



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:22 AM UTC

PDB ID : 5VOI / pdb_00005voi
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 : 2017-05-02
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

<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

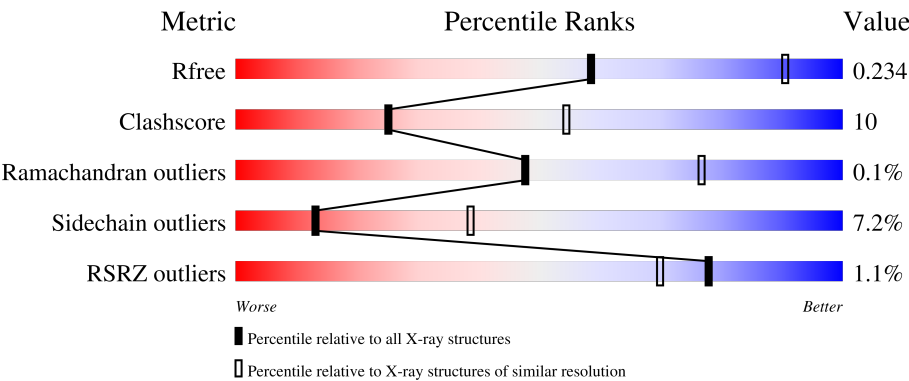
1 Overall quality at a glance i

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	315	54%16%28%
1	B	315	2% 53%15%30%
2	C	1119	% 72%24%
3	D	1524	% 72%23%
4	E	99	81%14%5%

Continued on next page...

Continued from previous page...

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	G	101	-	-	-	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 (CCD ID: ZN) (formula: Zn).

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

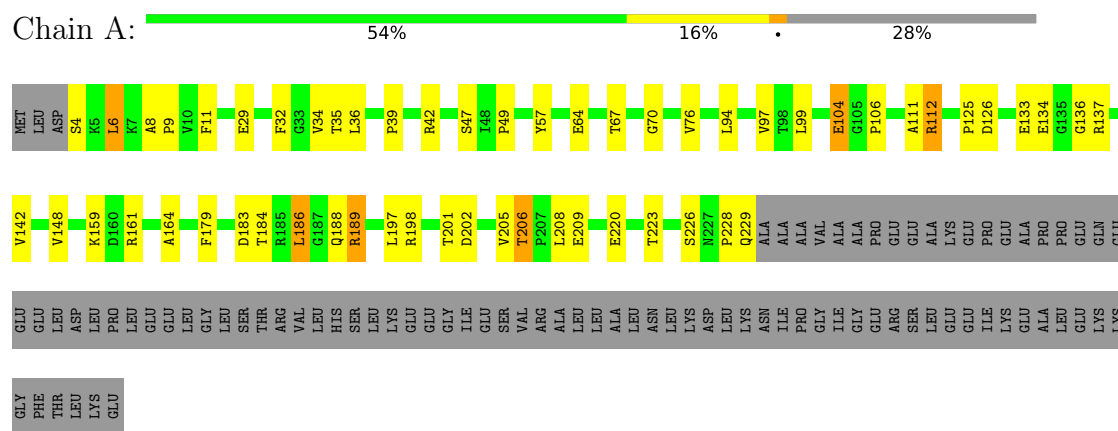
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

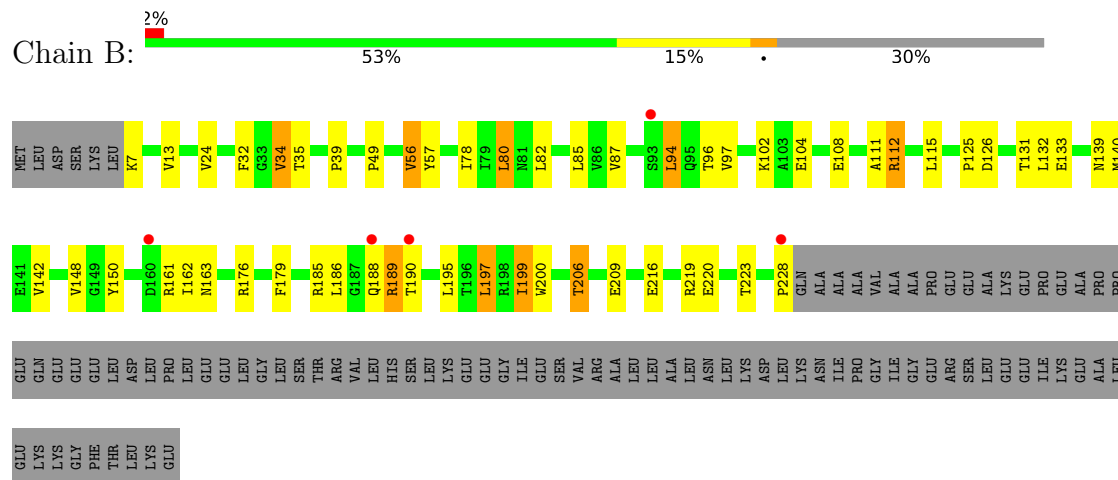
3 Residue-property plots [i](#)

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.

