



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:56 AM UTC

PDB ID : 6DCF / pdb_00006dcf
Title : Crystal structure of a Mycobacterium smegmatis transcription initiation complex with Rifampicin-resistant RNA polymerase and bound to kanglemycin A
Authors : Lilic, M.; Darst, S.A.; Campbell, E.A.
Deposited on : 2018-05-06
Resolution : 3.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

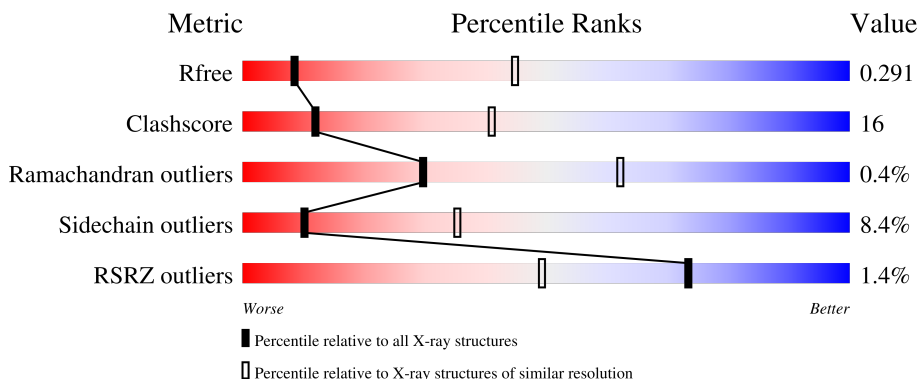
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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	J	114	
2	A	350	
2	B	350	
3	C	1169	

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Mol	Chain	Length	Quality of chain
4	D	1317	<p>61% 25% 11% 2%</p>
5	E	107	<p>45% 25% 7% 23%</p>
6	F	466	<p>49% 14% 36%</p>
7	O	31	<p>61% 39%</p>
8	P	26	<p>77% 23%</p>

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
10	SO4	C	1204	-	-	X	-
10	SO4	D	2006	-	-	X	-
10	SO4	D	2007	-	-	X	-
10	SO4	F	502	-	-	X	-
13	GLU	D	2008	-	-	X	-

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 23212 atoms, of which 12 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 RNA polymerase-binding protein RbpA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	J	85	662	416	120	124	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	219	1618	1022	276	318	2	0	0	0
2	B	225	1604	1009	280	313	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	858	6237	3909	1094	1205	29	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	447	LEU	SER	engineered mutation	UNP P60281

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	1176	8792	5494	1582	1678	38	0	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	E	82	624	396	107	121	0	0	0

- Molecule 6 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	297	2360	1480	428	445	7	0	0	0

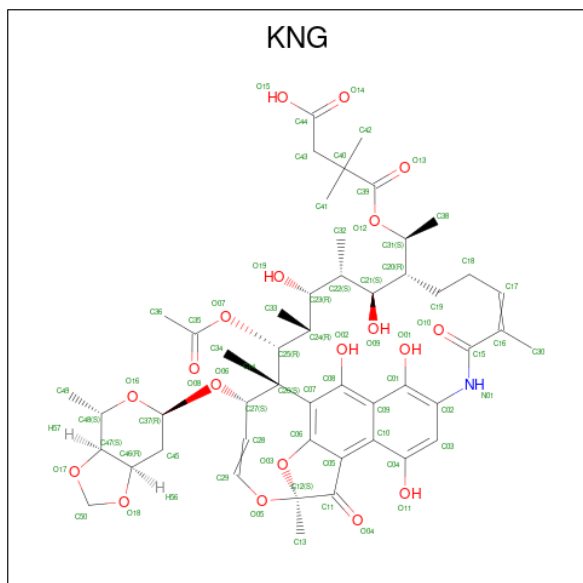
- Molecule 7 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
7	O	31	635	306	114	185	30	0	0	0

- Molecule 8 is a DNA chain called DNA (26-MER).

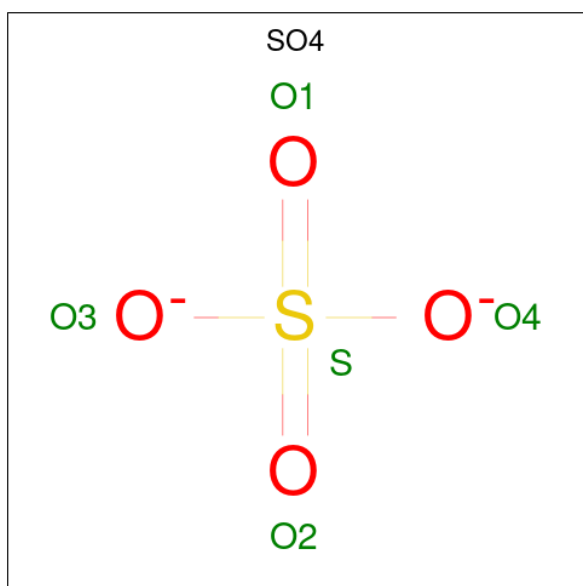
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
8	P	26	526	254	94	153	25	0	0	0

- Molecule 9 is Kanglemycin A (CCD ID: KNG) (formula: C₅₀H₆₇NO₁₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	C	1	70	50	1	19	0	0

- Molecule 10 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total O S 5 4 1	0	0
10	C	1	Total O S 5 4 1	0	0
10	C	1	Total O S 5 4 1	0	0
10	D	1	Total O S 5 4 1	0	0
10	D	1	Total O S 5 4 1	0	0
10	D	1	Total O S 5 4 1	0	0
10	D	1	Total O S 5 4 1	0	0
10	F	1	Total O S 5 4 1	0	0
10	F	1	Total O S 5 4 1	0	0

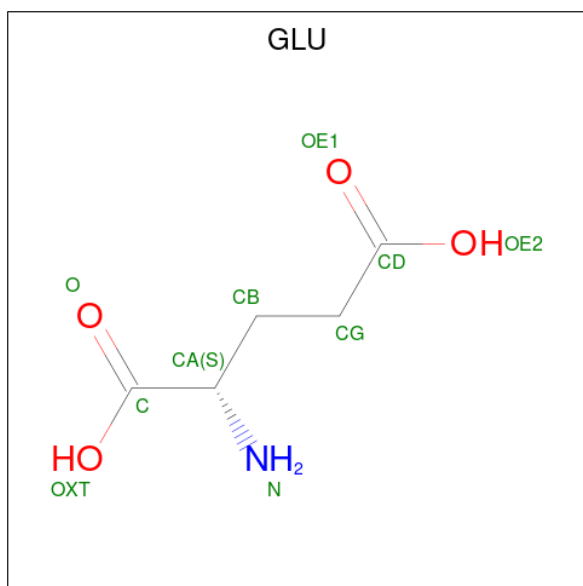
- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

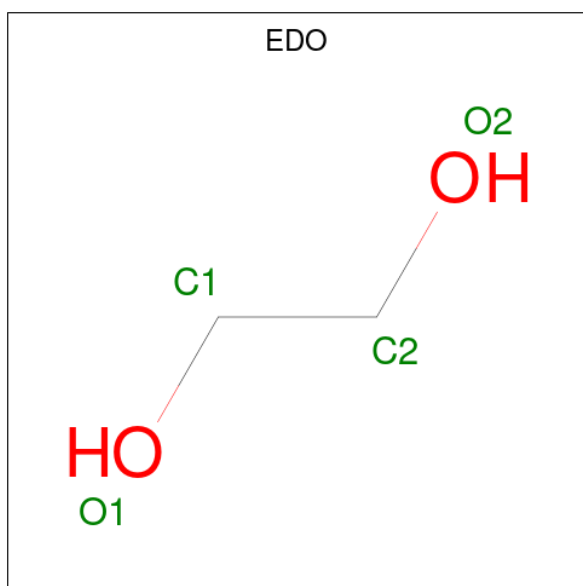
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	D	1	Total	Mg	0	0
			1	1		

- Molecule 13 is GLUTAMIC ACID (CCD ID: GLU) (formula: $C_5H_9NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
13	D	1	9	5	1	3	0	0

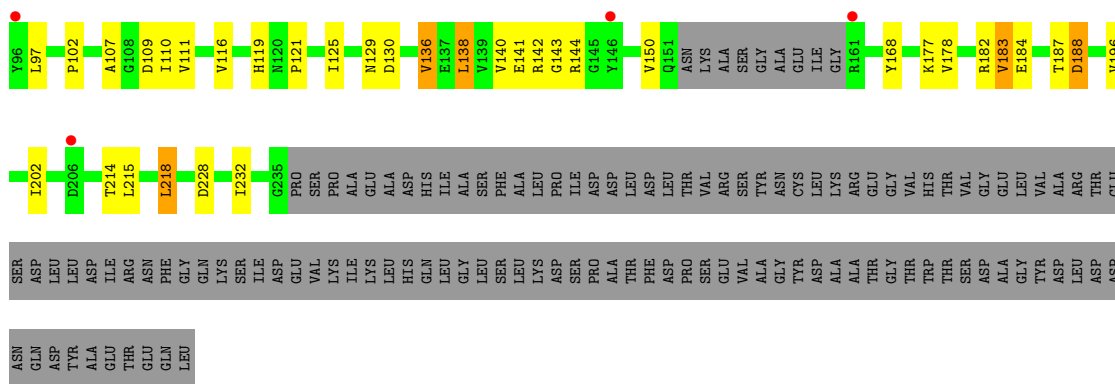
- Molecule 14 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



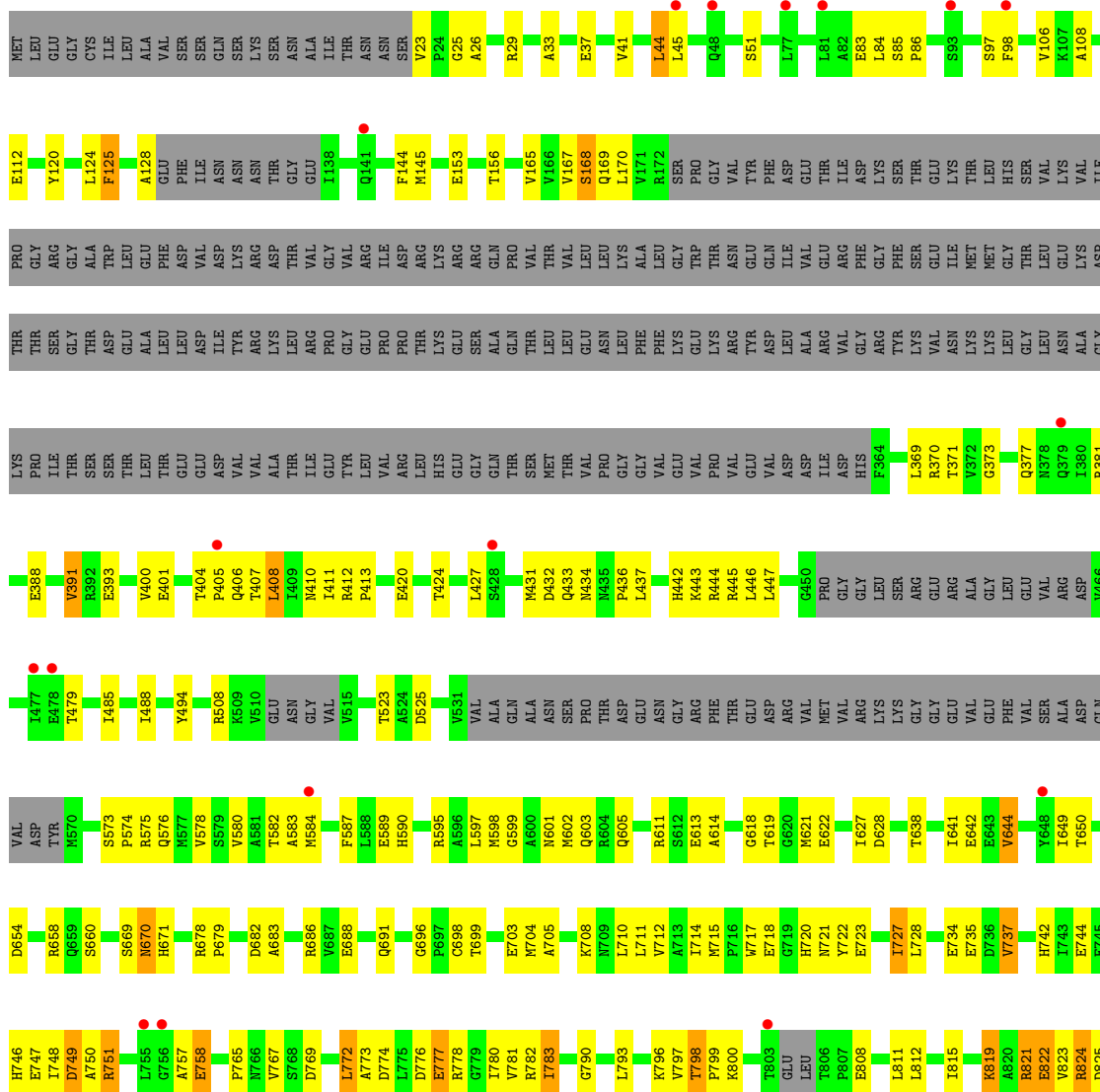
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	F	1	Total	C	H	O	0	0
			10	2	6	2		
14	F	1	Total	C	H	O	0	0
			10	2	6	2		

