



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 5, 2017 – 06:08 PM EST

PDB ID : 5VOI
Title : X-ray crystal structure of bacterial RNA polymerase and pyrG promoter complex
Authors : Murakami, K.S.; Shin, Y.; Turnbough Jr, C.L.; Molodtsov, V.
Deposited on : unknown
Resolution : 2.80 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

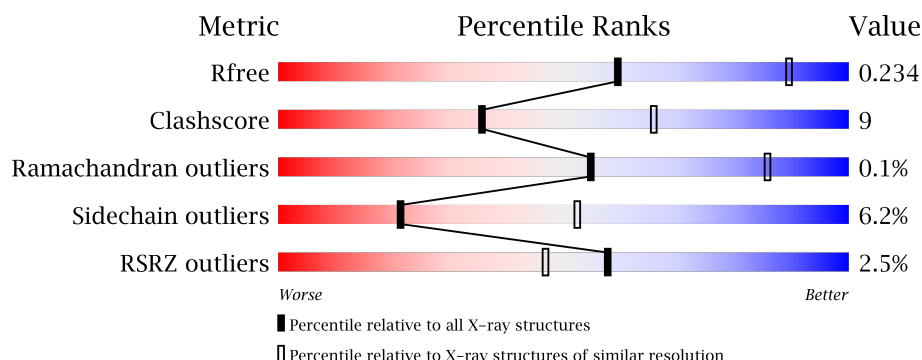
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	
6	G	22	
7	H	27	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	ZN	D	2002	-	-	X	-
9	MG	D	2004	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 28432 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	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	B	222	Total	C	N	O	S	0	0	0
			1750	1118	304	326	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0	0
			8770	5548	1564	1634	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1486	Total	C	N	O	S	0	0	0
			11738	7440	2067	2195	36			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2807	1770	509	524	4			

- Molecule 6 is a DNA chain called PyrG promoter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	18	Total	C	N	O	P	0	0	0
			368	175	71	104	18			

- Molecule 7 is a DNA chain called PyrG promoter.

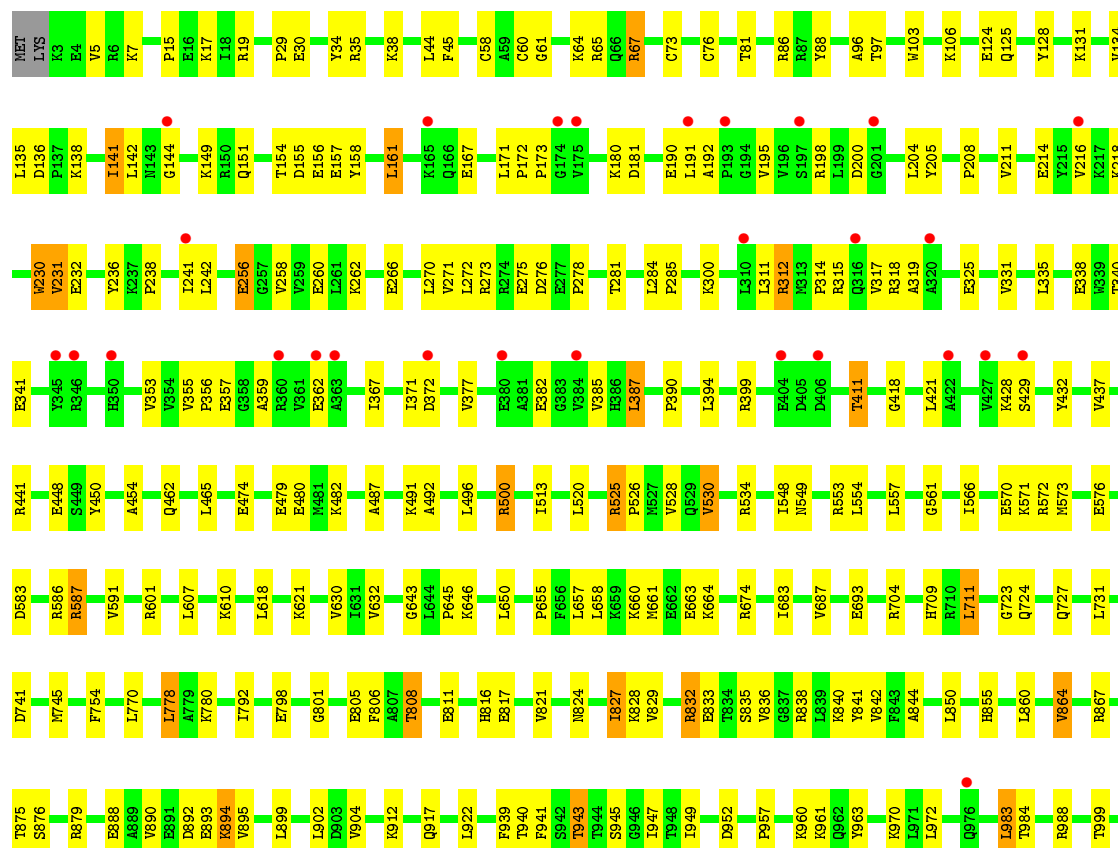
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	22	Total	C	N	O	P	0	0	0
			451	216	84	130	21			

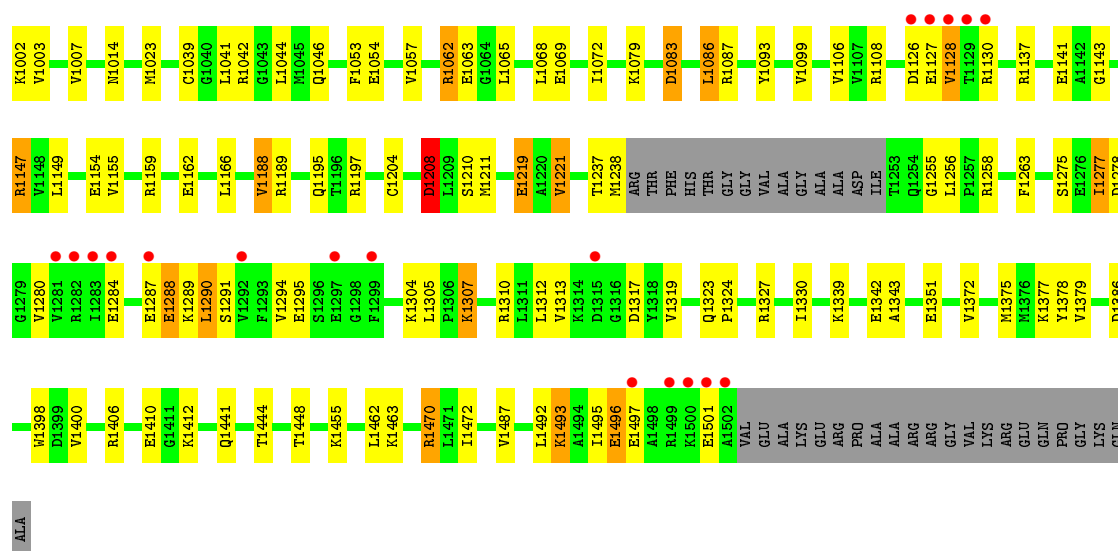
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

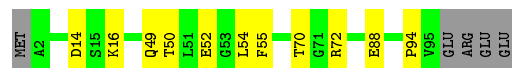
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	G	1	Total	Mg	0	0
			1	1		
9	D	2	Total	Mg	0	0
			2	2		





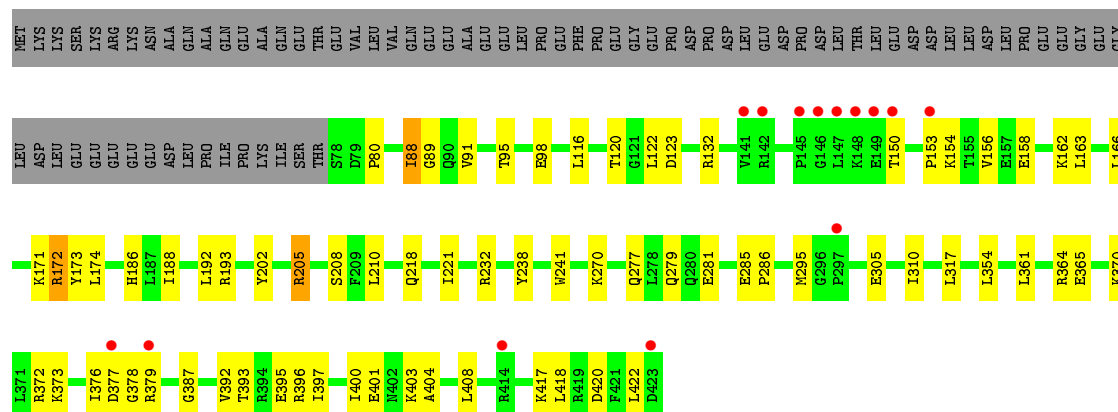
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 84% 11% 5%