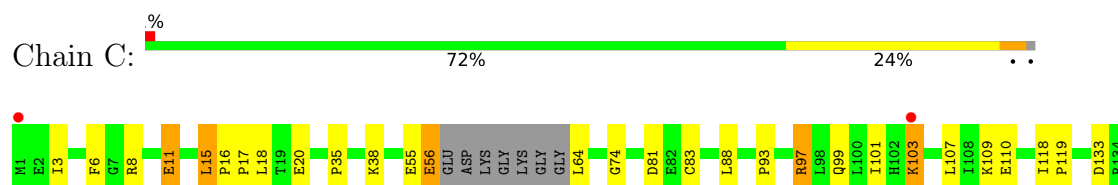
• Molecule 1: DNA-directed RNA polymerase subunit alpha

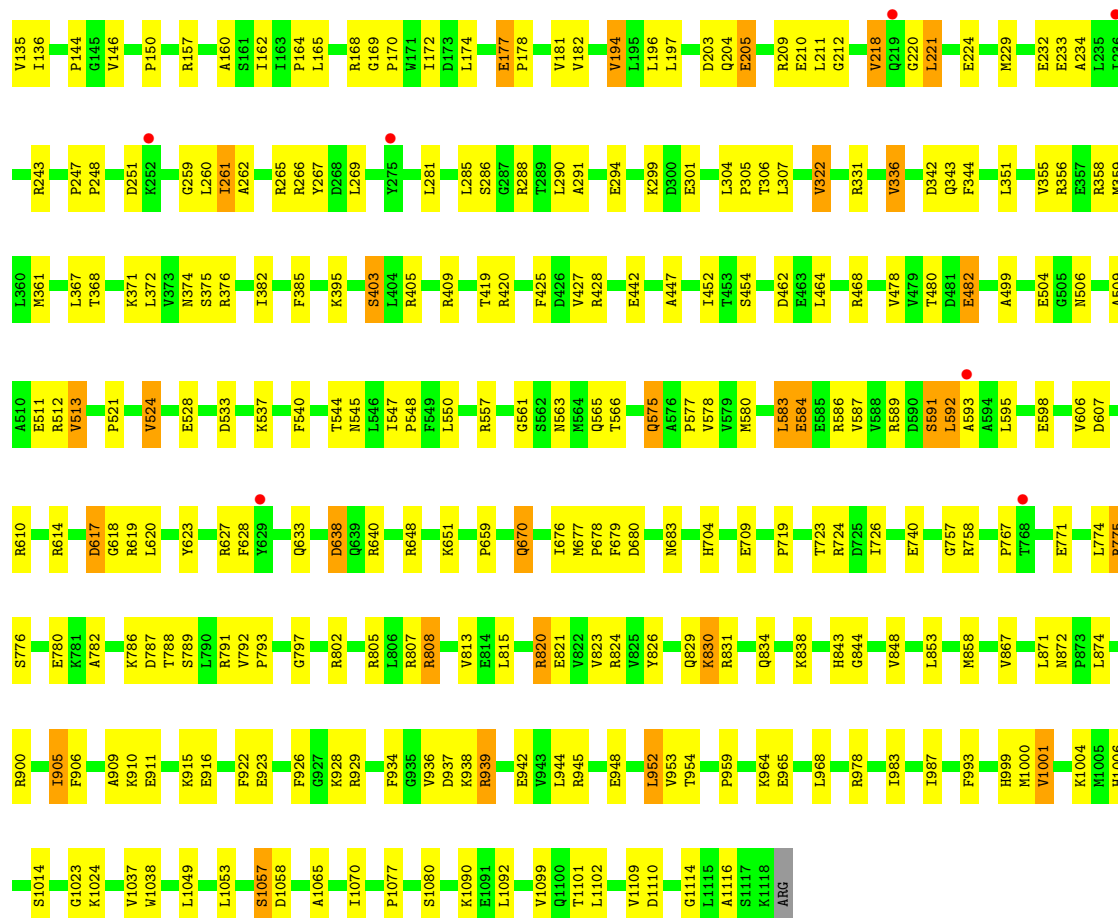


• Molecule 1: DNA-directed RNA polymerase subunit alpha

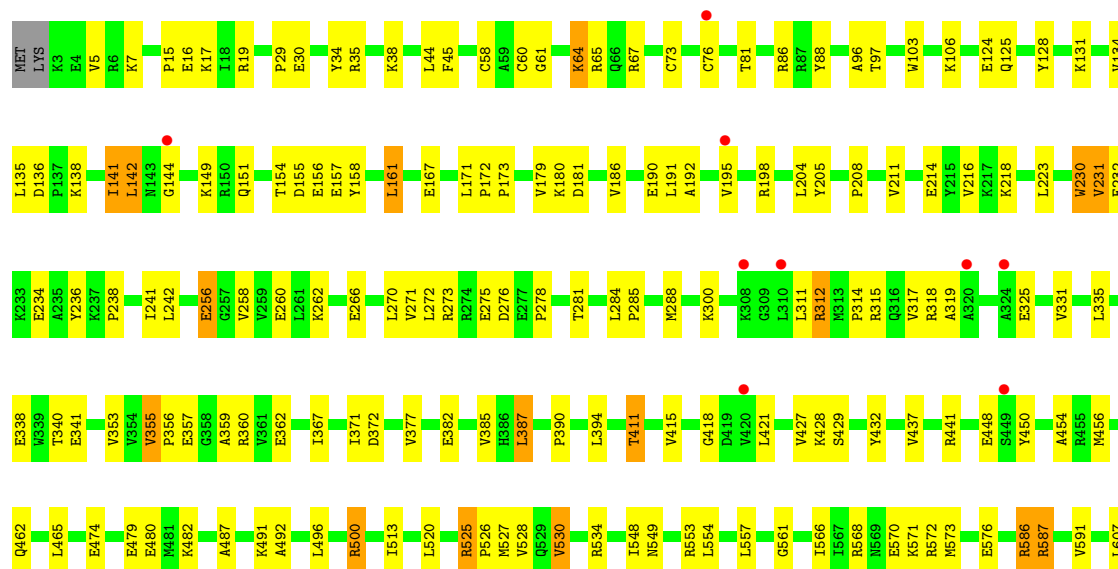