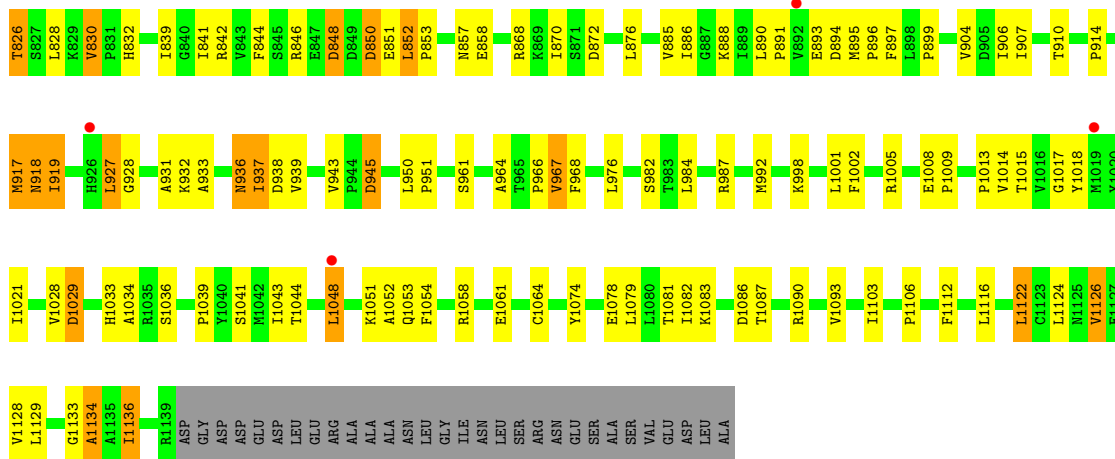
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	D	3	Total	O	0	0
			3	3		
15	F	2	Total	O	0	0
			2	2		
15	P	2	Total	O	0	0
			2	2		

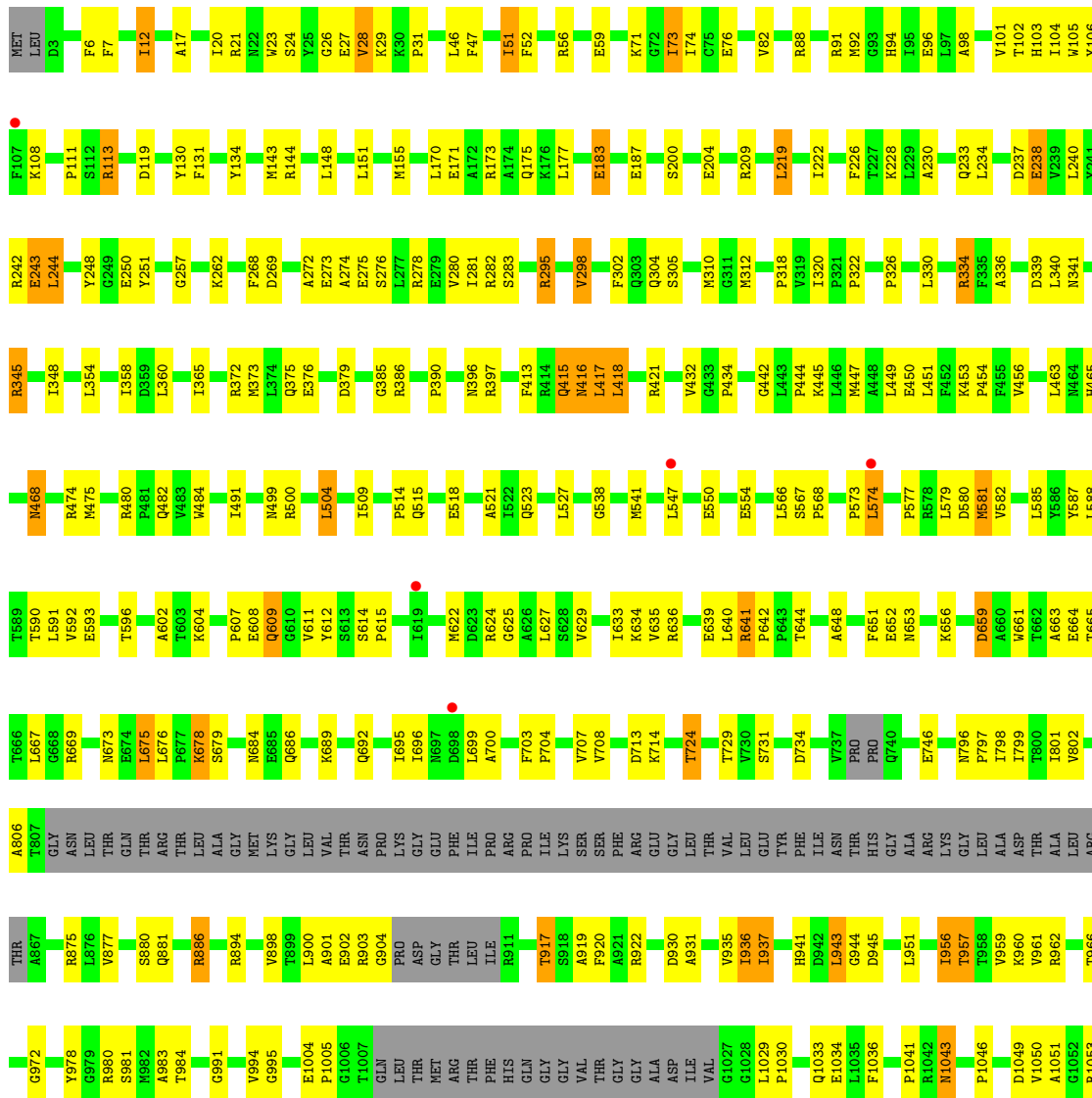


• Molecule 3: DNA-directed RNA polymerase subunit beta





• Molecule 4: DNA-directed RNA polymerase subunit beta'





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	129.25Å 160.91Å 136.86Å 90.00° 110.75° 90.00°	Depositor
Resolution (Å)	43.89 – 3.45 43.89 – 3.45	Depositor EDS
% Data completeness (in resolution range)	97.8 (43.89-3.45) 97.8 (43.89-3.45)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 3.13Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.252 , 0.290 0.255 , 0.291	Depositor DCC
R_{free} test set	1890 reflections (2.16%)	wwPDB-VP
Wilson B-factor (Å ²)	106.1	Xtrriage
Anisotropy	0.146	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 75.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23212	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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, EDO, SO4, ZN, KNG

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	J	0.12	0/676	0.42	0/918
2	A	0.10	0/1644	0.38	0/2245
2	B	0.11	0/1628	0.29	0/2229
3	C	0.11	0/6343	0.32	0/8636
4	D	0.11	0/8923	0.31	0/12103
5	E	0.13	0/637	0.38	0/868
6	F	0.09	0/2390	0.25	0/3223
7	O	0.20	0/712	0.39	0/1098
8	P	0.22	0/589	0.39	0/906
All	All	0.12	0/23542	0.32	0/32226