- Molecule 5: RNA polymerase sigma factor SigA

Chain F: 3% 65% 16% 18%



- Molecule 6: PyrG promoter

Chain G: 23% 50% 9% 18%



- Molecule 7: PyrG promoter

Chain H: 7% 30% 22% 30% 19%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.18Å 103.47Å 294.44Å 90.00° 99.14° 90.00°	Depositor
Resolution (Å)	29.74 – 2.80 29.74 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.74-2.80) 98.1 (29.74-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.80Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.192 , 0.236 0.191 , 0.234	Depositor DCC
R_{free} test set	1998 reflections (1.52%)	DCC
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-l 0.014 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h- 1/2*k-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28432	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.55	0/1814	0.78	0/2466
1	B	0.55	1/1782 (0.1%)	0.83	1/2424 (0.0%)
2	C	0.58	0/8937	0.82	5/12087 (0.0%)
3	D	0.59	1/11944 (0.0%)	0.81	6/16148 (0.0%)
4	E	0.55	0/775	0.77	0/1045
5	F	0.51	0/2852	0.73	0/3837
6	G	1.62	7/413 (1.7%)	1.24	3/634 (0.5%)
7	H	1.49	8/505 (1.6%)	1.45	8/776 (1.0%)
All	All	0.63	17/29022 (0.1%)	0.83	23/39417 (0.1%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	1	DT	C1'-N1	9.36	1.61	1.49
6	G	15	DC	N1-C2	8.71	1.48	1.40
6	G	12	DG	C3'-O3'	-8.08	1.33	1.44
7	H	17	DT	C1'-N1	7.82	1.59	1.49
6	G	15	DC	C4-C5	7.56	1.49	1.43
6	G	17	DA	C3'-O3'	-6.93	1.34	1.44
6	G	15	DC	C1'-N1	6.21	1.57	1.49
7	H	20	DG	C3'-O3'	-5.66	1.36	1.44
7	H	1	DT	C3'-O3'	5.48	1.51	1.44
6	G	14	DC	C4-C5	5.39	1.47	1.43
6	G	11	DA	C3'-O3'	-5.29	1.37	1.44
7	H	12	DC	C1'-N1	5.26	1.56	1.49
7	H	17	DT	N1-C2	5.15	1.42	1.38
7	H	16	DC	N1-C2	5.12	1.45	1.40
3	D	1039	CYS	CB-SG	-5.09	1.73	1.81
7	H	16	DC	C1'-N1	5.08	1.55	1.49
1	B	154	GLU	CB-CG	5.01	1.61	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	23	DG	O4'-C4'-C3'	-9.00	100.60	106.00
6	G	15	DC	O4'-C1'-N1	7.94	113.56	108.00
7	H	20	DG	O4'-C1'-N9	-7.58	102.70	108.00
7	H	10	DA	P-O3'-C3'	7.33	128.49	119.70
1	B	197	LEU	CA-CB-CG	7.17	131.79	115.30
6	G	15	DC	O4'-C4'-C3'	-6.76	101.80	104.50
7	H	1	DT	O4'-C1'-N1	6.46	112.53	108.00
2	C	107	LEU	CA-CB-CG	6.23	129.62	115.30
3	D	1208	ASP	CB-CG-OD1	6.07	123.77	118.30
2	C	134	ARG	NE-CZ-NH1	-5.76	117.42	120.30
7	H	22	DT	O4'-C1'-C2'	-5.76	101.29	105.90
3	D	583	ASP	CB-CG-OD2	-5.74	113.14	118.30
6	G	16	DA	O4'-C4'-C3'	-5.72	102.21	104.50
2	C	324	ASP	CB-CG-OD1	5.53	123.28	118.30
3	D	711	LEU	CA-CB-CG	-5.52	102.61	115.30
7	H	24	DC	O4'-C1'-N1	5.46	111.82	108.00
7	H	21	DA	O4'-C4'-C3'	-5.42	102.33	104.50
2	C	269	LEU	CA-CB-CG	5.42	127.75	115.30
3	D	1086	LEU	CA-CB-CG	5.17	127.20	115.30
2	C	661	SER	N-CA-CB	5.17	118.25	110.50
3	D	1147	ARG	NE-CZ-NH2	-5.12	117.74	120.30
7	H	3	DT	O4'-C1'-N1	5.05	111.53	108.00
3	D	601	ARG	NE-CZ-NH1	-5.01	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1782	0	1834	41	0
1	B	1750	0	1797	38	0
2	C	8770	0	8874	187	0
3	D	11738	0	11971	233	0
4	E	761	0	778	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	2807	0	2882	46	0
6	G	368	0	202	6	0
7	H	451	0	251	15	0
8	D	2	0	0	2	0
9	D	2	0	0	0	0
9	G	1	0	0	0	0
All	All	28432	0	28589	520	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (520) 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)
1:B:206:THR:HG22	1:B:209:GLU:H	1.29	0.98
2:C:628:PHE:H	2:C:638:ASP:HB2	1.34	0.92
3:D:76:CYS:HG	8:D:2002:ZN:ZN	0.82	0.91
1:B:112:ARG:NH1	1:B:126:ASP:OD1	2.03	0.90
3:D:61:GLY:O	3:D:64:LYS:NZ	2.08	0.85
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.59	0.84
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.11	0.84
3:D:67:ARG:HD2	5:F:379:ARG:HB2	1.60	0.83
2:C:905:ILE:HG23	2:C:906:PHE:HD2	1.44	0.81
2:C:97:ARG:NH1	2:C:110:GLU:OE1	2.16	0.79
2:C:683:ASN:HB3	2:C:872:ASN:HD22	1.48	0.78
3:D:1258:ARG:HH21	3:D:1351:GLU:HG2	1.49	0.77
2:C:1116:ALA:HB2	3:D:88:TYR:HB3	1.67	0.76
2:C:614:ARG:NH1	2:C:620:LEU:HD13	2.02	0.75
2:C:294:GLU:HB3	2:C:299:LYS:HD2	1.69	0.74
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.69	0.74
5:F:91:VAL:O	5:F:193:ARG:NH2	2.20	0.73
3:D:5:VAL:O	3:D:1470:ARG:NH2	2.21	0.73
2:C:547:ILE:O	2:C:905:ILE:HD11	1.89	0.73
2:C:55:GLU:O	2:C:56:GLU:HB3	1.87	0.73
5:F:397:ILE:HD12	5:F:400:ILE:HD11	1.69	0.73
3:D:832:ARG:HD2	3:D:833:GLU:H	1.53	0.73
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.20	0.72
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.72	0.72
2:C:229:MET:HB2	2:C:233:GLU:HB2	1.70	0.72
1:A:183:ASP:HA	2:C:938:LYS:HE3	1.71	0.72
3:D:216:VAL:HB	3:D:382:GLU:HG2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:73:CYS:HB3	3:D:76:CYS:SG	2.30	0.72
6:G:15:DC:H2'	6:G:16:DA:C8	2.24	0.72
2:C:740:GLU:HB3	2:C:805:ARG:NH1	2.04	0.71
1:B:185:ARG:HB3	1:B:190:THR:HG23	1.73	0.71
2:C:428:ARG:NH2	2:C:447:ALA:O	2.23	0.71
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.73	0.70
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.72	0.70
5:F:393:THR:HG22	5:F:395:GLU:H	1.55	0.70
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.73	0.70
5:F:270:LYS:HG2	5:F:295:MET:HE1	1.74	0.69
2:C:680:ASP:OD1	3:D:943:THR:HG21	1.93	0.68
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.27	0.68
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.75	0.68
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.75	0.68
2:C:169:GLY:O	7:H:12:DC:N4	2.26	0.68
1:A:201:THR:HG21	1:A:205:VAL:O	1.94	0.68
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.29	0.68
3:D:60:CYS:SG	3:D:76:CYS:HB3	2.34	0.67
2:C:775:ARG:HD3	2:C:782:ALA:HB2	1.74	0.67