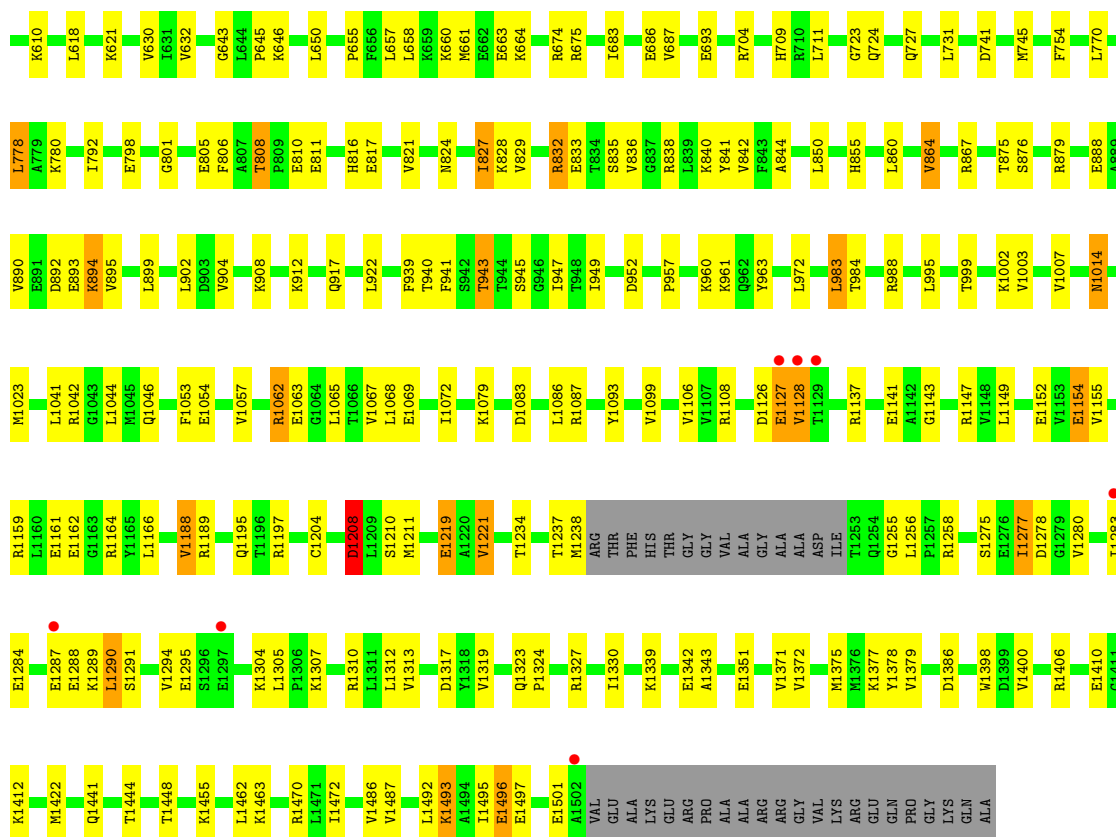
• Molecule 2: DNA-directed RNA polymerase subunit beta





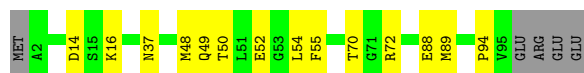
• Molecule 3: DNA-directed RNA polymerase subunit beta'