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	J	0	1
2	A	0	1
2	B	0	1
3	C	0	2
4	D	0	3
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	157	ALA	Peptide
2	B	183	VAL	Peptide
3	C	821	ARG	Peptide
3	C	822	GLU	Peptide
4	D	1177	LEU	Peptide
4	D	282	ARG	Peptide
4	D	936	ILE	Peptide
1	J	69	VAL	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	J	662	0	631	30	0
2	A	1618	0	1624	54	0
2	B	1604	0	1552	47	0
3	C	6237	0	5937	239	0
4	D	8792	0	8499	300	0
5	E	624	0	604	26	0
6	F	2360	0	2388	60	0
7	O	635	0	354	14	0
8	P	526	0	296	10	0
9	C	70	0	0	2	0
10	C	15	0	0	4	0
10	D	20	0	0	13	0
10	F	10	0	0	3	0
11	D	2	0	0	0	0
12	D	1	0	0	0	0
13	D	9	0	5	14	0
14	F	8	12	12	1	0
15	D	3	0	0	0	0
15	F	2	0	0	0	0
15	P	2	0	0	0	0
All	All	23200	12	21902	706	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 (706) 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:C:819:LYS:HE3	3:C:819:LYS:HA	1.29	1.08
1:J:68:ASP:O	1:J:70:PRO:HD3	1.57	1.05
4:D:1129:ARG:NH1	10:D:2007:SO4:O2	1.92	1.01
4:D:1129:ARG:NH1	10:D:2007:SO4:S	2.33	1.00
3:C:800:LYS:CB	3:C:822:GLU:HB3	1.91	0.99
3:C:822:GLU:HB2	3:C:823:VAL:CG1	1.98	0.94
4:D:1265:ILE:HG23	13:D:2008:GLU:HG2	1.51	0.93
4:D:894:ARG:NH1	10:D:2007:SO4:O1	2.02	0.92
3:C:717:TRP:H	3:C:721:ASN:HD21	1.12	0.90
4:D:1266:SER:HB2	13:D:2008:GLU:HA	1.54	0.90
4:D:527:LEU:HD21	4:D:581:MET:HE1	1.51	0.89
1:J:84:MET:HE3	6:F:272:LYS:HE2	1.60	0.83
3:C:822:GLU:HB2	3:C:823:VAL:HG12	1.61	0.83
4:D:1266:SER:CB	13:D:2008:GLU:HA	2.08	0.83
3:C:1015:THR:H	4:D:729:THR:HG21	1.43	0.82
1:J:42:VAL:HG13	4:D:74:ILE:HD12	1.61	0.81
3:C:758:GLU:HB3	3:C:799:PRO:HD3	1.63	0.81
2:A:89:ASP:O	2:A:91:GLU:N	2.14	0.80
6:F:210:LYS:NZ	10:F:502:SO4:O3	2.14	0.80
4:D:1265:ILE:HG23	13:D:2008:GLU:CG	2.12	0.79
2:B:60:LEU:H	2:B:60:LEU:HD13	1.47	0.79
3:C:937:ILE:HD13	3:C:939:VAL:HG13	1.64	0.79
4:D:47:PHE:O	4:D:88:ARG:NH2	2.15	0.78
6:F:426:THR:CG2	6:F:429:GLU:HG3	2.12	0.78
2:A:40:ARG:HD3	2:B:33:THR:HG22	1.67	0.77
2:A:97:LEU:HB3	2:A:136:VAL:HG22	1.66	0.77
4:D:936:ILE:HG12	4:D:937:ILE:HD12	1.67	0.77
2:A:88:ASP:N	2:A:88:ASP:OD1	2.16	0.76
3:C:125:PHE:HB3	3:C:144:PHE:HA	1.67	0.76
2:B:54:ILE:HG22	2:B:138:LEU:HB3	1.67	0.76
4:D:56:ARG:HG3	4:D:59:GLU:HB2	1.66	0.76
4:D:579:LEU:HA	4:D:806:ALA:HB1	1.66	0.76
2:A:56:ILE:HB	2:A:59:VAL:HG22	1.67	0.75
3:C:33:ALA:HB2	3:C:966:PRO:HG2	1.69	0.75
5:E:84:LEU:HB2	5:E:85:GLN:HE21	1.53	0.74
4:D:894:ARG:HH11	4:D:960:LYS:HZ3	1.35	0.74
4:D:641:ARG:NE	4:D:642:PRO:HD3	2.03	0.73
3:C:822:GLU:HB2	3:C:823:VAL:HG13	1.70	0.73
3:C:144:PHE:N	6:F:326:GLN:OE1	2.20	0.73
3:C:1079:LEU:HD23	3:C:1083:LYS:HD2	1.70	0.73
4:D:894:ARG:HB3	10:D:2007:SO4:O3	1.89	0.73
3:C:574:PRO:O	3:C:575:ARG:HG2	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:944:GLY:HA2	4:D:980:ARG:HH22	1.52	0.72
6:F:426:THR:OG1	8:P:19:DT:H3'	1.89	0.72
4:D:376:GLU:OE2	6:F:165:SER:OG	2.06	0.72
4:D:421:ARG:NH2	10:D:2005:SO4:O4	2.22	0.72
2:B:75:ASP:O	2:B:79:ASN:ND2	2.23	0.71
8:P:11:DA:H4'	8:P:12:DA:OP1	1.89	0.71
5:E:62:ASN:O	5:E:66:ASN:ND2	2.24	0.71
3:C:590:HIS:HB3	3:C:919:ILE:HG23	1.72	0.71
4:D:567:SER:HB2	4:D:574:LEU:HD13	1.72	0.71
7:O:12:DG:O6	8:P:14:DA:N6	2.24	0.71
4:D:700:ALA:HA	4:D:708:VAL:HG21	1.73	0.70
3:C:822:GLU:OE1	3:C:822:GLU:N	2.23	0.70
4:D:444:PRO:HD2	4:D:447:MET:HE2	1.73	0.70
6:F:404:THR:OG1	6:F:457:ARG:NH1	2.25	0.70
4:D:1160:ARG:NH2	10:D:2006:SO4:O1	2.24	0.70
6:F:438:ARG:NH1	8:P:20:DG:N7	2.39	0.70
6:F:426:THR:OG1	8:P:20:DG:OP2	2.09	0.70
3:C:742:HIS:HD2	3:C:868:ARG:HG3	1.57	0.70
3:C:798:THR:HG23	3:C:826:THR:HG21	1.73	0.69
7:O:19:DA:H2''	7:O:20:DT:O5'	1.92	0.69
4:D:922:ARG:HB3	4:D:961:VAL:HG11	1.74	0.69
3:C:611:ARG:NH2	3:C:735:GLU:O	2.26	0.69
3:C:641:ILE:HG21	3:C:644:VAL:HG13	1.74	0.69
5:E:40:LEU:HB3	5:E:50:LEU:HD11	1.75	0.69
3:C:819:LYS:HE3	3:C:819:LYS:CA	2.18	0.69
4:D:1129:ARG:NH1	10:D:2007:SO4:O3	2.25	0.69
4:D:894:ARG:HB3	10:D:2007:SO4:S	2.33	0.68
1:J:57:ARG:NH1	4:D:24:SER:O	2.27	0.68
4:D:1171:SER:HA	4:D:1176:PHE:O	1.93	0.68
3:C:391:VAL:HA	3:C:408:LEU:HD12	1.74	0.68
4:D:894:ARG:NH1	10:D:2007:SO4:S	2.66	0.68
3:C:708:LYS:HG3	3:C:737:VAL:HG23	1.76	0.67
4:D:365:ILE:HD12	4:D:365:ILE:H	1.60	0.67
6:F:210:LYS:NZ	10:F:502:SO4:S	2.68	0.67
4:D:442:GLY:HA3	4:D:523:GLN:HB2	1.76	0.67
3:C:649:ILE:HD11	3:C:679:PRO:HB3	1.77	0.66
1:J:68:ASP:C	1:J:70:PRO:HD3	2.19	0.66
3:C:774:ASP:HA	3:C:782:ARG:HH21	1.59	0.66
2:B:107:ALA:O	2:B:110:ILE:HG22	1.95	0.66
3:C:595:ARG:NH2	10:C:1203:SO4:O3	2.28	0.66
2:B:75:ASP:OD1	4:D:636:ARG:NH2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:750:ALA:HB3	3:C:858:GLU:H	1.61	0.66
5:E:84:LEU:HD12	5:E:84:LEU:H	1.61	0.66
4:D:1177:LEU:CB	4:D:1178:PRO:HD3	2.25	0.66
5:E:42:SER:OG	5:E:43:ARG:NH1	2.29	0.66
4:D:991:GLY:HA2	4:D:1265:ILE:HD12	1.78	0.65
8:P:11:DA:H2''	8:P:12:DA:C5'	2.26	0.65
3:C:751:ARG:CB	3:C:757:ALA:HB1	2.26	0.65
3:C:1043:ILE:HD12	3:C:1043:ILE:H	1.62	0.65
4:D:1144:ARG:HH12	4:D:1150:ILE:H	1.43	0.65
4:D:432:VAL:HG22	4:D:434:PRO:HD3	1.78	0.65
4:D:1220:SER:HB2	4:D:1244:ASP:OD2	1.97	0.65
4:D:20:ILE:HD13	4:D:318:PRO:HD3	1.77	0.65
4:D:238:GLU:OE1	6:F:175:LYS:NZ	2.29	0.65
4:D:972:GLY:N	10:D:2006:SO4:O4	2.24	0.65
4:D:1276:THR:HG22	5:E:102:GLU:HG3	1.77	0.65
7:O:19:DA:H4'	7:O:20:DT:OP1	1.96	0.65
4:D:527:LEU:CD2	4:D:581:MET:HE1	2.25	0.64
4:D:1266:SER:N	13:D:2008:GLU:HG3	2.12	0.64
3:C:1074:TYR:O	3:C:1078:GLU:HG2	1.96	0.64
4:D:951:LEU:HB3	4:D:956:ILE:HD11	1.79	0.64
3:C:895:MET:HG3	3:C:896:PRO:HD2	1.79	0.64
3:C:819:LYS:HA	3:C:819:LYS:CE	2.16	0.64
4:D:386:ARG:HH12	4:D:1231:THR:HG21	1.63	0.64
6:F:280:LYS:HG2	7:O:30:DC:OP2	1.97	0.64
2:A:22:VAL:HB	2:A:193:ILE:HG23	1.80	0.63
4:D:936:ILE:HG12	4:D:937:ILE:H	1.63	0.63
2:B:6:ARG:O	2:B:6:ARG:HG2	1.97	0.63
4:D:922:ARG:HB3	4:D:961:VAL:CG1	2.29	0.63
2:A:40:ARG:HH21	3:C:894:ASP:HB3	1.64	0.63
2:B:102:PRO:HG3	2:B:130:ASP:HA	1.81	0.63
3:C:619:THR:HG23	3:C:621:MET:H	1.63	0.63
6:F:426:THR:HG22	6:F:429:GLU:HG3	1.81	0.62
4:D:639:GLU:HG2	4:D:678:LYS:HD3	1.80	0.62
4:D:170:LEU:HD13	4:D:209:ARG:HH11	1.63	0.62
5:E:80:VAL:HG23	5:E:95:GLU:HG2	1.81	0.62
3:C:437:LEU:HB2	3:C:704:MET:HE2	1.80	0.62
4:D:797:PRO:O	4:D:801:ILE:HG13	1.99	0.62
1:J:25:ALA:N	1:J:26:PRO:HD3	2.14	0.62
4:D:1248:GLY:O	4:D:1252:ASN:ND2	2.32	0.62
3:C:23:VAL:HB	3:C:26:ALA:HB2	1.82	0.62
4:D:894:ARG:HD2	10:D:2007:SO4:O1	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:40:ARG:HH11	2:A:40:ARG:HB3	1.64	0.62
3:C:584:MET:HA	3:C:619:THR:HG21	1.82	0.62
4:D:155:MET:HE3	4:D:219:LEU:HD23	1.81	0.62
3:C:598:MET:O	3:C:602:MET:HG2	1.99	0.61
4:D:170:LEU:HD13	4:D:209:ARG:NH1	2.15	0.61
4:D:491:ILE:HG23	4:D:514:PRO:HG2	1.82	0.61
4:D:880:SER:O	4:D:995:GLY:HA3	2.00	0.61
4:D:641:ARG:NE	4:D:641:ARG:HA	2.15	0.61
4:D:886:ARG:NH1	13:D:2008:GLU:OE1	2.30	0.61
6:F:426:THR:HG1	8:P:20:DG:P	2.23	0.61
4:D:1266:SER:H	13:D:2008:GLU:HG3	1.65	0.61
4:D:920:PHE:HE1	4:D:945:ASP:HB2	1.66	0.60
4:D:661:TRP:CZ3	4:D:663:ALA:HB2	2.36	0.60
4:D:894:ARG:NH1	4:D:960:LYS:HZ3	2.00	0.60
2:A:2:LEU:HD11	2:B:142:ARG:HB2	1.83	0.60
4:D:170:LEU:HD11	4:D:209:ARG:HD3	1.82	0.60
4:D:798:ILE:O	4:D:802:VAL:HG23	2.01	0.60
3:C:108:ALA:HB1	3:C:112:GLU:HG2	1.83	0.59
3:C:758:GLU:HB3	3:C:798:THR:HA	1.84	0.59
3:C:1087:THR:HA	3:C:1090:ARG:NH1	2.16	0.59
1:J:109:ARG:NH2	6:F:214:GLN:OE1	2.36	0.59
2:A:43:LEU:HA	2:A:171:VAL:HG11	1.84	0.59
4:D:28:VAL:HG21	4:D:46:LEU:HD23	1.85	0.59
7:O:14:DG:H2"	7:O:15:DT:OP2	2.02	0.59
3:C:846:ARG:HE	3:C:857:ASN:HA	1.67	0.59
3:C:1124:LEU:HD11	4:D:105:TRP:HZ3	1.67	0.59
4:D:898:VAL:HG11	4:D:919:ALA:HB2	1.84	0.59
3:C:404:THR:HG23	3:C:407:THR:H	1.67	0.59
3:C:1129:LEU:HG	3:C:1134:ALA:O	2.03	0.59
3:C:170:LEU:HD12	3:C:369:LEU:H	1.68	0.59
1:J:79:ARG:NH2	7:O:25:DC:OP1	2.35	0.59
2:A:129:ASN:HD22	2:A:129:ASN:H	1.50	0.58
2:A:187:THR:O	2:A:188:ASP:OD1	2.21	0.58
3:C:388:GLU:O	3:C:391:VAL:HG22	2.02	0.58
2:A:146:TYR:HD1	2:A:167:ILE:HG12	1.68	0.58
3:C:98:PHE:HA	3:C:128:ALA:HB3	1.85	0.58
4:D:52:PHE:O	4:D:91:ARG:HD2	2.04	0.58
2:B:63:PHE:HD2	2:B:64:THR:HG23	1.67	0.58
2:B:74:THR:HG23	4:D:611:VAL:HG21	1.84	0.58
6:F:251:ARG:HB2	6:F:297:MET:HE1	1.86	0.58