3:D:1372:VAL:HA	3:D:1375:MET:HE3	1.75	0.67
1:A:104:GLU:OE2	1:A:137:ARG:NH1	2.28	0.67
3:D:520:LEU:O	3:D:525:ARG:NH1	2.27	0.67
3:D:58:CYS:HB2	3:D:76:CYS:SG	2.35	0.66
2:C:205:GLU:O	2:C:209:ARG:HG2	1.95	0.66
2:C:545:ASN:HB3	2:C:583:LEU:HD22	1.77	0.66
2:C:740:GLU:HB3	2:C:805:ARG:HH12	1.60	0.66
2:C:834:GLN:OE1	3:D:724:GLN:NE2	2.29	0.66
2:C:787:ASP:OD2	2:C:791:ARG:NH2	2.29	0.66
3:D:1258:ARG:NH2	3:D:1351:GLU:HG2	2.10	0.66
3:D:65:ARG:HD3	5:F:378:GLY:O	1.96	0.65
2:C:983:ILE:HG21	2:C:987:ILE:HD11	1.79	0.65
2:C:999:HIS:HB3	2:C:1004:LYS:HZ2	1.60	0.65
5:F:238:TYR:HH	7:H:1:DT:H6	1.44	0.65
2:C:521:PRO:HB3	3:D:1068:LEU:HD21	1.80	0.64
3:D:45:PHE:O	3:D:86:ARG:NH2	2.30	0.64
2:C:999:HIS:HB3	2:C:1004:LYS:NZ	2.11	0.64
3:D:658:LEU:HA	3:D:661:MET:HE3	1.79	0.64
2:C:614:ARG:NH2	2:C:618:GLY:O	2.31	0.64
2:C:805:ARG:HG3	2:C:823:VAL:HG22	1.81	0.63
5:F:372:ARG:HD3	5:F:401:GLU:OE2	1.98	0.63
3:D:181:ASP:HB2	3:D:205:TYR:CG	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:905:ILE:HG23	2:C:906:PHE:CD2	2.31	0.63
3:D:806:PHE:HB2	3:D:829:VAL:HG22	1.82	0.62
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.82	0.62
3:D:828:LYS:HG2	3:D:833:GLU:HB3	1.81	0.62
3:D:136:ASP:OD2	3:D:138:LYS:HE3	1.99	0.61
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.82	0.61
1:B:216:GLU:OE1	1:B:219:ARG:NH2	2.33	0.61
1:A:188:GLN:HG2	1:A:189:ARG:HG2	1.82	0.61
2:C:64:LEU:N	2:C:103:LYS:HE2	2.15	0.61
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.83	0.61
3:D:949:ILE:HD11	3:D:1023:MET:HE1	1.83	0.61
3:D:231:VAL:O	3:D:236:TYR:OH	2.19	0.60
3:D:1258:ARG:HH21	3:D:1351:GLU:CG	2.14	0.60
3:D:808:THR:O	3:D:811:GLU:HB2	2.01	0.60
2:C:221:LEU:HD11	2:C:307:LEU:HD21	1.81	0.60
2:C:1053:LEU:HA	3:D:621:LYS:HD2	1.84	0.59
3:D:828:LYS:HA	3:D:833:GLU:HA	1.84	0.59
3:D:841:TYR:HB2	3:D:864:VAL:HG22	1.85	0.59
1:A:228:PRO:HB3	1:B:13:VAL:HG21	1.84	0.59
2:C:591:SER:O	2:C:592:LEU:HB2	2.01	0.59
3:D:658:LEU:HD23	3:D:661:MET:HE1	1.84	0.59
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.83	0.59
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.28	0.58
3:D:1493:LYS:NZ	3:D:1496:GLU:HG3	2.18	0.58
1:A:11:PHE:O	1:B:228:PRO:HA	2.03	0.58
2:C:926:PHE:HE1	2:C:929:ARG:HH11	1.51	0.58
3:D:832:ARG:HD2	3:D:833:GLU:N	2.19	0.58
2:C:1001:VAL:HG13	3:D:630:VAL:HB	1.85	0.58
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.37	0.58
3:D:561:GLY:HA3	5:F:132:ARG:HD3	1.86	0.58
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.85	0.58
3:D:704:ARG:HB2	3:D:745:MET:HG2	1.84	0.58
1:A:220:GLU:O	1:A:223:THR:HB	2.04	0.58
2:C:405:ARG:HD2	2:C:442:GLU:OE2	2.04	0.58
3:D:805:GLU:HG3	3:D:828:LYS:HB2	1.85	0.58
3:D:832:ARG:NH2	3:D:833:GLU:O	2.36	0.58
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.86	0.57
3:D:1197:ARG:HB2	3:D:1398:TRP:CH2	2.39	0.57
3:D:1126:ASP:OD1	3:D:1128:VAL:HG13	2.03	0.57
1:A:226:SER:O	1:A:228:PRO:HD3	2.04	0.57
3:D:1044:LEU:HD12	3:D:1044:LEU:H	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:899:LEU:HD22	3:D:917:GLN:HB3	1.87	0.57
1:A:32:PHE:HA	1:A:35:THR:HB	1.85	0.57
1:A:133:GLU:OE2	2:C:606:VAL:N	2.37	0.57
3:D:960:LYS:NZ	3:D:1063:GLU:OE2	2.37	0.56
3:D:73:CYS:CB	3:D:76:CYS:SG	2.93	0.56
3:D:76:CYS:SG	8:D:2002:ZN:ZN	1.88	0.56
3:D:657:LEU:HG	3:D:661:MET:HE2	1.86	0.56
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.87	0.56
3:D:262:LYS:HE2	3:D:341:GLU:OE1	2.04	0.56
1:B:80:LEU:HG	3:D:844:ALA:HA	1.87	0.56
2:C:627:ARG:NH1	2:C:638:ASP:OD2	2.39	0.56
2:C:409:ARG:HD2	2:C:452:ILE:HG22	1.88	0.56
2:C:853:LEU:HB2	2:C:858:MET:CE	2.35	0.56
3:D:67:ARG:NH1	5:F:379:ARG:HD3	2.21	0.55
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.89	0.55
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.89	0.55
2:C:210:GLU:HG2	2:C:304:LEU:HD21	1.89	0.55
3:D:1211:MET:SD	4:E:16:LYS:HE3	2.46	0.55
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.89	0.55
3:D:892:ASP:OD1	3:D:894:LYS:HD2	2.06	0.55
4:E:49:GLN:OE1	4:E:54:LEU:HD12	2.07	0.55
5:F:188:ILE:HD13	5:F:221:ILE:HG12	1.89	0.55
2:C:146:VAL:HG22	2:C:162:ILE:HG12	1.88	0.54
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.21	0.54
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.41	0.54
3:D:371:ILE:HG13	5:F:232:ARG:NH1	2.22	0.54
5:F:120:THR:HG21	5:F:122:LEU:HD22	1.89	0.54
3:D:1310:ARG:HD2	3:D:1327:ARG:HD2	1.90	0.54
3:D:271:VAL:HG22	3:D:281:THR:HG23	1.90	0.54
2:C:3:ILE:HD13	2:C:900:ARG:HB2	1.89	0.54
3:D:58:CYS:SG	3:D:76:CYS:SG	3.06	0.54
1:B:80:LEU:HD11	3:D:842:VAL:HG12	1.88	0.54
7:H:21:DA:H5'	7:H:21:DA:C8	2.43	0.54
2:C:259:GLY:HA3	2:C:266:ARG:HH21	1.73	0.53
7:H:22:DT:H2"	7:H:23:DG:C8	2.43	0.53
1:A:70:GLY:HA3	1:A:136:GLY:HA2	1.90	0.53
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.89	0.53
3:D:180:LYS:NZ	3:D:357:GLU:OE1	2.37	0.53
6:G:6:DA:H5"	6:G:6:DA:H8	1.73	0.53
2:C:942:GLU:HG2	2:C:945:ARG:HH21	1.73	0.53
3:D:141:ILE:HG23	3:D:450:TYR:OH	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:210:GLU:HB3	2:C:211:LEU:HD12	1.90	0.53
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.91	0.53
2:C:767:PRO:HB2	2:C:771:GLU:HG2	1.90	0.53
2:C:136:ILE:HB	2:C:336:VAL:HG13	1.91	0.53
3:D:270:LEU:HD12	3:D:284:LEU:HD11	1.91	0.53
2:C:617:ASP:OD2	2:C:619:ARG:NE	2.30	0.52
3:D:860:LEU:O	3:D:876:SER:HB2	2.09	0.52
3:D:893:GLU:H	3:D:894:LYS:NZ	2.06	0.52
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	1.91	0.52
3:D:211:VAL:HG22	3:D:387:LEU:HD12	1.92	0.52
5:F:95:THR:HB	5:F:98:GLU:HG3	1.91	0.52
4:E:52:GLU:HB2	4:E:55:PHE:HE2	1.75	0.52
2:C:1065:ALA:HB1	2:C:1077:PRO:HG3	1.91	0.52