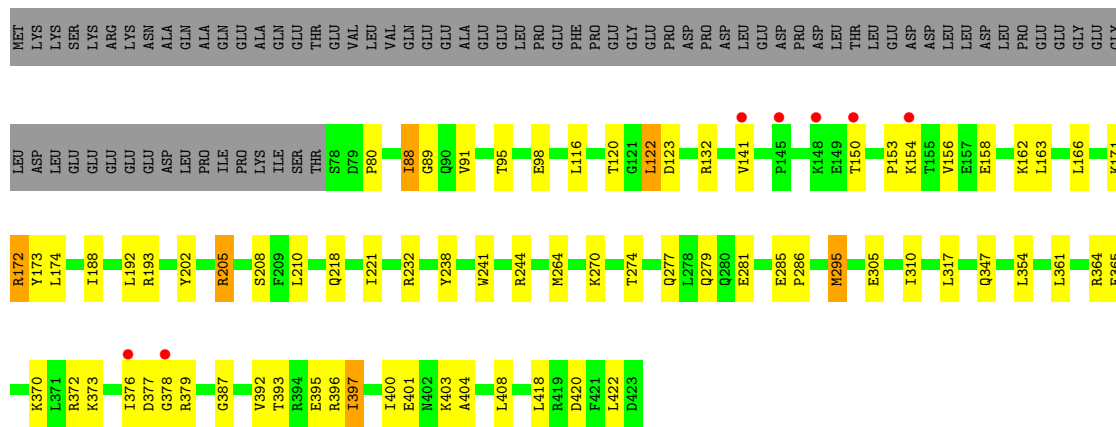
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 81% 14% 5%

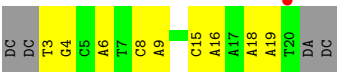


- Molecule 5: RNA polymerase sigma factor SigA

Chain F: 64% 16% 18%



- Molecule 6: PyrG promoter



● Molecule 7: PyrG promoter



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) 98.0 (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 0.193 , 0.234	Depositor DCC
R_{free} test set	2001 reflections (1.49%)	wwPDB-VP
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 , 55.4	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	0.51	0/1814	0.86	0/2466
1	B	0.50	0/1782	0.90	0/2424
2	C	0.55	0/8937	0.89	0/12087
3	D	0.56	0/11944	0.88	2/16148 (0.0%)
4	E	0.52	0/775	0.80	0/1045
5	F	0.47	0/2852	0.81	0/3837
6	G	0.75	0/413	0.75	0/634
7	H	0.70	0/505	0.94	1/776 (0.1%)
All	All	0.55	0/29022	0.87	3/39417 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1208	ASP	N-CA-C	-5.96	98.81	108.41
3	D	1154	GLU	CA-CB-CG	-5.54	103.02	114.10
7	H	10	DA	P-O3'-C3'	5.53	128.49	120.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1782	0	1834	42	0
1	B	1750	0	1797	42	0
2	C	8770	0	8874	191	0
3	D	11738	0	11971	245	0
4	E	761	0	778	10	0
5	F	2807	0	2882	50	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	543	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 10.