3:C:718:GLU:H	4:D:724:THR:CG2	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:426:THR:HG23	6:F:429:GLU:HG3	1.86	0.57
4:D:917:THR:HG21	4:D:1144:ARG:HH21	1.68	0.57
2:B:49:ALA:HA	2:B:142:ARG:HA	1.87	0.57
3:C:85:SER:HB2	3:C:97:SER:HA	1.85	0.57
5:E:27:ASP:OD2	5:E:28:THR:HG22	2.03	0.57
4:D:230:ALA:N	4:D:233:GLN:OE1	2.38	0.57
3:C:717:TRP:H	3:C:721:ASN:ND2	1.93	0.57
3:C:910:THR:HG21	4:D:729:THR:HA	1.87	0.57
4:D:119:ASP:HB2	4:D:295:ARG:NH1	2.20	0.57
5:E:76:VAL:HG22	5:E:77:GLY:H	1.69	0.57
4:D:269:ASP:HB3	4:D:272:ALA:HB3	1.86	0.57
3:C:1051:LYS:HG2	3:C:1052:ALA:H	1.69	0.56
4:D:183:GLU:O	4:D:187:GLU:HG2	2.04	0.56
6:F:426:THR:O	6:F:430:ILE:HG13	2.05	0.56
3:C:822:GLU:N	3:C:823:VAL:HG13	2.19	0.56
8:P:11:DA:H2''	8:P:12:DA:O5'	2.05	0.56
3:C:1036:SER:HB3	4:D:450:GLU:O	2.05	0.56
1:J:36:ASN:HD21	1:J:58:ASN:HD21	1.54	0.56
3:C:885:VAL:HG13	4:D:538:GLY:H	1.71	0.56
4:D:902:GLU:OE2	4:D:903:ARG:N	2.39	0.56
4:D:396:ASN:O	4:D:396:ASN:ND2	2.39	0.55
6:F:218:ASP:O	6:F:222:ILE:HG12	2.07	0.55
1:J:89:ARG:NH2	6:F:274:ASP:OD1	2.31	0.55
2:A:94:THR:HG22	2:A:139:VAL:HG22	1.87	0.55
4:D:415:GLN:O	4:D:415:GLN:HG2	2.06	0.55
4:D:1251:GLU:OE1	4:D:1251:GLU:N	2.37	0.55
7:O:2:DC:O2	8:P:25:DG:N2	2.34	0.55
3:C:433:GLN:O	3:C:669:SER:OG	2.22	0.55
3:C:638:THR:HG23	3:C:688:GLU:HA	1.88	0.55
4:D:937:ILE:HG23	4:D:941:HIS:HD2	1.72	0.55
6:F:409:GLU:HG2	6:F:448:THR:CG2	2.36	0.55
2:A:102:PRO:HD3	2:A:130:ASP:HA	1.89	0.55
3:C:45:LEU:HD21	3:C:443:LYS:HE3	1.87	0.55
3:C:433:GLN:NE2	3:C:670:ASN:OD1	2.33	0.55
3:C:479:THR:HG21	3:C:485:ILE:HG13	1.88	0.55
3:C:1116:LEU:HG	3:C:1126:VAL:HG21	1.88	0.55
4:D:1144:ARG:HH22	4:D:1150:ILE:H	1.55	0.55
3:C:708:LYS:NZ	3:C:737:VAL:O	2.38	0.55
4:D:1118:ASP:HB3	4:D:1121:GLU:HB2	1.89	0.55
3:C:914:PRO:HB3	4:D:798:ILE:HG23	1.88	0.55
3:C:1136:ILE:O	3:C:1136:ILE:HG13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:937:ILE:HG23	4:D:941:HIS:CD2	2.42	0.55
4:D:1225:ALA:HB1	4:D:1230:THR:HG23	1.88	0.54
3:C:939:VAL:HG11	3:C:943:VAL:HG12	1.89	0.54
3:C:669:SER:OG	3:C:670:ASN:N	2.39	0.54
3:C:1058:ARG:HH11	4:D:418:LEU:HA	1.72	0.54
4:D:274:ALA:O	4:D:278:ARG:HG2	2.06	0.54
4:D:463:LEU:HB2	4:D:465:HIS:HD2	1.73	0.54
4:D:956:ILE:HD12	4:D:956:ILE:O	2.07	0.54
7:O:15:DT:H1'	7:O:16:DT:H5''	1.89	0.54
4:D:302:PHE:HZ	4:D:312:MET:HE3	1.71	0.54
2:B:54:ILE:HA	2:B:138:LEU:HA	1.89	0.54
4:D:900:LEU:HB3	4:D:957:THR:O	2.07	0.54
4:D:373:MET:SD	6:F:256:LEU:HB3	2.47	0.54
1:J:68:ASP:O	1:J:70:PRO:CD	2.45	0.54
4:D:641:ARG:CZ	4:D:642:PRO:HD3	2.38	0.54
6:F:293:ILE:O	6:F:297:MET:HG3	2.08	0.54
2:B:86:SER:HB2	2:B:119:HIS:CE1	2.43	0.54
3:C:618:GLY:O	3:C:964:ALA:HA	2.08	0.54
4:D:1177:LEU:CB	4:D:1178:PRO:CD	2.86	0.54
5:E:26:TYR:O	5:E:26:TYR:CD1	2.60	0.54
5:E:29:PRO:HB2	5:E:34:ASN:HB2	1.90	0.54
3:C:37:GLU:OE1	3:C:494:TYR:OH	2.14	0.53
3:C:832:HIS:ND1	10:C:1204:SO4:O2	2.39	0.53
4:D:113:ARG:N	4:D:113:ARG:HD3	2.22	0.53
2:B:68:GLY:C	2:B:129:ASN:HB2	2.34	0.53
3:C:167:VAL:O	3:C:427:LEU:HD12	2.09	0.53
3:C:1053:GLN:HB3	3:C:1054:PHE:CD2	2.42	0.53
4:D:6:PHE:HA	4:D:1257:LYS:HE3	1.89	0.53
4:D:104:ILE:HD12	4:D:379:ASP:HB3	1.90	0.53
4:D:480:ARG:HB3	4:D:482:GLN:OE1	2.08	0.53
4:D:978:TYR:CE1	4:D:994:VAL:HG11	2.44	0.53
4:D:1275:PRO:HG3	5:E:76:VAL:HG11	1.91	0.53
2:B:97:LEU:HB3	2:B:136:VAL:HG13	1.90	0.53
4:D:499:ASN:HB2	4:D:509:ILE:HG12	1.89	0.53
4:D:966:THR:HG22	4:D:1129:ARG:HD2	1.90	0.53
2:A:87:SER:OG	2:A:116:VAL:HG12	2.08	0.53
4:D:103:HIS:HB3	4:D:106:TYR:HD2	1.73	0.53
4:D:444:PRO:HG3	4:D:521:ALA:O	2.09	0.53
4:D:651:PHE:HB3	4:D:653:ASN:OD1	2.09	0.53
6:F:409:GLU:HG2	6:F:448:THR:HG22	1.91	0.53
3:C:654:ASP:OD2	3:C:686:ARG:NH2	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:832:HIS:H	3:C:1053:GLN:HG2	1.74	0.52
4:D:1265:ILE:HG22	4:D:1267:ARG:HG2	1.90	0.52
6:F:338:ALA:HB1	6:F:343:ILE:O	2.09	0.52
4:D:222:ILE:HD13	4:D:243:GLU:HG2	1.91	0.52
4:D:1161:GLN:HA	4:D:1164:ARG:HD3	1.91	0.52
6:F:210:LYS:NZ	10:F:502:SO4:O1	2.35	0.52
3:C:1081:THR:O	3:C:1086:ASP:HB2	2.09	0.52
2:A:99:LYS:HG2	2:A:105:VAL:HG22	1.92	0.52
2:A:199:LYS:O	2:A:200:ASN:HB2	2.08	0.52
3:C:41:VAL:HG22	3:C:494:TYR:CE1	2.44	0.52
3:C:642:GLU:OE2	3:C:658:ARG:NH2	2.39	0.52
3:C:718:GLU:H	4:D:724:THR:HG22	1.73	0.52
4:D:330:LEU:N	4:D:334:ARG:O	2.38	0.52
4:D:796:ASN:HD22	4:D:799:ILE:H	1.58	0.52
4:D:903:ARG:HG3	4:D:904:GLY:N	2.25	0.52
3:C:650:THR:HG22	3:C:660:SER:OG	2.10	0.52
3:C:800:LYS:CB	3:C:822:GLU:CB	2.76	0.52
4:D:295:ARG:O	4:D:298:VAL:HG22	2.10	0.52
6:F:242:VAL:O	6:F:246:LYS:HG3	2.10	0.52
6:F:295:ARG:NH2	7:O:24:DG:O6	2.42	0.52
3:C:393:GLU:HG3	6:F:247:ARG:HH21	1.74	0.52
6:F:330:ARG:NH2	6:F:336:GLU:OE2	2.42	0.52
2:A:30:PHE:HZ	2:B:41:THR:HA	1.74	0.52
4:D:262:LYS:HG3	4:D:310:MET:HE1	1.91	0.52
1:J:92:GLU:OE1	1:J:92:GLU:N	2.42	0.52
1:J:67:GLY:O	1:J:68:ASP:O	2.28	0.51
2:A:151:GLN:H	2:A:151:GLN:NE2	2.09	0.51
3:C:896:PRO:HB2	3:C:1001:LEU:HD13	1.90	0.51
4:D:320:ILE:HG21	4:D:340:LEU:HD23	1.91	0.51
4:D:1222:LEU:HD23	4:D:1244:ASP:OD2	2.11	0.51
2:A:36:ASN:HB2	2:A:176:TYR:OH	2.10	0.51
3:C:1015:THR:OG1	4:D:731:SER:OG	2.26	0.51
4:D:875:ARG:HH12	4:D:1033:GLN:NE2	2.08	0.51
4:D:1129:ARG:O	4:D:1133:ILE:HG12	2.10	0.51
2:B:5:GLN:N	2:B:5:GLN:OE1	2.43	0.51
3:C:145:MET:O	3:C:411:ILE:HD12	2.10	0.51
3:C:917:MET:O	3:C:919:ILE:N	2.44	0.51
4:D:31:PRO:HB3	4:D:348:ILE:HG23	1.92	0.51
4:D:130:TYR:HE1	4:D:376:GLU:HG2	1.75	0.51
2:B:41:THR:O	2:B:45:SER:HB3	2.11	0.51
3:C:51:SER:OG	3:C:373:GLY:N	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:432:ASP:HA	3:C:671:HIS:HE1	1.75	0.51
2:A:40:ARG:NH2	3:C:894:ASP:HB3	2.24	0.51
3:C:622:GLU:OE1	3:C:622:GLU:N	2.34	0.51
3:C:1112:PHE:CE1	4:D:1255:ILE:HG22	2.46	0.51
4:D:500:ARG:HB2	4:D:541:MET:HG2	1.92	0.51
2:A:14:VAL:HG13	2:A:15:ALA:H	1.76	0.51
3:C:727:ILE:HG13	3:C:907:ILE:HB	1.93	0.51
4:D:692:GLN:O	4:D:696:ILE:HG12	2.10	0.51
3:C:106:VAL:HG11	3:C:120:TYR:CZ	2.46	0.50
3:C:767:VAL:HG23	3:C:772:LEU:HD11	1.92	0.50
1:J:44:PHE:HB2	4:D:74:ILE:O	2.11	0.50
3:C:728:LEU:HD22	3:C:906:ILE:HG22	1.94	0.50
3:C:917:MET:O	3:C:918:ASN:C	2.54	0.50
3:C:1002:PHE:HA	3:C:1009:PRO:HA	1.93	0.50
4:D:611:VAL:HA	4:D:634:LYS:O	2.10	0.50
6:F:190:ARG:HH12	6:F:228:ARG:HH11	1.60	0.50
2:B:143:GLY:HA3	2:B:168:TYR:CD2	2.47	0.50
2:B:183:VAL:HA	2:B:187:THR:HG22	1.93	0.50
4:D:1167:THR:OG1	4:D:1207:VAL:HG21	2.12	0.50
4:D:275:GLU:HG3	4:D:276:SER:N	2.26	0.50
4:D:656:LYS:CB	4:D:659:ASP:HB2	2.42	0.50
1:J:25:ALA:N	1:J:26:PRO:CD	2.75	0.50
3:C:587:PHE:HZ	3:C:927:LEU:HD12	1.77	0.50
3:C:742:HIS:CD2	3:C:868:ARG:HG3	2.42	0.50
4:D:173:ARG:NH2	4:D:204:GLU:OE1	2.44	0.50
4:D:602:ALA:HB2	4:D:608:GLU:HG3	1.92	0.50
3:C:1033:HIS:HA	10:C:1204:SO4:O1	2.12	0.50
3:C:1043:ILE:HG13	4:D:326:PRO:HG3	1.93	0.50
7:O:16:DT:H6	7:O:16:DT:H5'	1.77	0.50
3:C:765:PRO:HG3	3:C:825:ASP:HB2	1.94	0.49
4:D:504:LEU:HD23	4:D:1004:GLU:HG2	1.94	0.49
1:J:25:ALA:O	1:J:27:ARG:N	2.46	0.49
1:J:28:GLN:NE2	1:J:46:ASP:O	2.45	0.49
2:B:188:ASP:OD1	2:B:188:ASP:N	2.45	0.49
4:D:1168:ILE:O	4:D:1179:GLY:HA2	2.12	0.49
4:D:1252:ASN:HB3	4:D:1257:LYS:HB3	1.94	0.49
1:J:69:VAL:O	1:J:71:GLU:N	2.45	0.49
4:D:550:GLU:O	4:D:554:GLU:HG3	2.11	0.49
3:C:772:LEU:HD12	3:C:772:LEU:H	1.77	0.49
4:D:568:PRO:HB3	4:D:983:ALA:HB2	1.94	0.49
4:D:894:ARG:NH1	4:D:960:LYS:NZ	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:420:GLU:O	3:C:424:THR:OG1	2.21	0.49
4:D:222:ILE:CD1	4:D:243:GLU:HG2	2.43	0.49
3:C:406:GLN:NE2	6:F:326:GLN:HG2	2.28	0.49
4:D:665:THR:HG22	4:D:684:ASN:ND2	2.27	0.49
7:O:13:DT:H2''	7:O:14:DG:C8	2.47	0.49
2:A:144:ARG:HA	2:A:168:TYR:HB2	1.94	0.49
3:C:589:GLU:OE1	3:C:589:GLU:N	2.29	0.49
3:C:796:LYS:HB3	3:C:826:THR:O	2.13	0.49
4:D:21:ARG:NE	4:D:96:GLU:OE2	2.37	0.49
4:D:134:TYR:OH	4:D:242:ARG:NH2	2.46	0.49
4:D:339:ASP:CG	4:D:397:ARG:HH22	2.21	0.49
4:D:903:ARG:HG3	4:D:904:GLY:H	1.78	0.49
5:E:37:ILE:HD12	5:E:38:ASP:N	2.28	0.49
6:F:187:LEU:O	6:F:191:ILE:HG13	2.13	0.49
4:D:1265:ILE:CG2	4:D:1267:ARG:HG2	2.43	0.48
5:E:55:ALA:O	5:E:59:ARG:HG2	2.13	0.48
6:F:190:ARG:HH12	6:F:228:ARG:HE	1.61	0.48
6:F:426:THR:HG23	6:F:429:GLU:H	1.78	0.48
3:C:29:ARG:HG2	3:C:964:ALA:HB2	1.95	0.48
3:C:167:VAL:HG13	3:C:445:ARG:O	2.13	0.48