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	1.92	0.52
3:D:487:ALA:O	3:D:491:LYS:HG2	2.10	0.52
2:C:808:ARG:NH2	5:F:305:GLU:OE2	2.42	0.52
2:C:164:PRO:HA	2:C:269:LEU:HD12	1.92	0.51
3:D:1143:GLY:O	3:D:1147:ARG:HD2	2.09	0.51
2:C:395:LYS:HD3	2:C:403:SER:HB3	1.91	0.51
2:C:593:ALA:HB1	2:C:659:PRO:HD2	1.93	0.51
1:A:159:LYS:HE3	1:A:164:ALA:O	2.10	0.51
3:D:479:GLU:OE1	3:D:482:LYS:NZ	2.29	0.51
5:F:354:LEU:HD23	5:F:418:LEU:HD21	1.93	0.51
1:A:206:THR:HG22	1:A:209:GLU:H	1.75	0.51
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.93	0.51
2:C:802:ARG:HB2	2:C:826:TYR:HB2	1.92	0.51
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.46	0.51
3:D:208:PRO:HG2	3:D:353:VAL:HG21	1.92	0.51
3:D:44:LEU:O	3:D:525:ARG:NH2	2.34	0.51
1:A:64:GLU:OE2	2:C:830:LYS:NZ	2.44	0.51
3:D:142:LEU:HB2	3:D:161:LEU:HD11	1.93	0.51
3:D:520:LEU:HD23	3:D:525:ARG:HG2	1.93	0.51
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.93	0.51
2:C:109:LYS:HG2	2:C:368:THR:HG22	1.93	0.51
3:D:103:TRP:HB3	3:D:1448:THR:CG2	2.41	0.51
3:D:1289:LYS:HA	3:D:1307:LYS:HD2	1.92	0.51
3:D:318:ARG:NH1	3:D:338:GLU:OE1	2.43	0.51
2:C:243:ARG:NH1	7:H:10:DA:H61	2.09	0.51
1:A:49:PRO:HA	1:A:148:VAL:HG12	1.92	0.51
1:B:80:LEU:HB3	3:D:867:ARG:NH2	2.25	0.51
2:C:607:ASP:HB3	2:C:610:ARG:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1083:ASP:OD1	3:D:1238:MET:HB3	2.11	0.51
3:D:230:TRP:CZ2	3:D:232:GLU:HG2	2.46	0.51
2:C:74:GLY:HA3	2:C:93:PRO:HG2	1.93	0.50
3:D:474:GLU:OE2	3:D:500:ARG:NE	2.42	0.50
1:A:106:PRO:HG3	1:A:134:GLU:HG2	1.91	0.50
1:A:186:LEU:HB3	1:A:188:GLN:OE1	2.11	0.50
1:B:49:PRO:HA	1:B:148:VAL:HG12	1.93	0.50
1:B:57:TYR:CD1	1:B:161:ARG:HD2	2.46	0.50
2:C:212:GLY:HA2	2:C:218:VAL:HG21	1.93	0.50
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.93	0.50
3:D:963:TYR:CE2	3:D:1002:LYS:HD3	2.47	0.50
3:D:1288:GLU:O	3:D:1307:LYS:HE3	2.12	0.50
3:D:798:GLU:OE2	3:D:824:ASN:HB2	2.12	0.50
2:C:197:LEU:HD12	2:C:221:LEU:HD21	1.93	0.49
2:C:478:VAL:HG13	2:C:506:ASN:HB3	1.93	0.49
2:C:587:VAL:O	2:C:591:SER:HB3	2.12	0.49
1:B:56:VAL:HG21	1:B:82:LEU:HD13	1.94	0.49
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.52	0.49
2:C:513:VAL:HG22	2:C:524:VAL:HG12	1.94	0.49
2:C:577:PRO:HB3	2:C:993:PHE:CG	2.48	0.49
3:D:1093:TYR:OH	3:D:1441:GLN:OE1	2.18	0.49
1:B:94:LEU:HD12	1:B:96:THR:H	1.77	0.49
3:D:34:TYR:CZ	3:D:35:ARG:HG3	2.47	0.49
3:D:44:LEU:HB3	3:D:525:ARG:NH2	2.27	0.49
2:C:679:PHE:HA	3:D:943:THR:HB	1.95	0.49
1:B:179:PHE:HB3	1:B:197:LEU:HD23	1.93	0.49
1:B:32:PHE:HA	1:B:35:THR:HB	1.94	0.49
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.94	0.49
1:A:206:THR:HB	1:A:209:GLU:HG3	1.94	0.49
2:C:1006:HIS:HB2	2:C:1024:LYS:HG3	1.94	0.49
3:D:1219:GLU:HG2	3:D:1221:VAL:HG23	1.95	0.49
3:D:1263:PHE:HD2	3:D:1375:MET:HE2	1.78	0.49
5:F:392:VAL:HB	5:F:396:ARG:HG2	1.94	0.49
2:C:614:ARG:CZ	2:C:620:LEU:HD13	2.42	0.49
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.95	0.49
2:C:374:ASN:OD1	2:C:376:ARG:HG2	2.13	0.48
3:D:573:MET:SD	5:F:210:LEU:HB3	2.53	0.48
2:C:135:VAL:HG23	2:C:395:LYS:HG3	1.94	0.48
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.46	0.48
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	1.95	0.48
2:C:35:PRO:HG2	2:C:38:LYS:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:758:ARG:HH21	2:C:788:THR:HB	1.77	0.48
2:C:368:THR:H	2:C:371:LYS:HD2	1.78	0.48
2:C:767:PRO:CB	2:C:771:GLU:HG2	2.44	0.48
2:C:224:GLU:CD	2:C:224:GLU:H	2.16	0.48
2:C:211:LEU:HD21	2:C:307:LEU:HG	1.95	0.48
2:C:118:ILE:HD11	2:C:344:PHE:CE2	2.49	0.48
2:C:911:GLU:O	2:C:915:LYS:HG2	2.14	0.48
3:D:957:PRO:HG3	3:D:1007:VAL:HA	1.95	0.48
3:D:658:LEU:HD23	3:D:661:MET:CE	2.43	0.48
6:G:18:DA:H2'	6:G:19:DA:C8	2.49	0.48
2:C:563:ASN:O	2:C:566:THR:HB	2.14	0.48
3:D:1493:LYS:HZ2	3:D:1496:GLU:HG3	1.79	0.48
3:D:1053:PHE:CZ	3:D:1072:ILE:HD12	2.49	0.48
3:D:1237:THR:HG22	3:D:1238:MET:H	1.78	0.48
3:D:780:LYS:HE3	3:D:912:LYS:HD3	1.96	0.48
1:B:111:ALA:HB3	1:B:125:PRO:HA	1.95	0.48
2:C:286:SER:OG	2:C:301:GLU:OE2	2.19	0.48
2:C:580:MET:HB3	2:C:584:GLU:CD	2.34	0.48
3:D:1277:ILE:HG22	3:D:1278:ASP:H	1.78	0.48
7:H:23:DG:H2'	7:H:23:DG:O5'	2.14	0.48
2:C:6:PHE:CD2	2:C:909:ALA:HB2	2.48	0.47
3:D:1087:ARG:HG3	3:D:1256:LEU:HD23	1.96	0.47
3:D:1290:LEU:HD13	3:D:1291:SER:N	2.29	0.47
3:D:432:TYR:O	3:D:448:GLU:HA	2.14	0.47
3:D:939:PHE:O	3:D:943:THR:HG22	2.14	0.47
1:A:206:THR:HG22	1:A:208:LEU:N	2.29	0.47
3:D:1149:LEU:HG	3:D:1166:LEU:HD21	1.96	0.47
3:D:801:GLY:HA2	3:D:821:VAL:HG22	1.96	0.47
2:C:499:ALA:HB2	2:C:533:ASP:HB2	1.96	0.47
3:D:1237:THR:HG22	3:D:1238:MET:N	2.29	0.47
3:D:134:VAL:HG22	3:D:151:GLN:H	1.80	0.47
3:D:1386:ASP:HB3	3:D:1412:LYS:HD2	1.97	0.47
3:D:835:SER:OG	3:D:838:ARG:HG3	2.14	0.47
5:F:370:LYS:HB3	5:F:376:ILE:HG13	1.95	0.47
1:A:112:ARG:HG2	1:A:112:ARG:HH21	1.79	0.47
1:B:188:GLN:HG2	1:B:189:ARG:N	2.30	0.47
2:C:683:ASN:HB3	2:C:872:ASN:HB2	1.97	0.47
3:D:156:GLU:H	3:D:156:GLU:CD	2.17	0.47
3:D:664:LYS:NZ	3:D:693:GLU:OE1	2.24	0.47
1:B:188:GLN:HE21	1:B:189:ARG:HG3	1.80	0.47
2:C:617:ASP:OD1	2:C:617:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:258:VAL:HG12	3:D:273:ARG:O	2.15	0.47
3:D:167:GLU:O	3:D:394:LEU:HD12	2.15	0.47
3:D:557:LEU:HD13	3:D:566:ILE:HG22	1.96	0.47
2:C:285:LEU:HD13	2:C:301:GLU:OE1	2.15	0.47
2:C:926:PHE:HE1	2:C:929:ARG:NH1	2.10	0.47
3:D:44:LEU:HB3	3:D:525:ARG:HH21	1.80	0.47
3:D:816:HIS:CG	3:D:836:VAL:HG11	2.50	0.47
1:A:6:LEU:HB2	1:A:29:GLU:OE2	2.15	0.47
3:D:1046:GLN:N	3:D:1046:GLN:OE1	2.45	0.47
3:D:792:ILE:HD13	3:D:941:PHE:CE1	2.49	0.47