All (543) 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
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.54	0.88
3:D:949:ILE:HD11	3:D:1023:MET:HE1	1.57	0.86
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:1372:VAL:HA	3:D:1375:MET:HE3	1.59	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
5:F:270:LYS:HG2	5:F:295:MET:HE1	1.72	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
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
2:C:169:GLY:O	7:H:12:DC:N4	2.26	0.68
2:C:704:HIS:CE1	2:C:1000:MET:HE1	2.29	0.68
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.75	0.68
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.29	0.68
1:A:201:THR:HG21	1:A:205:VAL:O	1.94	0.68
3:D:60:CYS:SG	3:D:76:CYS:HB3	2.34	0.67
3:D:657:LEU:HG	3:D:661:MET:HE2	1.76	0.67
2:C:775:ARG:HD3	2:C:782:ALA:HB2	1.74	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
3:D:284:LEU:HD22	3:D:288:MET:HE2	1.76	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
2:C:521:PRO:HB3	3:D:1068:LEU:HD21	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:905:ILE:HG23	2:C:906:PHE:CD2	2.31	0.63
1:B:78:ILE:HG21	1:B:140:MET:HE1	1.80	0.62
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
4:E:37:ASN:HD22	4:E:89:MET:HE1	1.64	0.62
3:D:1371:VAL:HG12	3:D:1375:MET:HE2	1.80	0.62
3:D:658:LEU:HA	3:D:661:MET:HE3	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
3:D:223:LEU:HD11	3:D:288:MET:HE1	1.80	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:456:MET:HE1	3:D:568:ARG:NE	2.16	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:693:GLU:HG2	4:E:48:MET:HE1	1.86	0.57
3:D:899:LEU:HD22	3:D:917:GLN:HB3	1.87	0.57
3:D:1044:LEU:H	3:D:1044:LEU:HD12	1.68	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
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
3:D:1493:LYS:HZ2	3:D:1496:GLU:HG3	1.71	0.55
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:224:GLU:CD	2:C:224:GLU:H	2.16	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
2:C:580:MET:HB3	2:C:584:GLU:CD	2.34	0.52
5:F:295:MET:HA	5:F:295:MET:HE2	1.92	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
3:D:156:GLU:CD	3:D:156:GLU:H	2.17	0.52
4:E:52:GLU:HB2	4:E:55:PHE:HE2	1.75	0.52
2:C:808:ARG:NH2	5:F:305:GLU:OE2	2.42	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: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:44:LEU:O	3:D:525:ARG:NH2	2.34	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:356:ARG:HA	2:C:359:MET:HE2	1.93	0.51
2:C:109:LYS:HG2	2:C:368:THR:HG22	1.93	0.51
2:C:243:ARG:NH1	7:H:10:DA:H61	2.09	0.51
3:D:103:TRP:HB3	3:D:1448:THR:CG2	2.41	0.51
3:D:318:ARG:NH1	3:D:338:GLU:OE1	2.43	0.51
3:D:1289:LYS:HA	3:D:1307:LYS:HD2	1.92	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
3:D:230:TRP:CZ2	3:D:232:GLU:HG2	2.46	0.51
3:D:1083:ASP:OD1	3:D:1238:MET:HB3	2.11	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
1:B:188:GLN:CD	1:B:188:GLN:H	2.20	0.50
3:D:1208:ASP:OD2	3:D:1211:MET:HE2	2.11	0.50
3:D:963:TYR:CE2	3:D:1002:LYS:HD3	2.47	0.50
3:D:664:LYS:NZ	3:D:693:GLU:OE1	2.24	0.50
3:D:798:GLU:OE2	3:D:824:ASN:HB2	2.12	0.50
3:D:1288:GLU:O	3:D:1307:LYS:HE3	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
3:D:1342:GLU:CD	3:D:1342:GLU:H	2.21	0.49
1:B:94:LEU:HD12	1:B:96:THR:H	1.77	0.49
2:C:679:PHE:HA	3:D:943:THR:HB	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:32:PHE:HA	1:B:35:THR:HB	1.94	0.49
1:B:179:PHE:HB3	1:B:197:LEU:HD23	1.93	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
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:361:MET:HE1	5:F:244:ARG:CZ	2.43	0.48
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:35:PRO:HG2	2:C:38:LYS:HD3	1.96	0.48
2:C:758:ARG:HH21	2:C:788:THR:HB	1.77	0.48
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	1.95	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
3:D:658:LEU:HD23	3:D:661:MET:CE	2.43	0.48
2:C:118:ILE:HD11	2:C:344:PHE:CE2	2.49	0.48
2:C:211:LEU:HD21	2:C:307:LEU:HG	1.95	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
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:988:ARG:HH22	3:D:1054:GLU:CD	2.22	0.48