3:C:169:GLN:O	3:C:370:ARG:N	2.45	0.48
4:D:1266:SER:H	13:D:2008:GLU:HA	1.78	0.48
4:D:1276:THR:HG23	5:E:101:LEU:HA	1.96	0.48
2:A:68:GLY:O	2:A:129:ASN:ND2	2.46	0.48
4:D:577:PRO:HB3	4:D:581:MET:HE2	1.95	0.48
4:D:614:SER:HB2	4:D:615:PRO:HD2	1.94	0.48
4:D:1266:SER:H	13:D:2008:GLU:CA	2.25	0.48
2:B:107:ALA:HB2	2:B:125:ILE:HD11	1.95	0.48
4:D:651:PHE:C	4:D:653:ASN:H	2.22	0.48
4:D:991:GLY:HA2	4:D:1265:ILE:CD1	2.43	0.48
2:B:24:GLU:HA	2:B:25:PRO:HA	1.70	0.48
4:D:930:ASP:OD1	4:D:931:ALA:N	2.47	0.48
4:D:1278:GLU:OE2	4:D:1278:GLU:N	2.46	0.48
2:B:84:VAL:HG22	2:B:119:HIS:CD2	2.48	0.48
4:D:917:THR:CG2	4:D:1144:ARG:HH21	2.26	0.48
4:D:1220:SER:OG	4:D:1223:SER:HB3	2.13	0.48
6:F:228:ARG:HD3	14:F:504:EDO:H22	1.95	0.48
4:D:612:TYR:HE1	4:D:633:ILE:HG21	1.79	0.48
4:D:894:ARG:HG3	10:D:2007:SO4:O4	2.14	0.48
4:D:1127:GLY:O	4:D:1131:VAL:HG23	2.13	0.48
2:B:74:THR:HG21	4:D:611:VAL:HG11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:73:ILE:O	4:D:82:VAL:HG12	2.13	0.48
4:D:1034:GLU:OE2	4:D:1041:PRO:HA	2.14	0.48
3:C:400:VAL:HG23	3:C:401:GLU:HG2	1.95	0.48
3:C:998:LYS:HB3	3:C:1013:PRO:HB2	1.95	0.48
2:A:158:GLU:O	2:A:160:GLY:N	2.47	0.47
4:D:415:GLN:H	4:D:415:GLN:NE2	2.12	0.47
4:D:566:LEU:HA	4:D:573:PRO:HA	1.96	0.47
4:D:886:ARG:HH12	13:D:2008:GLU:CD	2.21	0.47
4:D:886:ARG:HH22	13:D:2008:GLU:HG2	1.78	0.47
3:C:167:VAL:HG12	3:C:168:SER:N	2.29	0.47
4:D:151:LEU:HD13	4:D:226:PHE:HE2	1.79	0.47
4:D:734:ASP:O	4:D:798:ILE:HD12	2.14	0.47
4:D:1144:ARG:NH1	4:D:1150:ILE:H	2.11	0.47
3:C:590:HIS:HB3	3:C:919:ILE:CG2	2.42	0.47
3:C:812:LEU:HD11	6:F:398:LEU:HD21	1.95	0.47
4:D:577:PRO:HB3	4:D:581:MET:HB2	1.96	0.47
3:C:584:MET:HA	3:C:619:THR:CG2	2.43	0.47
3:C:584:MET:HE3	3:C:622:GLU:HG3	1.97	0.47
3:C:642:GLU:CD	3:C:658:ARG:HH21	2.22	0.47
4:D:237:ASP:O	4:D:238:GLU:HB3	2.13	0.47
4:D:336:ALA:HA	6:F:359:ILE:O	2.14	0.47
2:A:40:ARG:HH11	2:B:33:THR:HG22	1.79	0.47
3:C:83:GLU:OE2	3:C:381:ARG:NH2	2.43	0.47
3:C:891:PRO:HG2	3:C:894:ASP:OD1	2.15	0.47
2:A:14:VAL:HG13	2:A:18:ARG:HG3	1.96	0.47
3:C:808:GLU:OE1	3:C:808:GLU:N	2.46	0.47
2:A:59:VAL:HG11	2:A:73:VAL:HG21	1.97	0.47
3:C:710:LEU:HD13	3:C:1021:ILE:HG12	1.96	0.47
3:C:711:LEU:HD23	3:C:904:VAL:HA	1.97	0.47
4:D:432:VAL:HG13	4:D:434:PRO:HD3	1.97	0.47
4:D:607:PRO:O	4:D:609:GLN:NE2	2.47	0.47
4:D:894:ARG:HD2	4:D:960:LYS:HZ3	1.79	0.47
4:D:1029:LEU:N	4:D:1030:PRO:HD2	2.30	0.47
4:D:1043:ASN:OD1	4:D:1043:ASN:N	2.47	0.47
6:F:444:ILE:O	6:F:448:THR:HG23	2.15	0.47
2:B:54:ILE:CG2	2:B:138:LEU:HB3	2.41	0.47
4:D:1050:VAL:HG22	4:D:1051:ALA:H	1.80	0.47
2:A:12:GLU:O	2:A:19:SER:HB2	2.15	0.47
3:C:84:LEU:HD13	3:C:84:LEU:O	2.14	0.47
4:D:17:ALA:O	4:D:21:ARG:HG3	2.15	0.47
4:D:468:ASN:H	4:D:468:ASN:HD22	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1004:GLU:N	4:D:1005:PRO:HD2	2.30	0.47
4:D:1086:ARG:HB2	4:D:1086:ARG:CZ	2.45	0.47
3:C:722:TYR:HB3	4:D:432:VAL:HG21	1.97	0.47
4:D:143:MET:HG2	4:D:251:TYR:CE2	2.49	0.47
4:D:240:LEU:O	4:D:244:LEU:HB2	2.14	0.47
4:D:624:ARG:HG2	4:D:625:GLY:H	1.80	0.47
4:D:900:LEU:HD23	4:D:959:VAL:HG23	1.97	0.47
4:D:936:ILE:O	4:D:937:ILE:C	2.57	0.47
4:D:937:ILE:HD12	4:D:937:ILE:H	1.80	0.47
4:D:1275:PRO:HB3	5:E:79:LEU:HD11	1.95	0.47
7:O:15:DT:H2''	7:O:16:DT:OP2	2.15	0.47
3:C:895:MET:HE2	3:C:895:MET:HB2	1.76	0.46
3:C:945:ASP:OD1	3:C:945:ASP:N	2.48	0.46
4:D:170:LEU:CD1	4:D:209:ARG:HD3	2.45	0.46
2:B:86:SER:HB2	2:B:119:HIS:NE2	2.30	0.46
3:C:51:SER:HB2	3:C:371:THR:OG1	2.16	0.46
4:D:641:ARG:HA	4:D:641:ARG:CZ	2.45	0.46
2:A:146:TYR:CG	3:C:734:GLU:HG2	2.51	0.46
3:C:851:GLU:C	3:C:852:LEU:HD13	2.41	0.46
4:D:98:ALA:HB3	4:D:354:LEU:HD23	1.98	0.46
4:D:102:THR:OG1	4:D:375:GLN:NE2	2.48	0.46
4:D:675:LEU:HG	4:D:714:LYS:HB3	1.97	0.46
6:F:307:PRO:O	6:F:311:VAL:HG23	2.16	0.46
2:A:66:VAL:O	2:A:69:VAL:HG22	2.16	0.46
3:C:573:SER:HB2	3:C:574:PRO:HD2	1.97	0.46
3:C:936:ASN:HD22	3:C:938:ASP:H	1.64	0.46
3:C:1005:ARG:NH2	10:C:1202:SO4:O2	2.46	0.46
3:C:950:LEU:HG	3:C:951:PRO:HD2	1.97	0.46
3:C:852:LEU:HB2	3:C:853:PRO:HD2	1.96	0.46
4:D:268:PHE:CE1	4:D:273:GLU:HG3	2.50	0.46
4:D:669:ARG:O	4:D:673:ASN:ND2	2.35	0.46
2:B:63:PHE:CD1	4:D:604:LYS:HA	2.51	0.46
3:C:670:ASN:OD1	3:C:670:ASN:N	2.48	0.46
3:C:1082:ILE:HD12	3:C:1093:VAL:HG21	1.97	0.46
8:P:11:DA:H2''	8:P:12:DA:H5''	1.98	0.46
2:A:177:LYS:HG3	2:A:193:ILE:CD1	2.46	0.46
3:C:777:GLU:H	3:C:777:GLU:HG3	1.43	0.46
4:D:238:GLU:O	4:D:238:GLU:HG2	2.16	0.46
4:D:877:VAL:O	4:D:881:GLN:HB3	2.16	0.46
4:D:961:VAL:HG12	4:D:962:ARG:O	2.15	0.46
2:A:30:PHE:CZ	2:B:41:THR:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:773:ALA:O	3:C:782:ARG:NH2	2.49	0.46
3:C:1122:LEU:HD13	3:C:1122:LEU:HA	1.85	0.46
4:D:447:MET:O	4:D:451:LEU:HB2	2.16	0.46
6:F:452:LEU:O	6:F:458:SER:HB3	2.16	0.46
3:C:622:GLU:HB3	3:C:703:GLU:HB2	1.97	0.45
3:C:1103:ILE:CD1	4:D:547:LEU:HB3	2.46	0.45
2:B:107:ALA:HB2	2:B:125:ILE:CD1	2.46	0.45
3:C:748:ILE:HB	3:C:828:LEU:HD22	1.97	0.45
4:D:113:ARG:NH2	4:D:1236:ASP:OD1	2.49	0.45
5:E:35:PRO:HG2	5:E:40:LEU:HD11	1.97	0.45
6:F:233:LEU:HD23	6:F:270:VAL:HG13	1.97	0.45
3:C:627:ILE:HG13	3:C:628:ASP:OD1	2.16	0.45
3:C:932:LYS:HG2	3:C:1018:TYR:CE2	2.51	0.45
4:D:1086:ARG:HB2	4:D:1086:ARG:NH1	2.32	0.45
5:E:30:LEU:O	5:E:33:THR:HG22	2.17	0.45
2:A:175:THR:OG1	3:C:899:PRO:O	2.22	0.45
3:C:1126:VAL:HG12	4:D:12:ILE:HG22	1.98	0.45
4:D:612:TYR:HB2	4:D:635:VAL:HG12	1.96	0.45
3:C:29:ARG:HH21	3:C:703:GLU:CD	2.24	0.45
3:C:715:MET:HG2	3:C:1014:VAL:HG11	1.99	0.45
3:C:848:ASP:OD1	3:C:848:ASP:N	2.49	0.45
3:C:1039:PRO:HG2	3:C:1048:LEU:HD21	1.98	0.45
2:A:89:ASP:C	2:A:91:GLU:N	2.69	0.45
3:C:488:ILE:HD13	9:C:1201:KNG:C02	2.47	0.45
3:C:1041:SER:HB3	3:C:1044:THR:O	2.16	0.45
5:E:37:ILE:H	5:E:37:ILE:HG13	1.59	0.45
2:A:72:ASP:OD1	2:A:74:THR:HG22	2.17	0.45
3:C:410:ASN:O	3:C:413:PRO:HD2	2.17	0.45
3:C:578:VAL:HG13	3:C:582:THR:HB	1.98	0.45
3:C:783:ILE:HG22	3:C:841:ILE:HD13	1.99	0.45
3:C:1058:ARG:NH1	4:D:418:LEU:HA	2.31	0.45
4:D:1162:MET:HE2	4:D:1211:ILE:HG23	1.99	0.45
4:D:981:SER:HB3	4:D:984:THR:OG1	2.17	0.45
1:J:44:PHE:CD1	1:J:44:PHE:N	2.85	0.44
7:O:29:DA:H1'	7:O:30:DC:H5'	1.98	0.44
9:C:1201:KNG:O19	9:C:1201:KNG:O09	2.35	0.44
4:D:886:ARG:NH2	13:D:2008:GLU:HB3	2.32	0.44
3:C:106:VAL:HG11	3:C:120:TYR:CE1	2.52	0.44
3:C:444:ARG:HH12	3:C:580:VAL:HG23	1.83	0.44
4:D:82:VAL:O	4:D:82:VAL:HG13	2.17	0.44
4:D:943:LEU:HD23	4:D:943:LEU:HA	1.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:ILE:HG23	2:B:136:VAL:HB	1.98	0.44
3:C:167:VAL:HB	3:C:427:LEU:HD13	1.99	0.44
3:C:842:ARG:HH21	3:C:844:PHE:HE1	1.66	0.44
3:C:1034:ALA:HB2	4:D:447:MET:HG3	2.00	0.44
1:J:82:TRP:CE2	6:F:199:GLN:HG2	2.53	0.44
3:C:870:ILE:HD11	3:C:886:ILE:HD11	1.98	0.44
5:E:80:VAL:HG22	5:E:100:LEU:HD22	1.99	0.44
3:C:436:PRO:HD2	3:C:698:CYS:HB2	1.99	0.44
4:D:579:LEU:O	4:D:580:ASP:OD1	2.36	0.44
4:D:704:PRO:HG2	4:D:707:VAL:HG23	1.98	0.44
5:E:26:TYR:O	5:E:27:ASP:C	2.60	0.44
6:F:430:ILE:O	6:F:433:VAL:HG13	2.17	0.44
2:A:64:THR:OG1	2:A:65:THR:N	2.50	0.44
3:C:583:ALA:O	3:C:619:THR:HG21	2.17	0.44
3:C:749:ASP:OD1	3:C:749:ASP:N	2.49	0.44
3:C:714:ILE:HG22	3:C:910:THR:HG22	1.99	0.44
4:D:673:ASN:HA	4:D:676:LEU:HD13	1.99	0.44
2:B:32:TYR:CD1	3:C:1005:ARG:HB3	2.53	0.43
3:C:712:VAL:HG12	3:C:1017:GLY:O	2.18	0.43
3:C:1029:ASP:N	3:C:1029:ASP:OD1	2.48	0.43
4:D:31:PRO:HB2	4:D:345:ARG:HG2	1.99	0.43
4:D:71:LYS:HA	4:D:82:VAL:HG13	1.99	0.43
3:C:432:ASP:HA	3:C:671:HIS:CE1	2.52	0.43
4:D:1144:ARG:HH22	4:D:1150:ILE:N	2.15	0.43
4:D:1249:LEU:HB3	4:D:1260:PRO:HD2	2.00	0.43
5:E:57:ARG:O	5:E:57:ARG:HD3	2.18	0.43
5:E:87:LYS:H	5:E:87:LYS:HG2	1.58	0.43
2:A:197:GLU:OE1	3:C:987:ARG:NH1	2.37	0.43
2:B:28:PRO:HA	2:B:29:GLY:HA2	1.46	0.43
2:B:45:SER:OG	2:B:214:THR:HG21	2.17	0.43
2:B:56:ILE:HG22	2:B:57:ASP:H	1.82	0.43
3:C:796:LYS:HG2	3:C:826:THR:HG23	1.99	0.43
3:C:936:ASN:N	3:C:982:SER:OG	2.39	0.43
4:D:200:SER:O	4:D:204:GLU:HG3	2.18	0.43
4:D:1153:LYS:O	4:D:1157:VAL:HG23	2.18	0.43
3:C:721:ASN:ND2	3:C:721:ASN:H	2.17	0.43
3:C:821:ARG:NE	3:C:822:GLU:OE1	2.51	0.43
4:D:1144:ARG:HH12	4:D:1150:ILE:N	2.12	0.43
1:J:82:TRP:CZ2	6:F:199:GLN:HG2	2.53	0.43