5:F:172:ARG:HG3	5:F:173:TYR:N	2.30	0.47
1:B:150:TYR:HB3	3:D:855:HIS:ND1	2.30	0.46
2:C:1057:SER:HB3	2:C:1058:ASP:H	1.49	0.46
3:D:840:LYS:HE3	3:D:841:TYR:OH	2.16	0.46
4:E:70:THR:OG1	4:E:72:ARG:HG3	2.15	0.46
2:C:11:GLU:OE1	2:C:537:LYS:HE2	2.16	0.46
2:C:168:ARG:O	2:C:267:TYR:HA	2.14	0.46
4:E:52:GLU:OE1	4:E:52:GLU:N	2.43	0.46
3:D:879:ARG:HD3	3:D:902:LEU:O	2.15	0.46
5:F:166:LEU:O	5:F:171:LYS:HD2	2.15	0.46
1:A:94:LEU:HD21	1:A:97:VAL:CG2	2.45	0.46
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.15	0.46
3:D:1319:VAL:HG12	3:D:1323:GLN:NE2	2.31	0.46
3:D:242:LEU:HD23	3:D:285:PRO:HG3	1.97	0.46
1:B:161:ARG:HG3	1:B:162:ILE:O	2.15	0.46
1:B:24:VAL:HA	1:B:195:LEU:O	2.15	0.46
2:C:157:ARG:HA	2:C:157:ARG:HD3	1.78	0.46
3:D:534:ARG:HB3	3:D:534:ARG:HE	1.47	0.46
5:F:193:ARG:HB3	7:H:7:DG:H5"	1.98	0.46
2:C:797:GLY:O	2:C:829:GLN:NE2	2.49	0.46
3:D:103:TRP:HB3	3:D:1448:THR:HG21	1.97	0.46
3:D:711:LEU:HD13	3:D:778:LEU:CD1	2.46	0.46
2:C:776:SER:CB	5:F:373:LYS:NZ	2.79	0.46
1:B:176:ARG:HG2	1:B:200:TRP:CZ3	2.51	0.46
1:A:70:GLY:N	2:C:607:ASP:OD1	2.49	0.46
2:C:598:GLU:O	2:C:651:LYS:HG3	2.16	0.46
3:D:273:ARG:HB3	3:D:278:PRO:HA	1.98	0.46
6:G:8:DC:H2"	6:G:9:DA:C8	2.51	0.46
2:C:948:GLU:HB3	2:C:953:VAL:HG23	1.97	0.45
2:C:999:HIS:ND1	2:C:1004:LYS:NZ	2.61	0.45
3:D:1462:LEU:HD22	3:D:1472:ILE:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.99	0.45
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.98	0.45
3:D:418:GLY:N	3:D:429:SER:O	2.33	0.45
3:D:1290:LEU:HA	3:D:1290:LEU:HD22	1.71	0.45
1:B:188:GLN:CD	1:B:188:GLN:H	2.20	0.45
2:C:937:ASP:OD1	2:C:939:ARG:HG2	2.16	0.45
2:C:425:PHE:CE2	3:D:1086:LEU:HD12	2.51	0.45
3:D:411:THR:HB	3:D:437:VAL:H	1.82	0.45
5:F:154:LYS:O	5:F:158:GLU:HG3	2.16	0.45
5:F:202:TYR:O	5:F:205:ARG:HG3	2.16	0.45
2:C:99:GLN:OE1	2:C:101:ILE:HD11	2.16	0.45
2:C:118:ILE:HG12	2:C:382:ILE:HD13	1.99	0.45
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.64	0.45
3:D:1275:SER:OG	3:D:1294:VAL:HG21	2.16	0.45
3:D:103:TRP:CZ2	3:D:1444:THR:HG22	2.52	0.45
3:D:844:ALA:O	3:D:867:ARG:HB3	2.17	0.45
2:C:838:LYS:HE3	3:D:741:ASP:O	2.16	0.45
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.96	0.45
7:H:17:DT:H2''	7:H:18:DC:H5'	1.99	0.45
2:C:243:ARG:NH2	7:H:9:DG:O6	2.48	0.45
2:C:203:ASP:OD2	2:C:204:GLN:N	2.50	0.45
2:C:356:ARG:HA	2:C:359:MET:HE2	1.99	0.45
2:C:557:ARG:HG3	2:C:844:GLY:HA3	1.99	0.45
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.52	0.45
5:F:89:GLY:HA3	7:H:7:DG:C6	2.52	0.45
1:A:57:TYR:CG	1:A:161:ARG:HD2	2.51	0.45
2:C:260:LEU:O	2:C:261:ILE:HD12	2.17	0.45
2:C:678:PRO:HA	2:C:683:ASN:HD22	1.82	0.45
2:C:911:GLU:OE1	3:D:1062:ARG:NH1	2.50	0.45
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.99	0.45
2:C:150:PRO:HG3	2:C:322:VAL:HG11	1.99	0.44
2:C:617:ASP:HB2	2:C:619:ARG:HG2	1.98	0.44
3:D:1342:GLU:CD	3:D:1342:GLU:H	2.21	0.44
3:D:15:PRO:O	3:D:19:ARG:HG3	2.18	0.44
3:D:214:GLU:HB3	3:D:340:THR:HB	1.98	0.44
2:C:775:ARG:HG3	2:C:780:GLU:O	2.18	0.44
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.98	0.44
4:E:14:ASP:OD2	4:E:14:ASP:N	2.50	0.44
2:C:983:ILE:HG21	2:C:987:ILE:CD1	2.47	0.44
2:C:290:LEU:O	2:C:301:GLU:HB2	2.17	0.44
3:D:172:PRO:HA	3:D:173:PRO:HD3	1.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:236:TYR:CZ	3:D:242:LEU:HD12	2.52	0.44
2:C:1001:VAL:CG1	3:D:630:VAL:HB	2.46	0.44
5:F:88:ILE:HG23	5:F:193:ARG:HG2	1.98	0.44
1:A:201:THR:HG22	1:A:202:ASP:N	2.32	0.44
2:C:194:VAL:HG22	2:C:221:LEU:HD23	1.99	0.44
3:D:141:ILE:HD11	3:D:144:GLY:HA2	2.00	0.44
2:C:683:ASN:HB3	2:C:872:ASN:ND2	2.25	0.44
3:D:530:VAL:HG22	3:D:534:ARG:O	2.17	0.44
3:D:660:LYS:HD3	3:D:663:GLU:OE1	2.18	0.44
3:D:658:LEU:HD11	3:D:674:ARG:HH11	1.83	0.44
3:D:1280:VAL:HG12	3:D:1295:GLU:O	2.17	0.44
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.17	0.44
3:D:29:PRO:HG3	3:D:549:ASN:OD1	2.17	0.44
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.99	0.44
1:A:94:LEU:HD21	1:A:97:VAL:HG23	1.99	0.43
1:B:206:THR:HG22	1:B:209:GLU:N	2.13	0.43
1:B:94:LEU:HD11	1:B:97:VAL:HG23	2.00	0.43
2:C:281:LEU:HD11	2:C:306:THR:HG22	1.99	0.43
2:C:858:MET:HB2	2:C:858:MET:HE3	1.84	0.43
2:C:676:ILE:HA	2:C:871:LEU:O	2.18	0.43
3:D:1053:PHE:CE1	3:D:1072:ILE:HG23	2.52	0.43
3:D:1386:ASP:CB	3:D:1412:LYS:HD2	2.48	0.43
3:D:418:GLY:O	3:D:428:LYS:HD3	2.18	0.43
2:C:805:ARG:NH2	2:C:821:GLU:OE1	2.49	0.43
3:D:171:LEU:HD22	3:D:390:PRO:HG2	1.99	0.43
3:D:192:ALA:HB3	3:D:195:VAL:HB	2.01	0.43
3:D:683:ILE:HG23	3:D:687:VAL:HG21	2.00	0.43
3:D:827:ILE:O	3:D:833:GLU:HA	2.18	0.43
7:H:21:DA:H5'	7:H:21:DA:H8	1.82	0.43
2:C:757:GLY:HA2	2:C:789:SER:OG	2.18	0.43
3:D:256:GLU:OE2	3:D:300:LYS:HE2	2.17	0.43
3:D:553:ARG:HD2	3:D:570:GLU:OE2	2.17	0.43
3:D:893:GLU:H	3:D:894:LYS:HZ3	1.65	0.43
5:F:162:LYS:HE3	5:F:162:LYS:HB2	1.75	0.43
2:C:144:PRO:HG2	2:C:165:LEU:HD23	2.00	0.43
2:C:936:VAL:HG11	2:C:959:PRO:CB	2.46	0.43
2:C:677:MET:HB3	2:C:987:ILE:HD13	1.99	0.43
3:D:988:ARG:HH22	3:D:1054:GLU:CD	2.22	0.43
3:D:128:TYR:CZ	3:D:587:ARG:HD3	2.53	0.43
7:H:20:DG:H2''	7:H:21:DA:C8	2.54	0.43
1:B:85:LEU:HG	1:B:87:VAL:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:771:GLU:O	2:C:771:GLU:HG3	2.18	0.43
2:C:858:MET:HG2	2:C:867:VAL:O	2.18	0.43
3:D:125:GLN:HB3	3:D:131:LYS:HB2	2.00	0.43
3:D:1377:LYS:HE3	3:D:1378:TYR:OH	2.19	0.43
3:D:480:GLU:HG2	3:D:492:ALA:HB2	2.00	0.43
2:C:723:THR:OG1	2:C:724:ARG:N	2.52	0.43
3:D:38:LYS:HD3	3:D:38:LYS:HA	1.77	0.43
5:F:397:ILE:CD1	5:F:400:ILE:HD11	2.43	0.43
1:B:188:GLN:HG2	1:B:189:ARG:HG3	2.00	0.43
3:D:1154:GLU:HG2	3:D:1159:ARG:HA	1.99	0.43