3:D:780:LYS:HE3	3:D:912:LYS:HD3	1.96	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
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
3:D:1277:ILE:HG22	3:D:1278:ASP:H	1.78	0.48
7:H:23:DG:O5'	7:H:23:DG:H2'	2.14	0.48
2:C:6:PHE:CD2	2:C:909:ALA:HB2	2.48	0.47
3:D:432:TYR:O	3:D:448:GLU:HA	2.14	0.47
3:D:527:MET:HB2	3:D:527:MET:HE2	1.76	0.47
3:D:939:PHE:O	3:D:943:THR:HG22	2.14	0.47
3:D:1087:ARG:HG3	3:D:1256:LEU:HD23	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1290:LEU:HD13	3:D:1291:SER:N	2.29	0.47
1:A:206:THR:HG22	1:A:208:LEU:N	2.29	0.47
3:D:801:GLY:HA2	3:D:821:VAL:HG22	1.96	0.47
3:D:1149:LEU:HG	3:D:1166:LEU:HD21	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:835:SER:OG	3:D:838:ARG:HG3	2.14	0.47
3:D:1386:ASP:HB3	3:D:1412:LYS:HD2	1.97	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
2:C:683:ASN:HB3	2:C:872:ASN:HB2	1.97	0.47
2:C:853:LEU:HB2	2:C:858:MET:CE	2.35	0.47
1:B:188:GLN:HE21	1:B:189:ARG:HG3	1.80	0.47
2:C:285:LEU:HD13	2:C:301:GLU:OE1	2.15	0.47
2:C:361:MET:HE1	5:F:244:ARG:NH2	2.30	0.47
2:C:617:ASP:OD1	2:C:617:ASP:N	2.47	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:167:GLU:O	3:D:394:LEU:HD12	2.15	0.47
3:D:258:VAL:HG12	3:D:273:ARG:O	2.15	0.47
3:D:557:LEU:HD13	3:D:566:ILE:HG22	1.96	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:792:ILE:HD13	3:D:941:PHE:CE1	2.49	0.47
3:D:1046:GLN:OE1	3:D:1046:GLN:N	2.45	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
1:B:188:GLN:HG2	1:B:189:ARG:N	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:456:MET:HE1	3:D:568:ARG:CZ	2.46	0.46
3:D:693:GLU:CG	4:E:48:MET:HE1	2.45	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:242:LEU:HD23	3:D:285:PRO:HG3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:24:VAL:HA	1:B:195:LEU:O	2.15	0.46
1:B:161:ARG:HG3	1:B:162:ILE:O	2.15	0.46
2:C:157:ARG:HA	2:C:157:ARG:HD3	1.78	0.46
3:D:534:ARG:HE	3:D:534:ARG:HB3	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
2:C:776:SER:CB	5:F:373:LYS:NZ	2.79	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
1:A:70:GLY:N	2:C:607:ASP:OD1	2.49	0.46
1:B:176:ARG:HG2	1:B:200:TRP:CZ3	2.51	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:355:VAL:HG11	3:D:385:VAL:HG21	1.98	0.45
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.99	0.45
3:D:418:GLY:N	3:D:429:SER:O	2.33	0.45
3:D:1462:LEU:HD22	3:D:1472:ILE:HB	1.98	0.45
3:D:1290:LEU:HD22	3:D:1290:LEU:HA	1.71	0.45
3:D:1422:MET:HB3	3:D:1422:MET:HE2	1.80	0.45
2:C:425:PHE:CE2	3:D:1086:LEU:HD12	2.51	0.45
2:C:937:ASP:OD1	2:C:939:ARG:HG2	2.16	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: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
3:D:1208:ASP:OD1	3:D:1208:ASP:C	2.60	0.45
3:D:1275:SER:OG	3:D:1294:VAL:HG21	2.16	0.45
2:C:243:ARG:NH2	7:H:9:DG:O6	2.48	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:203:ASP:OD2	2:C:204:GLN:N	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:893:GLU:H	3:D:894:LYS:HZ3	1.62	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
1:A:64:GLU:OE2	2:C:830:LYS:NZ	2.44	0.44
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:15:PRO:O	3:D:19:ARG:HG3	2.18	0.44
2:C:229:MET:HE3	2:C:234:ALA:HA	1.99	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
1:B:102:LYS:HG2	1:B:139:ASN:CG	2.42	0.44
4:E:14:ASP:OD2	4:E:14:ASP:N	2.50	0.44
1:B:112:ARG:NH1	1:B:126:ASP:CG	2.74	0.44
2:C:983:ILE:HG21	2:C:987:ILE:CD1	2.47	0.44
3:D:16:GLU:CD	3:D:16:GLU:H	2.26	0.44
2:C:290:LEU:O	2:C:301:GLU:HB2	2.17	0.44
2:C:1001:VAL:CG1	3:D:630:VAL:HB	2.46	0.44
3:D:172:PRO:HA	3:D:173:PRO:HD3	1.91	0.44
3:D:236:TYR:CZ	3:D:242:LEU:HD12	2.52	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:658:LEU:HD11	3:D:674:ARG:HH11	1.83	0.44
3:D:660:LYS:HD3	3:D:663:GLU:OE1	2.18	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
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
1:A:94:LEU:HD21	1:A:97:VAL:HG23	1.99	0.43
1:B:94:LEU:HD11	1:B:97:VAL:HG23	2.00	0.43
1:B:206:THR:HG22	1:B:209:GLU:N	2.13	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:281:LEU:HD11	2:C:306:THR:HG22	1.99	0.43