2:A:157:ALA:O	2:A:158:GLU:O	2.37	0.43
3:C:1008:GLU:H	3:C:1008:GLU:HG2	1.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:MET:HB2	2:B:138:LEU:CD1	2.48	0.43
3:C:895:MET:O	3:C:897:PHE:HD1	2.02	0.43
4:D:24:SER:HB2	4:D:94:HIS:HB3	2.01	0.43
4:D:113:ARG:HH12	4:D:1236:ASP:CG	2.27	0.43
4:D:922:ARG:HD2	4:D:961:VAL:HG11	2.00	0.43
1:J:59:GLY:O	4:D:29:LYS:NZ	2.35	0.43
2:A:177:LYS:O	2:A:193:ILE:HD12	2.19	0.43
2:B:119:HIS:C	2:B:121:PRO:HD3	2.43	0.43
3:C:821:ARG:O	3:C:822:GLU:C	2.62	0.43
4:D:587:TYR:O	4:D:590:THR:HG22	2.19	0.43
4:D:633:ILE:HD13	4:D:635:VAL:HG13	2.01	0.43
6:F:200:LYS:O	6:F:204:LEU:HG	2.18	0.43
3:C:1061:GLU:HA	3:C:1064:CYS:HB2	1.99	0.43
4:D:1041:PRO:HB3	4:D:1116:ALA:HB3	2.01	0.43
4:D:1235:THR:O	4:D:1239:ILE:HG13	2.19	0.43
6:F:431:GLY:O	6:F:435:GLY:N	2.49	0.43
4:D:341:ASN:O	4:D:345:ARG:HB2	2.19	0.43
4:D:639:GLU:CG	4:D:678:LYS:HD3	2.47	0.43
2:B:41:THR:HG21	2:B:215:LEU:HG	2.01	0.43
4:D:171:GLU:O	4:D:175:GLN:HB2	2.19	0.43
4:D:1049:ASP:HB2	4:D:1078:TYR:OH	2.19	0.43
1:J:81:HIS:CE1	6:F:195:LEU:HD11	2.53	0.42
3:C:776:ASP:HB3	3:C:782:ARG:HG2	2.00	0.42
3:C:777:GLU:OE1	3:C:778:ARG:HD3	2.19	0.42
4:D:1129:ARG:CZ	10:D:2007:SO4:O3	2.67	0.42
1:J:81:HIS:CG	6:F:195:LEU:HD11	2.55	0.42
3:C:641:ILE:HG22	3:C:683:ALA:HA	2.00	0.42
3:C:790:GLY:H	3:C:830:VAL:HG22	1.83	0.42
3:C:899:PRO:HB2	3:C:992:MET:HE1	2.01	0.42
3:C:933:ALA:O	3:C:984:LEU:HB2	2.18	0.42
3:C:1078:GLU:OE1	3:C:1082:ILE:HD11	2.19	0.42
4:D:240:LEU:HD23	4:D:240:LEU:C	2.44	0.42
4:D:445:LYS:HB2	4:D:484:TRP:CZ3	2.53	0.42
4:D:648:ALA:O	4:D:652:GLU:HB2	2.19	0.42
3:C:144:PHE:O	3:C:411:ILE:HG21	2.19	0.42
3:C:780:ILE:HD12	3:C:781:VAL:O	2.20	0.42
4:D:27:GLU:HB2	4:D:94:HIS:CE1	2.54	0.42
4:D:661:TRP:HZ3	4:D:663:ALA:HB2	1.80	0.42
4:D:734:ASP:OD2	4:D:797:PRO:HG2	2.19	0.42
4:D:1132:GLN:HG2	4:D:1159:VAL:HG12	1.99	0.42
4:D:1230:THR:HG22	4:D:1234:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:443:GLN:O	6:F:447:LYS:HG2	2.19	0.42
2:A:162:ILE:HG13	2:A:162:ILE:O	2.19	0.42
3:C:601:ASN:O	3:C:605:GLN:HG3	2.18	0.42
3:C:822:GLU:CB	3:C:823:VAL:HA	2.49	0.42
4:D:304:GLN:HG3	4:D:305:SER:N	2.35	0.42
4:D:386:ARG:NH1	4:D:1231:THR:HG21	2.33	0.42
4:D:1036:PHE:HB3	4:D:1211:ILE:HD13	2.00	0.42
2:A:205:ARG:H	2:A:205:ARG:HG3	1.43	0.42
3:C:597:LEU:HD23	3:C:597:LEU:C	2.45	0.42
3:C:611:ARG:HB3	3:C:708:LYS:NZ	2.33	0.42
4:D:1126:GLN:OE1	4:D:1130:GLU:HG2	2.19	0.42
3:C:876:LEU:HD23	3:C:1021:ILE:HD12	2.01	0.42
4:D:1152:ASP:O	4:D:1156:GLU:HG3	2.19	0.42
3:C:404:THR:OG1	3:C:405:PRO:HD2	2.19	0.42
4:D:26:GLY:HA3	4:D:51:ILE:HG22	2.00	0.42
4:D:177:LEU:C	4:D:177:LEU:HD13	2.45	0.42
3:C:811:LEU:O	3:C:815:ILE:HG12	2.19	0.42
3:C:899:PRO:HD2	3:C:992:MET:SD	2.59	0.42
3:C:1082:ILE:HG23	3:C:1106:PRO:HB3	2.01	0.42
4:D:475:MET:HE3	4:D:475:MET:HB2	1.93	0.42
4:D:581:MET:O	4:D:585:LEU:HG	2.20	0.42
4:D:622:MET:HG3	4:D:629:VAL:HG22	2.01	0.42
4:D:900:LEU:O	4:D:901:ALA:HB3	2.19	0.42
1:J:57:ARG:HA	4:D:26:GLY:HA2	2.02	0.42
2:B:52:THR:OG1	2:B:141:GLU:HG2	2.19	0.42
3:C:85:SER:HA	3:C:86:PRO:HA	1.74	0.42
3:C:1081:THR:O	3:C:1086:ASP:N	2.50	0.42
4:D:108:LYS:HG3	4:D:108:LYS:O	2.20	0.42
4:D:451:LEU:HD12	4:D:451:LEU:HA	1.92	0.42
4:D:1221:TRP:NE1	4:D:1244:ASP:HB2	2.34	0.42
6:F:325:LEU:C	6:F:325:LEU:HD23	2.44	0.42
3:C:156:THR:HG22	3:C:165:VAL:HG22	2.02	0.42
3:C:431:MET:HA	3:C:442:HIS:CE1	2.55	0.42
2:A:12:GLU:O	2:A:13:THR:HG23	2.20	0.41
2:A:45:SER:HB3	2:B:232:ILE:HD11	2.01	0.41
3:C:872:ASP:HA	3:C:886:ILE:HB	2.01	0.41
4:D:278:ARG:HA	4:D:278:ARG:HD2	1.76	0.41
4:D:734:ASP:N	4:D:734:ASP:OD1	2.52	0.41
4:D:937:ILE:HD13	4:D:951:LEU:HG	2.02	0.41
4:D:1046:PRO:HD2	4:D:1113:MET:HB2	2.01	0.41
6:F:272:LYS:HE3	7:O:25:DC:P	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:408:LEU:HD13	3:C:408:LEU:O	2.19	0.41
4:D:47:PHE:CD1	4:D:322:PRO:HB3	2.54	0.41
4:D:130:TYR:O	4:D:372:ARG:HD3	2.21	0.41
4:D:591:LEU:HD22	4:D:592:VAL:N	2.35	0.41
4:D:695:ILE:O	4:D:699:LEU:HG	2.19	0.41
5:E:66:ASN:O	5:E:67:GLN:HB2	2.19	0.41
1:J:88:ARG:HG3	1:J:89:ARG:N	2.36	0.41
2:A:107:ALA:HB3	2:A:120:ASN:O	2.21	0.41
4:D:796:ASN:HB3	4:D:799:ILE:HB	2.02	0.41
5:E:37:ILE:O	5:E:41:LEU:HG	2.21	0.41
2:B:31:GLY:HA3	2:B:178:VAL:HG11	2.02	0.41
3:C:720:HIS:CE1	3:C:888:LYS:HD2	2.56	0.41
4:D:415:GLN:OE1	4:D:417:LEU:HB2	2.21	0.41
1:J:102:LEU:O	1:J:105:ILE:HG23	2.20	0.41
3:C:433:GLN:HE21	3:C:670:ASN:CG	2.23	0.41
3:C:613:GLU:O	3:C:705:ALA:HB1	2.21	0.41
4:D:385:GLY:HA3	4:D:390:PRO:HG3	2.02	0.41
4:D:1144:ARG:NH2	4:D:1150:ILE:H	2.19	0.41
4:D:1236:ASP:OD1	4:D:1236:ASP:N	2.54	0.41
6:F:183:GLU:O	6:F:187:LEU:HG	2.20	0.41
6:F:328:LEU:HD21	6:F:336:GLU:OE1	2.21	0.41
1:J:69:VAL:O	1:J:69:VAL:HG13	2.20	0.41
1:J:101:ARG:O	1:J:105:ILE:HG22	2.20	0.41
3:C:696:GLY:N	3:C:699:THR:OG1	2.49	0.41
3:C:850:ASP:O	3:C:852:LEU:HD13	2.21	0.41
3:C:917:MET:HE3	3:C:917:MET:HB3	1.56	0.41
3:C:931:ALA:HB1	3:C:961:SER:O	2.20	0.41
3:C:1074:TYR:CZ	4:D:1258:LEU:HD21	2.56	0.41
4:D:111:PRO:HD2	4:D:1232:ARG:NH1	2.35	0.41
6:F:241:VAL:HG22	6:F:289:ILE:HD13	2.03	0.41
2:A:24:GLU:HA	2:A:25:PRO:HA	1.90	0.41
3:C:51:SER:OG	3:C:371:THR:HG23	2.20	0.41
3:C:411:ILE:HD11	6:F:325:LEU:HD22	2.02	0.41
3:C:614:ALA:HA	3:C:705:ALA:HB2	2.03	0.41
3:C:758:GLU:HB2	3:C:797:VAL:O	2.20	0.41
4:D:591:LEU:HD13	4:D:591:LEU:C	2.45	0.41
4:D:686:GLN:O	4:D:686:GLN:HG3	2.21	0.41
4:D:1165:ARG:HA	4:D:1182:THR:O	2.19	0.41
6:F:373:LEU:HD23	6:F:373:LEU:O	2.21	0.41
3:C:412:ARG:N	3:C:413:PRO:HD2	2.35	0.41
3:C:714:ILE:O	3:C:910:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:798:THR:OG1	3:C:824:ARG:O	2.37	0.41
1:J:78:PRO:O	1:J:80:THR:HG23	2.21	0.41
2:B:97:LEU:HB2	2:B:110:ILE:HG13	2.03	0.41
3:C:25:GLY:HA3	3:C:691:GLN:HG3	2.02	0.41
3:C:718:GLU:H	4:D:724:THR:HG21	1.86	0.41
3:C:1028:VAL:HG23	3:C:1029:ASP:OD1	2.21	0.41
4:D:23:TRP:HB3	4:D:92:MET:HE3	2.01	0.41
4:D:582:VAL:HG21	4:D:689:LYS:HD3	2.03	0.41
4:D:641:ARG:HE	4:D:642:PRO:HD3	1.81	0.41
4:D:679:SER:HB3	4:D:703:PHE:HZ	1.86	0.41
4:D:978:TYR:CE1	4:D:1153:LYS:HD3	2.56	0.41
4:D:1100:LEU:C	4:D:1100:LEU:HD23	2.46	0.41
4:D:1266:SER:HB3	13:D:2008:GLU:CB	2.51	0.41
5:E:65:TYR:HE1	5:E:78:PRO:HD3	1.84	0.41
2:A:70:LYS:HB3	2:A:71:GLU:OE1	2.20	0.41
2:A:147:VAL:HG12	2:A:168:TYR:HE1	1.86	0.41
3:C:165:VAL:HG11	3:C:443:LYS:HG2	2.03	0.41
3:C:599:GLY:O	3:C:603:GLN:HG3	2.20	0.41
3:C:850:ASP:OD1	3:C:850:ASP:N	2.54	0.41
4:D:131:PHE:CZ	4:D:257:GLY:HA3	2.55	0.41
4:D:453:LYS:HB3	4:D:454:PRO:HD3	2.03	0.41
4:D:1036:PHE:HA	4:D:1162:MET:HE1	2.02	0.41
6:F:258:LEU:HD22	6:F:293:ILE:HG23	2.03	0.40
2:B:95:MET:HE2	2:B:140:VAL:HG21	2.03	0.40
3:C:781:VAL:N	3:C:793:LEU:O	2.54	0.40
3:C:928:GLY:HA3	3:C:1018:TYR:O	2.21	0.40
3:C:967:VAL:HG23	3:C:968:PHE:H	1.86	0.40
3:C:1133:GLY:O	3:C:1134:ALA:C	2.64	0.40
4:D:886:ARG:HH22	13:D:2008:GLU:CB	2.34	0.40
2:A:26:LEU:HD22	2:B:218:LEU:HD11	2.03	0.40
3:C:523:THR:HG23	3:C:525:ASP:H	1.87	0.40
3:C:573:SER:O	3:C:576:GLN:HG3	2.20	0.40
3:C:722:TYR:O	3:C:723:GLU:HB2	2.20	0.40
3:C:750:ALA:O	3:C:751:ARG:O	2.40	0.40
3:C:822:GLU:CB	3:C:823:VAL:HG13	2.47	0.40
4:D:415:GLN:H	4:D:415:GLN:CD	2.30	0.40
4:D:664:GLU:HG3	4:D:664:GLU:O	2.21	0.40
4:D:1151:HIS:CE1	4:D:1153:LYS:HE3	2.56	0.40
2:A:33:THR:HG21	2:B:40:ARG:HG2	2.03	0.40
2:A:130:ASP:OD1	2:A:130:ASP:N	2.54	0.40
3:C:44:LEU:H	3:C:44:LEU:HG	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1053:ARG:NH2	4:D:1105:HIS:HB2	2.36	0.40
6:F:247:ARG:HA	6:F:247:ARG:NH1	2.36	0.40
6:F:397:GLN:O	6:F:401:VAL:HG23	2.21	0.40
2:A:70:LYS:NZ	3:C:682:ASP:OD1	2.49	0.40
2:A:75:ASP:OD2	3:C:678:ARG:NH1	2.53	0.40
3:C:744:GLU:HG3	3:C:746:HIS:HE1	1.86	0.40
3:C:1061:GLU:HG2	4:D:416:ASN:O	2.22	0.40
4:D:103:HIS:HB3	4:D:106:TYR:CD2	2.56	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	J	83/114 (73%)	74 (89%)	7 (8%)	2 (2%)	4	29
2	A	217/350 (62%)	207 (95%)	7 (3%)	3 (1%)	9	38
2	B	221/350 (63%)	211 (96%)	10 (4%)	0	100	100
3	C	844/1169 (72%)	804 (95%)	37 (4%)	3 (0%)	30	62
4	D	1160/1317 (88%)	1114 (96%)	43 (4%)	3 (0%)	36	67
5	E	80/107 (75%)	72 (90%)	8 (10%)	0	100	100
6	F	293/466 (63%)	293 (100%)	0	0	100	100
All	All	2898/3873 (75%)	2775 (96%)	112 (4%)	11 (0%)	30	62