3:D:1463:LYS:HE2	3:D:1463:LYS:HB3	1.82	0.43
2:C:243:ARG:HH12	7:H:10:DA:H61	1.66	0.43
1:A:47:SER:O	1:A:49:PRO:HD3	2.19	0.43
3:D:1339:LYS:HB3	3:D:1343:ALA:CB	2.49	0.43
3:D:1406:ARG:O	3:D:1410:GLU:HB2	2.19	0.43
2:C:524:VAL:HG13	2:C:528:GLU:HB2	2.01	0.43
5:F:241:TRP:CZ2	7:H:1:DT:H4'	2.54	0.43
5:F:88:ILE:HA	5:F:88:ILE:HD12	1.69	0.43
1:A:6:LEU:HD22	1:A:6:LEU:HA	1.93	0.42
2:C:550:LEU:HB3	2:C:905:ILE:HG13	2.01	0.42
1:A:4:SER:O	1:A:189:ARG:NH2	2.52	0.42
2:C:1070:ILE:HG21	3:D:655:PRO:HB2	2.01	0.42
2:C:261:ILE:CG2	2:C:291:ALA:HB3	2.49	0.42
5:F:277:GLN:O	5:F:281:GLU:HG2	2.19	0.42
1:B:104:GLU:HA	1:B:132:LEU:HD23	2.01	0.42
2:C:177:GLU:HG3	2:C:178:PRO:HD2	2.00	0.42
3:D:266:GLU:OE2	3:D:315:ARG:HG3	2.19	0.42
3:D:465:LEU:HD12	3:D:513:ILE:HD13	2.00	0.42
5:F:116:LEU:HA	5:F:116:LEU:HD23	1.85	0.42
1:B:162:ILE:O	1:B:163:ASN:HB2	2.19	0.42
2:C:18:LEU:HA	2:C:18:LEU:HD23	1.85	0.42
2:C:614:ARG:HH11	2:C:620:LEU:HD13	1.83	0.42
2:C:944:LEU:HD23	2:C:944:LEU:HA	1.86	0.42
3:D:1237:THR:HB	3:D:1255:GLY:HA3	2.00	0.42
3:D:17:LYS:HE3	3:D:17:LYS:HB2	1.63	0.42
2:C:419:THR:HG22	2:C:420:ARG:H	1.84	0.42
2:C:922:PHE:CD2	2:C:964:LYS:HD2	2.53	0.42
2:C:952:LEU:HD12	2:C:952:LEU:HA	1.81	0.42
3:D:645:PRO:HB3	3:D:723:GLY:O	2.20	0.42
2:C:726:ILE:HD11	2:C:757:GLY:HA3	2.01	0.42
3:D:526:PRO:HB2	3:D:528:VAL:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:387:GLY:HA2	5:F:397:ILE:HD13	2.02	0.42
1:A:97:VAL:HG12	1:A:99:LEU:HD12	2.01	0.42
1:A:39:PRO:HG3	1:B:39:PRO:CG	2.50	0.42
2:C:304:LEU:HB3	2:C:305:PRO:HD3	2.02	0.42
3:D:236:TYR:H	3:D:319:ALA:HB3	1.84	0.42
3:D:367:ILE:HB	3:D:377:VAL:HG12	2.01	0.42
5:F:408:LEU:HD23	5:F:408:LEU:HA	1.83	0.42
2:C:17:PRO:HB2	2:C:20:GLU:HB3	2.01	0.42
2:C:482:GLU:O	2:C:482:GLU:HG3	2.20	0.42
2:C:719:PRO:HB3	2:C:820:ARG:NE	2.34	0.42
3:D:1065:LEU:HD23	3:D:1069:GLU:HB3	2.01	0.42
1:A:36:LEU:HD23	1:A:36:LEU:HA	1.83	0.42
2:C:540:PHE:HB3	2:C:544:THR:HB	2.02	0.42
2:C:83:CYS:HA	2:C:88:LEU:HB2	2.02	0.42
3:D:58:CYS:CB	3:D:76:CYS:SG	3.07	0.42
1:A:64:GLU:HG2	1:A:76:VAL:HG22	2.02	0.42
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	2.02	0.42
2:C:367:LEU:HA	2:C:371:LYS:HD2	2.01	0.42
1:A:228:PRO:HB3	1:B:13:VAL:CG2	2.48	0.41
2:C:575:GLN:HG3	2:C:670:GLN:HA	2.01	0.41
3:D:945:SER:OG	3:D:947:ILE:HG12	2.20	0.41
5:F:80:PRO:HB2	5:F:210:LEU:HD11	2.01	0.41
2:C:261:ILE:HG22	2:C:262:ALA:N	2.35	0.41
3:D:462:GLN:HB2	3:D:513:ILE:HG21	2.02	0.41
3:D:607:LEU:HA	3:D:607:LEU:HD23	1.79	0.41
2:C:269:LEU:HB2	2:C:288:ARG:O	2.19	0.41
2:C:792:VAL:HA	2:C:793:PRO:HD3	1.93	0.41
3:D:876:SER:OG	3:D:879:ARG:HG3	2.20	0.41
1:B:197:LEU:HD13	1:B:199:ILE:HD11	2.02	0.41
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.55	0.41
2:C:355:VAL:O	2:C:359:MET:HG3	2.20	0.41
2:C:561:GLY:O	2:C:565:GLN:HG3	2.20	0.41
2:C:595:LEU:HD12	2:C:595:LEU:HA	1.89	0.41
3:D:566:ILE:HD11	5:F:192:LEU:HD21	2.03	0.41
3:D:97:THR:OG1	3:D:571:LYS:HE2	2.19	0.41
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.75	0.41
2:C:170:PRO:HD2	2:C:267:TYR:CE1	2.55	0.41
3:D:1014:ASN:OD1	3:D:1014:ASN:N	2.53	0.41
2:C:1023:GLY:HA2	6:G:18:DA:OP2	2.21	0.41
2:C:15:LEU:HA	2:C:16:PRO:HD3	1.97	0.41
2:C:1101:THR:OG1	2:C:1109:VAL:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:351:LEU:HD12	2:C:375:SER:HA	2.03	0.41
2:C:6:PHE:CE2	2:C:909:ALA:HB2	2.56	0.41
3:D:134:VAL:HG23	3:D:149:LYS:HA	2.03	0.41
3:D:241:ILE:HG12	3:D:312:ARG:NH1	2.35	0.41
3:D:983:LEU:HD13	3:D:988:ARG:HB2	2.03	0.41
2:C:548:PRO:O	2:C:843:HIS:HE1	2.03	0.41
1:B:115:LEU:HA	1:B:115:LEU:HD23	1.80	0.41
2:C:1090:LYS:HD3	2:C:1090:LYS:HA	1.87	0.41
3:D:1487:VAL:HG11	3:D:1492:LEU:HD23	2.03	0.41
3:D:731:LEU:HD23	3:D:731:LEU:HA	1.77	0.41
3:D:940:THR:O	3:D:943:THR:HG23	2.21	0.41
5:F:317:LEU:HD23	5:F:317:LEU:HA	1.85	0.41
2:C:1070:ILE:CG2	3:D:655:PRO:HB2	2.51	0.41
3:D:949:ILE:HD11	3:D:1023:MET:CE	2.49	0.41
3:D:988:ARG:NH2	3:D:1054:GLU:OE2	2.53	0.41
6:G:3:DT:H2"	6:G:4:DG:C8	2.56	0.41
7:H:20:DG:H2"	7:H:21:DA:H5'	2.03	0.41
2:C:598:GLU:HG3	2:C:623:TYR:OH	2.21	0.40
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.56	0.40
1:A:106:PRO:CG	1:A:134:GLU:HG2	2.51	0.40
1:B:7:LYS:HB3	1:B:7:LYS:NZ	2.35	0.40
2:C:118:ILE:HA	2:C:119:PRO:HD3	1.96	0.40
3:D:1197:ARG:HB2	3:D:1398:TRP:CZ2	2.56	0.40
3:D:1493:LYS:HZ1	3:D:1496:GLU:HG3	1.86	0.40
3:D:154:THR:OG1	3:D:157:GLU:HG3	2.21	0.40
3:D:586:ARG:HD3	3:D:586:ARG:HH11	1.70	0.40
5:F:270:LYS:HE2	5:F:295:MET:HE2	2.03	0.40
1:A:42:ARG:NH2	1:B:34:VAL:HG22	2.36	0.40
2:C:181:VAL:HG23	2:C:220:GLY:O	2.22	0.40
3:D:1208:ASP:OD1	3:D:1208:ASP:C	2.60	0.40
3:D:770:LEU:HB2	3:D:1210:SER:HA	2.03	0.40
3:D:895:VAL:HG11	3:D:922:LEU:HD21	2.04	0.40
3:D:961:LYS:HE3	3:D:961:LYS:HB2	1.86	0.40
5:F:393:THR:HG22	5:F:395:GLU:N	2.30	0.40
1:A:111:ALA:HB3	1:A:125:PRO:HA	2.03	0.40
3:D:1106:VAL:O	3:D:1108:ARG:HG3	2.21	0.40
3:D:1312:LEU:HD12	3:D:1324:PRO:HB2	2.03	0.40
3:D:850:LEU:HD23	3:D:850:LEU:HA	1.85	0.40
3:D:999:THR:O	3:D:1003:VAL:HG13	2.21	0.40
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.90	0.40
2:C:954:THR:HG23	2:C:965:GLU:OE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1377:LYS:HE3	3:D:1378:TYR:CZ	2.57	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	224/315 (71%)	222 (99%)	2 (1%)	0	100	100
1	B	220/315 (70%)	215 (98%)	5 (2%)	0	100	100
2	C	1107/1119 (99%)	1084 (98%)	23 (2%)	0	100	100
3	D	1482/1524 (97%)	1457 (98%)	24 (2%)	1 (0%)	55	86
4	E	92/99 (93%)	89 (97%)	2 (2%)	1 (1%)	17	47
5	F	344/423 (81%)	341 (99%)	3 (1%)	0	100	100
All	All	3469/3795 (91%)	3408 (98%)	59 (2%)	2 (0%)	55	86