2:C:676:ILE:HA	2:C:871:LEU:O	2.18	0.43
3:D:418:GLY:O	3:D:428:LYS:HD3	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
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:1161:GLU:CD	3:D:1164:ARG:HB2	2.43	0.43
5:F:162:LYS:HB2	5:F:162:LYS:HE3	1.75	0.43
2:C:144:PRO:HG2	2:C:165:LEU:HD23	2.00	0.43
2:C:677:MET:HB3	2:C:987:ILE:HD13	1.99	0.43
2:C:936:VAL:HG11	2:C:959:PRO:CB	2.46	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
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:480:GLU:HG2	3:D:492:ALA:HB2	2.00	0.43
3:D:1377:LYS:HE3	3:D:1378:TYR:OH	2.19	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
3:D:223:LEU:CD1	3:D:288:MET:HE1	2.47	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
2:C:243:ARG:HH12	7:H:10:DA:H61	1.66	0.43
3:D:1154:GLU:HG2	3:D:1159:ARG:HA	1.99	0.43
3:D:1463:LYS:HB3	3:D:1463:LYS:HE2	1.82	0.43
1:A:47:SER:O	1:A:49:PRO:HD3	2.19	0.43
3:D:704:ARG:HB2	3:D:745:MET:HE2	2.00	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:88:ILE:HD12	5:F:88:ILE:HA	1.69	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:241:TRP:CZ2	7:H:1:DT:H4'	2.54	0.43
5:F:270:LYS:O	5:F:274:THR:OG1	2.33	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
1:A:64:GLU:CD	2:C:830:LYS:HZ2	2.25	0.42
2:C:261:ILE:CG2	2:C:291:ALA:HB3	2.49	0.42
2:C:1070:ILE:HG21	3:D:655:PRO:HB2	2.01	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:HD23	5:F:116:LEU:HA	1.85	0.42
1:B:162:ILE:O	1:B:163:ASN:HB2	2.19	0.42
2:C:18:LEU:HD23	2:C:18:LEU:HA	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:17:LYS:HE3	3:D:17:LYS:HB2	1.63	0.42
3:D:1237:THR:HB	3:D:1255:GLY:HA3	2.00	0.42
5:F:264:MET:HE2	5:F:264:MET:HB2	1.87	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
5:F:387:GLY:HA2	5:F:397:ILE:HD13	2.02	0.42
1:A:39:PRO:HG3	1:B:39:PRO:CG	2.50	0.42
1:A:97:VAL:HG12	1:A:99:LEU:HD12	2.01	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:HG3	2:C:482:GLU:O	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:83:CYS:HA	2:C:88:LEU:HB2	2.02	0.42
2:C:540:PHE:HB3	2:C:544:THR:HB	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:367:LEU:HA	2:C:371:LYS:HD2	2.01	0.42
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	2.02	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
5:F:238:TYR:OH	7:H:1:DT:H6	2.03	0.41
1:B:220:GLU:O	1:B:223:THR:OG1	2.34	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: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
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.55	0.41
3:D:97:THR:OG1	3:D:571:LYS:HE2	2.19	0.41
3:D:566:ILE:HD11	5:F:192:LEU:HD21	2.03	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:284:LEU:CD2	3:D:288:MET:HE2	2.47	0.41
3:D:1014:ASN:OD1	3:D:1014:ASN:N	2.53	0.41
2:C:15:LEU:HA	2:C:16:PRO:HD3	1.97	0.41
2:C:1023:GLY:HA2	6:G:18:DA:OP2	2.21	0.41
2:C:6:PHE:CE2	2:C:909:ALA:HB2	2.56	0.41
2:C:261:ILE:HG22	2:C:262:ALA:N	2.35	0.41
2:C:351:LEU:HD12	2:C:375:SER:HA	2.03	0.41
2:C:1101:THR:OG1	2:C:1109:VAL:O	2.39	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:HD23	1:B:115:LEU:HA	1.80	0.41
2:C:1070:ILE:CG2	3:D:655:PRO:HB2	2.51	0.41
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.87	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1487:VAL:HG11	3:D:1492:LEU:HD23	2.03	0.41
5:F:317:LEU:HD23	5:F:317:LEU:HA	1.85	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:NZ	1:B:7:LYS:HB3	2.35	0.40
2:C:118:ILE:HA	2:C:119:PRO:HD3	1.96	0.40
3:D:154:THR:OG1	3:D:157:GLU:HG3	2.21	0.40
3:D:586:ARG:HH11	3:D:586:ARG:HD3	1.70	0.40
3:D:1197:ARG:HB2	3:D:1398:TRP:CZ2	2.56	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: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: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
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
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
3:D:1127:GLU:CD	3:D:1127:GLU:H	2.30	0.40
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%)	48	77
4	E	92/99 (93%)	89 (97%)	2 (2%)	1 (1%)	11	36
5	F	344/423 (81%)	341 (99%)	3 (1%)	0	100	100
All	All	3469/3795 (91%)	3408 (98%)	59 (2%)	2 (0%)	48	77