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	68	ASP
2	A	90	ASP
3	C	751	ARG

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Mol	Chain	Res	Type
2	A	158	GLU
3	C	918	ASN
3	C	1134	ALA
4	D	283	SER
4	D	937	ILE
1	J	70	PRO
2	A	159	ILE
4	D	281	ILE

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	J	66/98 (67%)	59 (89%)	7 (11%)	6	27
2	A	177/297 (60%)	157 (89%)	20 (11%)	5	25
2	B	165/297 (56%)	138 (84%)	27 (16%)	2	14
3	C	623/984 (63%)	575 (92%)	48 (8%)	12	38
4	D	876/1095 (80%)	808 (92%)	68 (8%)	11	37
5	E	63/86 (73%)	56 (89%)	7 (11%)	6	26
6	F	248/379 (65%)	238 (96%)	10 (4%)	28	55
All	All	2218/3236 (68%)	2031 (92%)	187 (8%)	10	35

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	44	PHE
1	J	69	VAL
1	J	76	LYS
1	J	97	LEU
1	J	100	GLU
1	J	104	LEU
1	J	105	ILE
2	A	2	LEU
2	A	14	VAL

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Mol	Chain	Res	Type
2	A	22	VAL
2	A	34	LEU
2	A	40	ARG
2	A	54	ILE
2	A	74	THR
2	A	88	ASP
2	A	111	VAL
2	A	116	VAL
2	A	117	THR
2	A	129	ASN
2	A	135	GLU
2	A	140	VAL
2	A	150	VAL
2	A	151	GLN
2	A	158	GLU
2	A	193	ILE
2	A	205	ARG
2	A	215	LEU
2	B	6	ARG
2	B	34	LEU
2	B	38	LEU
2	B	42	LEU
2	B	43	LEU
2	B	56	ILE
2	B	59	VAL
2	B	60	LEU
2	B	71	GLU
2	B	85	VAL
2	B	86	SER
2	B	88	ASP
2	B	109	ASP
2	B	111	VAL
2	B	116	VAL
2	B	136	VAL
2	B	138	LEU
2	B	144	ARG
2	B	150	VAL
2	B	177	LYS
2	B	182	ARG
2	B	184	GLU
2	B	188	ASP
2	B	196	VAL

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Mol	Chain	Res	Type
2	B	202	ILE
2	B	218	LEU
2	B	228	ASP
3	C	44	LEU
3	C	124	LEU
3	C	125	PHE
3	C	153	GLU
3	C	168	SER
3	C	377	GLN
3	C	391	VAL
3	C	408	LEU
3	C	434	ASN
3	C	446	LEU
3	C	447	LEU
3	C	508	ARG
3	C	644	VAL
3	C	670	ASN
3	C	727	ILE
3	C	737	VAL
3	C	747	GLU
3	C	749	ASP
3	C	758	GLU
3	C	769	ASP
3	C	772	LEU
3	C	777	GLU
3	C	783	ILE
3	C	798	THR
3	C	819	LYS
3	C	824	ARG
3	C	826	THR
3	C	830	VAL
3	C	839	ILE
3	C	848	ASP
3	C	850	ASP
3	C	852	LEU
3	C	890	LEU
3	C	893	GLU
3	C	917	MET
3	C	919	ILE
3	C	927	LEU
3	C	936	ASN
3	C	937	ILE

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Mol	Chain	Res	Type
3	C	945	ASP
3	C	967	VAL
3	C	976	LEU
3	C	1029	ASP
3	C	1048	LEU
3	C	1122	LEU
3	C	1126	VAL
3	C	1128	VAL
3	C	1136	ILE
4	D	7	PHE
4	D	12	ILE
4	D	28	VAL
4	D	51	ILE
4	D	73	ILE
4	D	76	GLU
4	D	101	VAL
4	D	113	ARG
4	D	144	ARG
4	D	148	LEU
4	D	183	GLU
4	D	219	LEU
4	D	228	LYS
4	D	234	LEU
4	D	238	GLU
4	D	243	GLU
4	D	244	LEU
4	D	248	TYR
4	D	250	GLU
4	D	280	VAL
4	D	295	ARG
4	D	298	VAL
4	D	334	ARG
4	D	345	ARG
4	D	358	ILE
4	D	360	LEU
4	D	413	PHE
4	D	415	GLN
4	D	416	ASN
4	D	417	LEU
4	D	418	LEU
4	D	449	LEU
4	D	456	VAL

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Mol	Chain	Res	Type
4	D	468	ASN
4	D	474	ARG
4	D	504	LEU
4	D	515	GLN
4	D	518	GLU
4	D	574	LEU
4	D	581	MET
4	D	588	LEU
4	D	593	GLU
4	D	596	THR
4	D	609	GLN
4	D	627	LEU
4	D	640	LEU
4	D	641	ARG
4	D	644	THR
4	D	659	ASP
4	D	667	LEU
4	D	675	LEU
4	D	678	LYS
4	D	713	ASP
4	D	724	THR
4	D	746	GLU
4	D	886	ARG
4	D	917	THR
4	D	935	VAL
4	D	943	LEU
4	D	956	ILE
4	D	957	THR
4	D	1043	ASN
4	D	1077	VAL
4	D	1180	SER
4	D	1208	LEU
4	D	1219	ASP
4	D	1222	LEU
4	D	1249	LEU
5	E	27	ASP
5	E	37	ILE
5	E	50	LEU
5	E	85	GLN
5	E	87	LYS
5	E	101	LEU
5	E	102	GLU

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Mol	Chain	Res	Type
6	F	313	VAL
6	F	343	ILE
6	F	344	THR
6	F	348	VAL
6	F	420	THR
6	F	433	VAL
6	F	452	LEU
6	F	453	ARG
6	F	459	GLN
6	F	460	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	58	ASN
2	A	129	ASN
2	A	151	GLN
2	B	36	ASN
2	B	79	ASN
2	B	226	ASN
3	C	160	ASN
3	C	406	GLN
3	C	434	ASN
3	C	576	GLN
3	C	603	GLN
3	C	671	HIS
3	C	721	ASN
3	C	742	HIS
3	C	746	HIS
3	C	911	HIS
3	C	936	ASN
3	C	1025	HIS
3	C	1057	GLN
3	C	1068	GLN
4	D	165	GLN
4	D	207	GLN
4	D	213	GLN
4	D	303	GLN
4	D	304	GLN
4	D	329	GLN
4	D	368	ASN
4	D	410	GLN