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	94	PRO
3	D	530	VAL

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	199/273 (73%)	189 (95%)	10 (5%)	28	62
1	B	195/273 (71%)	186 (95%)	9 (5%)	31	65
2	C	936/941 (100%)	872 (93%)	64 (7%)	18	47
3	D	1253/1279 (98%)	1167 (93%)	86 (7%)	18	46
4	E	83/88 (94%)	82 (99%)	1 (1%)	75	94
5	F	301/371 (81%)	286 (95%)	15 (5%)	28	62
All	All	2967/3225 (92%)	2782 (94%)	185 (6%)	21	52

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	34	VAL
1	A	67	THR
1	A	104	GLU
1	A	126	ASP
1	A	142	VAL
1	A	184	THR
1	A	186	LEU
1	A	189	ARG
1	A	229	GLN
1	B	34	VAL
1	B	80	LEU
1	B	112	ARG
1	B	133	GLU
1	B	142	VAL
1	B	186	LEU
1	B	197	LEU
1	B	199	ILE
1	B	206	THR
2	C	8	ARG
2	C	11	GLU
2	C	15	LEU
2	C	56	GLU
2	C	81	ASP
2	C	97	ARG
2	C	103	LYS
2	C	107	LEU
2	C	133	ASP
2	C	141	HIS
2	C	168	ARG