All (2) Ramachandran outliers are listed below:

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

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	199/273 (73%)	187 (94%)	12 (6%)	17	47
1	B	195/273 (71%)	183 (94%)	12 (6%)	16	45
2	C	936/941 (100%)	862 (92%)	74 (8%)	11	35
3	D	1253/1279 (98%)	1155 (92%)	98 (8%)	11	35
4	E	83/88 (94%)	82 (99%)	1 (1%)	63	87
5	F	301/371 (81%)	283 (94%)	18 (6%)	17	47
All	All	2967/3225 (92%)	2752 (93%)	215 (7%)	13	39

All (215) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	104	GLU
1	A	112	ARG
1	A	126	ASP
1	A	142	VAL
1	A	184	THR
1	A	186	LEU
1	A	189	ARG
1	A	206	THR
1	A	229	GLN
1	B	34	VAL
1	B	56	VAL
1	B	80	LEU
1	B	94	LEU
1	B	112	ARG
1	B	133	GLU
1	B	142	VAL
1	B	186	LEU
1	B	189	ARG
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	172	ILE
2	C	177	GLU
2	C	182	VAL
2	C	194	VAL
2	C	196	LEU
2	C	205	GLU
2	C	218	VAL
2	C	221	LEU
2	C	232	GLU
2	C	251	ASP
2	C	261	ILE
2	C	265	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	322	VAL
2	C	331	ARG
2	C	336	VAL
2	C	342	ASP
2	C	358	ARG
2	C	372	LEU
2	C	403	SER
2	C	427	VAL
2	C	454	SER
2	C	464	LEU
2	C	480	THR
2	C	482	GLU
2	C	511	GLU
2	C	512	ARG
2	C	513	VAL
2	C	524	VAL
2	C	575	GLN
2	C	578	VAL
2	C	583	LEU
2	C	584	GLU
2	C	586	ARG
2	C	589	ARG
2	C	591	SER
2	C	592	LEU
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	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	820	ARG
2	C	830	LYS
2	C	848	VAL
2	C	905	ILE
2	C	910	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	916	GLU
2	C	923	GLU
2	C	928	LYS
2	C	939	ARG
2	C	952	LEU
2	C	968	LEU
2	C	978	ARG
2	C	1001	VAL
2	C	1014	SER
2	C	1057	SER
2	C	1080	SER
3	D	30	GLU
3	D	64	LYS
3	D	81	THR
3	D	106	LYS
3	D	135	LEU
3	D	141	ILE
3	D	142	LEU
3	D	155	ASP
3	D	161	LEU
3	D	179	VAL
3	D	186	VAL
3	D	190	GLU
3	D	191	LEU
3	D	198	ARG
3	D	204	LEU
3	D	230	TRP
3	D	231	VAL
3	D	234	GLU
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	355	VAL
3	D	360	ARG
3	D	362	GLU
3	D	372	ASP
3	D	387	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	411	THR
3	D	415	VAL
3	D	421	LEU
3	D	427	VAL
3	D	500	ARG
3	D	525	ARG
3	D	548	ILE
3	D	572	ARG
3	D	576	GLU
3	D	586	ARG
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	675	ARG
3	D	686	GLU
3	D	709	HIS
3	D	754	PHE
3	D	778	LEU
3	D	808	THR
3	D	810	GLU
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	908	LYS
3	D	943	THR
3	D	972	LEU
3	D	983	LEU
3	D	984	THR
3	D	995	LEU
3	D	1014	ASN
3	D	1041	LEU
3	D	1062	ARG
3	D	1067	VAL
3	D	1079	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	1127	GLU
3	D	1128	VAL
3	D	1152	GLU
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	1234	THR
3	D	1277	ILE
3	D	1283	ILE
3	D	1284	GLU
3	D	1287	GLU
3	D	1290	LEU
3	D	1304	LYS
3	D	1305	LEU
3	D	1313	VAL
3	D	1317	ASP
3	D	1455	LYS
3	D	1486	VAL
3	D	1493	LYS
3	D	1496	GLU
3	D	1501	GLU
4	E	50	THR
5	F	88	ILE
5	F	122	LEU
5	F	123	ASP
5	F	141	VAL
5	F	150	THR
5	F	172	ARG
5	F	205	ARG
5	F	208	SER
5	F	218	GLN
5	F	279	GLN
5	F	295	MET
5	F	310	ILE
5	F	347	GLN
5	F	364	ARG
5	F	377	ASP
5	F	397	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	F	420	ASP
5	F	422	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	HIS
1	B	81	ASN
1	B	221	HIS
2	C	117	HIS
2	C	130	ASN
2	C	187	ASN
2	C	567	GLN
2	C	962	GLN
2	C	991	GLN
3	D	348	GLN
3	D	350	HIS
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 oligosaccharides 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.44	0 100 100	43, 64, 95, 117	0
1	B	222/315 (70%)	-0.15	5 (2%) 61 51	43, 76, 114, 141	0
2	C	1111/1119 (99%)	-0.38	9 (0%) 82 75	23, 56, 125, 169	0
3	D	1486/1524 (97%)	-0.20	16 (1%) 78 70	23, 64, 127, 154	0
4	E	94/99 (94%)	-0.54	0 100 100	31, 58, 96, 129	0
5	F	346/423 (81%)	0.03	7 (2%) 65 56	38, 86, 133, 171	0
6	G	18/22 (81%)	0.01	1 (5%) 30 23	46, 75, 164, 175	0
7	H	22/27 (81%)	-0.01	0 100 100	58, 91, 140, 171	0
All	All	3525/3844 (91%)	-0.25	38 (1%) 78 70	23, 65, 125, 175	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	190	THR	3.5
1	B	93	SER	3.4
6	G	20	DT	3.3
3	D	420	VAL	2.8
5	F	141	VAL	2.8
2	C	1	MET	2.8
5	F	145	PRO	2.8
3	D	1128	VAL	2.7
5	F	154	LYS	2.7
1	B	160	ASP	2.7
3	D	144	GLY	2.6
3	D	310	LEU	2.6
2	C	219	GLN	2.6
3	D	308	LYS	2.4
3	D	1502	ALA	2.4
2	C	103	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	F	148	LYS	2.4
3	D	320	ALA	2.3
3	D	1297	GLU	2.3
5	F	376	ILE	2.3
2	C	593	ALA	2.3
3	D	1127	GLU	2.3
2	C	629	TYR	2.3
3	D	1283	ILE	2.2
1	B	228	PRO	2.2
3	D	1287	GLU	2.2
5	F	150	THR	2.2
3	D	324	ALA	2.2
3	D	76	CYS	2.2
3	D	195	VAL	2.1
5	F	378	GLY	2.1
1	B	188	GLN	2.1
3	D	1129	THR	2.1
3	D	449	SER	2.0
2	C	768	THR	2.0
2	C	236	ILE	2.0
2	C	252	LYS	2.0
2	C	275	TYR	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(Å ²)	Q<0.9
9	MG	G	101	1/1	0.65	0.59	91,91,91,91	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	MG	D	2004	1/1	0.92	0.25	52,52,52,52	0
8	ZN	D	2002	1/1	0.93	0.21	238,238,238,238	0
9	MG	D	2003	1/1	0.95	0.13	44,44,44,44	0
8	ZN	D	2001	1/1	0.99	0.12	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.