43	138, 193, 227, 277	0
1	B	218/239 (91%)	-0.45	2 (0%) 81 57	133, 191, 230, 261	0
2	C	1335/1342 (99%)	-0.42	9 (0%) 84 63	93, 170, 229, 271	0
3	D	1236/1409 (87%)	-0.43	10 (0%) 82 60	99, 176, 247, 304	0
4	E	79/91 (86%)	-0.61	0 100 100	144, 183, 238, 268	0
5	F	318/612 (51%)	-0.49	1 (0%) 90 76	128, 190, 250, 265	0
6	M	21/21 (100%)	-0.49	0 100 100	151, 194, 226, 256	0
7	N	29/29 (100%)	-0.41	0 100 100	139, 222, 253, 255	0
8	T	24/24 (100%)	-0.32	1 (4%) 40 25	125, 223, 249, 259	0
All	All	3491/4006 (87%)	-0.43	27 (0%) 82 60	93, 179, 240, 304	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	85	LEU	3.2
2	C	516	ASP	3.1
2	C	826	ASP	2.7
3	D	675	ALA	2.7
3	D	1320	ILE	2.6
3	D	730	ALA	2.6
2	C	311	CYS	2.5
1	A	81	ILE	2.4
2	C	1323	PHE	2.3
2	C	1326	LEU	2.3
3	D	1332	LEU	2.3
3	D	1349	GLU	2.3
1	A	88	LEU	2.3
2	C	1318	GLY	2.2
2	C	429	MET	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	631	TYR	2.1
2	C	492	MET	2.1
3	D	741	ALA	2.1
1	A	173	VAL	2.1
3	D	690	ASN	2.1
3	D	676	GLY	2.1
1	B	102	LEU	2.0
3	D	1257	VAL	2.0
5	F	265	GLN	2.0
8	T	11	DA	2.0
1	B	144	ILE	2.0
2	C	460	ALA	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
9	MG	D	1501	1/1	0.97	0.06	83,83,83,83	0
10	ZN	D	1502	1/1	1.00	0.02	162,162,162,162	0
10	ZN	D	1503	1/1	1.00	0.04	185,185,185,185	0

6.5 Other polymers [i](#)

There are no such residues in this entry.