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Mol	Chain	Res	Type
2	C	177	GLU
2	C	205	GLU
2	C	221	LEU
2	C	232	GLU
2	C	251	ASP
2	C	322	VAL
2	C	331	ARG
2	C	342	ASP
2	C	358	ARG
2	C	372	LEU
2	C	403	SER
2	C	427	VAL
2	C	434	HIS
2	C	454	SER
2	C	464	LEU
2	C	480	THR
2	C	482	GLU
2	C	512	ARG
2	C	524	VAL
2	C	557	ARG
2	C	575	GLN
2	C	583	LEU
2	C	586	ARG
2	C	589	ARG
2	C	591	SER
2	C	592	LEU
2	C	610	ARG
2	C	617	ASP
2	C	633	GLN
2	C	638	ASP
2	C	640	ARG
2	C	648	ARG
2	C	670	GLN
2	C	771	GLU
2	C	774	LEU
2	C	775	ARG
2	C	786	LYS
2	C	807	ARG
2	C	808	ARG
2	C	813	VAL
2	C	815	LEU
2	C	830	LYS

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Mol	Chain	Res	Type
2	C	848	VAL
2	C	916	GLU
2	C	923	GLU
2	C	928	LYS
2	C	939	ARG
2	C	942	GLU
2	C	952	LEU
2	C	968	LEU
2	C	1001	VAL
2	C	1014	SER
2	C	1057	SER
3	D	30	GLU
3	D	67	ARG
3	D	81	THR
3	D	106	LYS
3	D	135	LEU
3	D	141	ILE
3	D	155	ASP
3	D	161	LEU
3	D	190	GLU
3	D	191	LEU
3	D	198	ARG
3	D	200	ASP
3	D	204	LEU
3	D	230	TRP
3	D	231	VAL
3	D	256	GLU
3	D	272	LEU
3	D	275	GLU
3	D	276	ASP
3	D	312	ARG
3	D	325	GLU
3	D	331	VAL
3	D	335	LEU
3	D	362	GLU
3	D	372	ASP
3	D	387	LEU
3	D	399	ARG
3	D	411	THR
3	D	421	LEU
3	D	500	ARG
3	D	525	ARG

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Mol	Chain	Res	Type
3	D	548	ILE
3	D	572	ARG
3	D	576	GLU
3	D	587	ARG
3	D	591	VAL
3	D	610	LYS
3	D	618	LEU
3	D	632	VAL
3	D	646	LYS
3	D	650	LEU
3	D	709	HIS
3	D	754	PHE
3	D	778	LEU
3	D	808	THR
3	D	817	GLU
3	D	827	ILE
3	D	832	ARG
3	D	864	VAL
3	D	875	THR
3	D	894	LYS
3	D	904	VAL
3	D	943	THR
3	D	970	LYS
3	D	972	LEU
3	D	983	LEU
3	D	984	THR
3	D	1041	LEU
3	D	1062	ARG
3	D	1079	LYS
3	D	1083	ASP
3	D	1127	GLU
3	D	1128	VAL
3	D	1130	ARG
3	D	1155	VAL
3	D	1162	GLU
3	D	1188	VAL
3	D	1195	GLN
3	D	1208	ASP
3	D	1219	GLU
3	D	1221	VAL
3	D	1277	ILE
3	D	1284	GLU

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Mol	Chain	Res	Type
3	D	1287	GLU
3	D	1288	GLU
3	D	1290	LEU
3	D	1304	LYS
3	D	1305	LEU
3	D	1307	LYS
3	D	1313	VAL
3	D	1317	ASP
3	D	1455	LYS
3	D	1470	ARG
3	D	1493	LYS
3	D	1496	GLU
3	D	1501	GLU
4	E	50	THR
5	F	88	ILE
5	F	123	ASP
5	F	150	THR
5	F	172	ARG
5	F	186	HIS
5	F	205	ARG
5	F	208	SER
5	F	218	GLN
5	F	279	GLN
5	F	310	ILE
5	F	364	ARG
5	F	377	ASP
5	F	417	LYS
5	F	420	ASP
5	F	422	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	HIS
1	B	81	ASN
2	C	204	GLN
3	D	1195	GLN
3	D	1359	GLN
5	F	279	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 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	226/315 (71%)	-0.51	1 (0%) 92 90	43, 64, 95, 117	0
1	B	222/315 (70%)	-0.35	4 (1%) 69 60	43, 76, 114, 141	0
2	C	1111/1119 (99%)	-0.34	21 (1%) 67 58	23, 56, 125, 169	0
3	D	1486/1524 (97%)	-0.16	47 (3%) 48 37	23, 64, 127, 154	0
4	E	94/99 (94%)	-0.53	0 100 100	31, 58, 96, 129	0
5	F	346/423 (81%)	-0.10	14 (4%) 39 28	38, 86, 133, 171	0
6	G	18/22 (81%)	0.03	0 100 100	46, 75, 164, 175	0
7	H	22/27 (81%)	-0.06	2 (9%) 10 5	58, 91, 140, 171	0
All	All	3525/3844 (91%)	-0.25	89 (2%) 58 47	23, 65, 125, 175	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1128	VAL	5.6
3	D	1297	GLU	5.1
5	F	147	LEU	5.0
3	D	144	GLY	4.7
5	F	150	THR	4.5
5	F	149	GLU	4.5
5	F	148	LYS	4.5
3	D	422	ALA	4.0
2	C	296	GLY	4.0
2	C	219	GLN	3.8
3	D	427	VAL	3.7
3	D	406	ASP	3.6
3	D	1499	ARG	3.6
5	F	414	ARG	3.5
2	C	188	LYS	3.5
5	F	145	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
2	C	1	MET	3.4
3	D	1287	GLU	3.3
2	C	295	ASP	3.3
3	D	310	LEU	3.2
5	F	141	VAL	3.1
2	C	811	PRO	3.1
1	A	187	GLY	3.1
2	C	365	ASP	3.0
2	C	104	ASP	3.0
3	D	320	ALA	3.0
3	D	1497	GLU	2.9
2	C	362	GLY	2.9
3	D	1502	ALA	2.9
3	D	1500	LYS	2.8
3	D	216	VAL	2.8
3	D	241	ILE	2.8
2	C	203	ASP	2.8
3	D	1127	GLU	2.8
1	B	188	GLN	2.7
5	F	146	GLY	2.7
3	D	360	ARG	2.7
3	D	404	GLU	2.6
3	D	1129	THR	2.6
2	C	293	PHE	2.6
3	D	197	SER	2.6
5	F	423	ASP	2.6
2	C	232	GLU	2.6
3	D	350	HIS	2.6
7	H	24	DC	2.5
1	B	190	THR	2.5
7	H	25	DA	2.5
3	D	193	PRO	2.4
1	B	189	ARG	2.4
5	F	153	PRO	2.4
3	D	174	GLY	2.4
3	D	362	GLU	2.4
2	C	249	LYS	2.4
3	D	165	LYS	2.4
2	C	103	LYS	2.3
3	D	345	TYR	2.3
3	D	1126	ASP	2.3
3	D	976	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	93	SER	2.3
5	F	142	ARG	2.3
2	C	766	GLU	2.3
3	D	175	VAL	2.2
3	D	1299	PHE	2.2
3	D	1501	GLU	2.2
3	D	1282	ARG	2.2
3	D	1283	ILE	2.2
3	D	1130	ARG	2.2
3	D	1281	VAL	2.2
3	D	346	ARG	2.2
5	F	377	ASP	2.2
3	D	201	GLY	2.2
3	D	372	ASP	2.2
3	D	384	VAL	2.2
3	D	1315	ASP	2.1
3	D	316	GLN	2.1
3	D	380	GLU	2.1
3	D	1284	GLU	2.1
2	C	775	ARG	2.1
2	C	194	VAL	2.1
3	D	1292	VAL	2.1
2	C	247	PRO	2.1
2	C	764	GLU	2.1
3	D	363	ALA	2.1
5	F	297	PRO	2.1
2	C	254	VAL	2.0
2	C	298	PHE	2.0
3	D	191	LEU	2.0
5	F	379	ARG	2.0
3	D	429	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
9	MG	D	2004	1/1	0.93	0.48	9.81	52,52,52,52	0
8	ZN	D	2001	1/1	0.98	0.18	1.66	77,77,77,77	0
8	ZN	D	2002	1/1	0.94	0.33	1.54	238,238,238,238	0
9	MG	D	2003	1/1	0.97	0.19	-	44,44,44,44	0
9	MG	G	101	1/1	0.87	0.58	-	91,91,91,91	0

6.5 Other polymers

There are no such residues in this entry.