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Mol	Chain	Res	Type
4	D	464	ASN
4	D	465	HIS
4	D	468	ASN
4	D	564	ASN
4	D	609	GLN
4	D	684	ASN
4	D	692	GLN
4	D	796	ASN
4	D	897	ASN
4	D	1033	GLN
4	D	1105	HIS
4	D	1140	GLN
4	D	1146	GLN
4	D	1161	GLN
5	E	34	ASN
5	E	66	ASN
5	E	85	GLN
5	E	103	HIS
6	F	215	GLN
6	F	353	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 16 ligands modelled in this entry, 3 are monoatomic - leaving 13 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	EDO	F	503	-	3,3,3	0.43	0	2,2,2	0.36	0
10	SO4	F	501	-	4,4,4	0.24	0	6,6,6	0.07	0
10	SO4	D	2006	-	4,4,4	0.23	0	6,6,6	0.12	0
10	SO4	D	2004	-	4,4,4	0.23	0	6,6,6	0.07	0
10	SO4	C	1204	-	4,4,4	0.24	0	6,6,6	0.07	0
10	SO4	F	502	-	4,4,4	0.24	0	6,6,6	0.10	0
10	SO4	C	1203	-	4,4,4	0.23	0	6,6,6	0.16	0
10	SO4	D	2005	-	4,4,4	0.23	0	6,6,6	0.05	0
9	KNG	C	1201	-	75,75,75	2.70	17 (22%)	107,114,114	1.71	16 (14%)
10	SO4	D	2007	-	4,4,4	0.22	0	6,6,6	1.06	0
10	SO4	C	1202	-	4,4,4	0.24	0	6,6,6	0.08	0
13	GLU	D	2008	-	7,8,9	1.03	0	4,9,11	1.25	0
14	EDO	F	504	-	3,3,3	0.43	0	2,2,2	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	EDO	F	503	-	-	1/1/1/1	-
9	KNG	C	1201	-	-	26/76/113/113	0/5/6/6
13	GLU	D	2008	-	-	2/6/7/9	-
14	EDO	F	504	-	-	0/1/1/1	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1201	KNG	O04-C11	12.36	1.40	1.21
9	C	1201	KNG	C17-C16	9.63	1.53	1.33
9	C	1201	KNG	O03-C06	9.50	1.55	1.37
9	C	1201	KNG	C15-N01	4.91	1.45	1.35
9	C	1201	KNG	O12-C31	-4.09	1.40	1.46
9	C	1201	KNG	C12-C11	-3.97	1.39	1.54
9	C	1201	KNG	C04-C10	-3.73	1.36	1.43
9	C	1201	KNG	O18-C50	3.67	1.47	1.41
9	C	1201	KNG	C06-C07	3.56	1.45	1.39
9	C	1201	KNG	O17-C50	3.30	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1201	KNG	O12-C39	3.30	1.40	1.34
9	C	1201	KNG	O07-C25	-2.98	1.40	1.44
9	C	1201	KNG	C05-C10	2.77	1.48	1.42
9	C	1201	KNG	O03-C12	-2.72	1.36	1.45
9	C	1201	KNG	C08-C09	2.48	1.50	1.43
9	C	1201	KNG	O10-C15	-2.45	1.18	1.23
9	C	1201	KNG	O07-C35	2.45	1.40	1.35

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1201	KNG	C18-C17-C16	-7.57	111.22	128.94
9	C	1201	KNG	O04-C11-C05	-5.06	122.30	131.63
9	C	1201	KNG	O07-C35-C36	4.75	119.57	111.09
9	C	1201	KNG	O03-C06-C07	4.58	128.92	121.16
9	C	1201	KNG	C12-C11-C05	4.19	115.41	107.30
9	C	1201	KNG	C50-O17-C47	-3.68	100.70	106.31
9	C	1201	KNG	O12-C39-C40	3.29	119.18	112.03
9	C	1201	KNG	C10-C05-C11	3.01	140.10	133.64
9	C	1201	KNG	C49-C48-C47	-2.98	108.95	113.39
9	C	1201	KNG	C06-C05-C11	-2.76	100.25	106.79
9	C	1201	KNG	C24-C23-C22	-2.62	111.04	115.41
9	C	1201	KNG	C26-C25-C24	-2.50	109.64	114.68
9	C	1201	KNG	O18-C50-O17	2.38	111.63	107.44
9	C	1201	KNG	C38-C31-C20	-2.32	109.25	113.39
9	C	1201	KNG	C30-C16-C15	2.28	120.80	115.22
9	C	1201	KNG	C25-O07-C35	-2.05	114.53	117.72

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	1201	KNG	C18-C19-C20-C21
9	C	1201	KNG	O06-C27-C28-C29
9	C	1201	KNG	C39-C40-C43-C44
9	C	1201	KNG	C41-C40-C43-C44
9	C	1201	KNG	C42-C40-C43-C44
9	C	1201	KNG	C40-C39-O12-C31
9	C	1201	KNG	O13-C39-O12-C31
9	C	1201	KNG	C22-C23-C24-C33
9	C	1201	KNG	O19-C23-C24-C25
9	C	1201	KNG	O19-C23-C24-C33

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Mol	Chain	Res	Type	Atoms
9	C	1201	KNG	C22-C23-C24-C25
9	C	1201	KNG	O12-C39-C40-C43
9	C	1201	KNG	O10-C15-C16-C30
9	C	1201	KNG	O12-C39-C40-C42
9	C	1201	KNG	C26-C27-C28-C29
9	C	1201	KNG	C31-C20-C21-O09
9	C	1201	KNG	C18-C19-C20-C31
9	C	1201	KNG	N01-C15-C16-C30
9	C	1201	KNG	O10-C15-C16-C17
13	D	2008	GLU	OE2-CD-CG-CB
13	D	2008	GLU	OE1-CD-CG-CB
9	C	1201	KNG	O13-C39-C40-C43
9	C	1201	KNG	C21-C22-C23-C24
9	C	1201	KNG	C19-C20-C31-O12
14	F	503	EDO	O1-C1-C2-O2
9	C	1201	KNG	C34-C26-C27-O06
9	C	1201	KNG	C25-C26-C27-O06
9	C	1201	KNG	C28-C27-O06-C37
9	C	1201	KNG	N01-C15-C16-C17

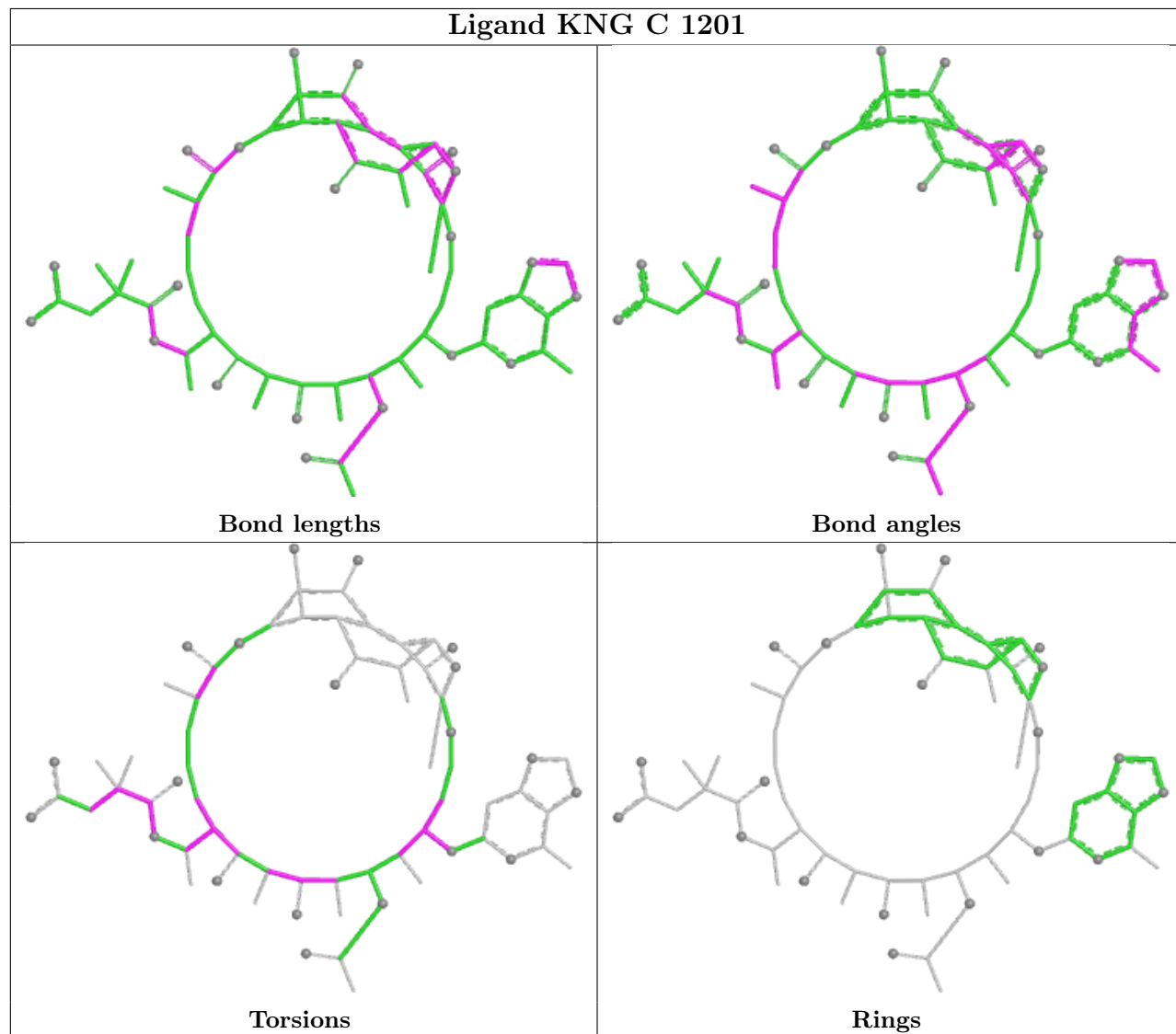
There are no ring outliers.

10 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	2006	SO4	2	0
10	C	1204	SO4	2	0
10	F	502	SO4	3	0
10	C	1203	SO4	1	0
10	D	2005	SO4	1	0
9	C	1201	KNG	2	0
10	D	2007	SO4	10	0
10	C	1202	SO4	1	0
13	D	2008	GLU	14	0
14	F	504	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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	J	85/114 (74%)	-0.07	0 100 100	76, 135, 173, 199	0
2	A	219/350 (62%)	0.15	3 (1%) 73 49	75, 115, 159, 186	0
2	B	225/350 (64%)	0.24	7 (3%) 51 31	88, 141, 164, 175	0
3	C	858/1169 (73%)	0.13	21 (2%) 59 37	49, 116, 175, 200	0
4	D	1176/1317 (89%)	-0.03	8 (0%) 84 64	50, 104, 180, 218	0
5	E	82/107 (76%)	-0.00	2 (2%) 59 37	73, 108, 188, 213	0
6	F	297/466 (63%)	-0.06	2 (0%) 84 64	52, 101, 138, 168	0
7	O	31/31 (100%)	-0.46	0 100 100	76, 108, 149, 160	0
8	P	26/26 (100%)	-0.48	0 100 100	97, 109, 155, 169	0
All	All	2999/3930 (76%)	0.04	43 (1%) 73 49	49, 112, 171, 218	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	478	GLU	4.8
6	F	385	ALA	4.6
3	C	379	GLN	3.3
3	C	98	PHE	3.1
2	A	188	ASP	3.0
2	B	21	PHE	3.0
3	C	756	GLY	2.9
2	A	220	GLY	2.9
4	D	1256	GLY	2.8
2	B	146	TYR	2.8
3	C	141	GLN	2.7
3	C	405	PRO	2.7
2	B	73	VAL	2.7
4	D	1230	THR	2.6
3	C	755	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
4	D	547	LEU	2.5
4	D	1191	ASN	2.5
3	C	93	SER	2.5
6	F	384	VAL	2.5
3	C	926	HIS	2.5
3	C	1019	MET	2.4
4	D	574	LEU	2.4
5	E	53	TYR	2.3
3	C	77	LEU	2.3
3	C	81	LEU	2.3
2	B	96	TYR	2.3
2	A	196	VAL	2.3
4	D	698	ASP	2.2
4	D	619	ILE	2.2
2	B	161	ARG	2.2
3	C	892	VAL	2.2
3	C	48	GLN	2.2
3	C	584	MET	2.2
3	C	428	SER	2.2
3	C	477	ILE	2.1
3	C	803	THR	2.1
4	D	107	PHE	2.1
3	C	648	TYR	2.1
3	C	45	LEU	2.0
2	B	206	ASP	2.0
2	B	59	VAL	2.0
3	C	1048	LEU	2.0
5	E	70	ASP	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.

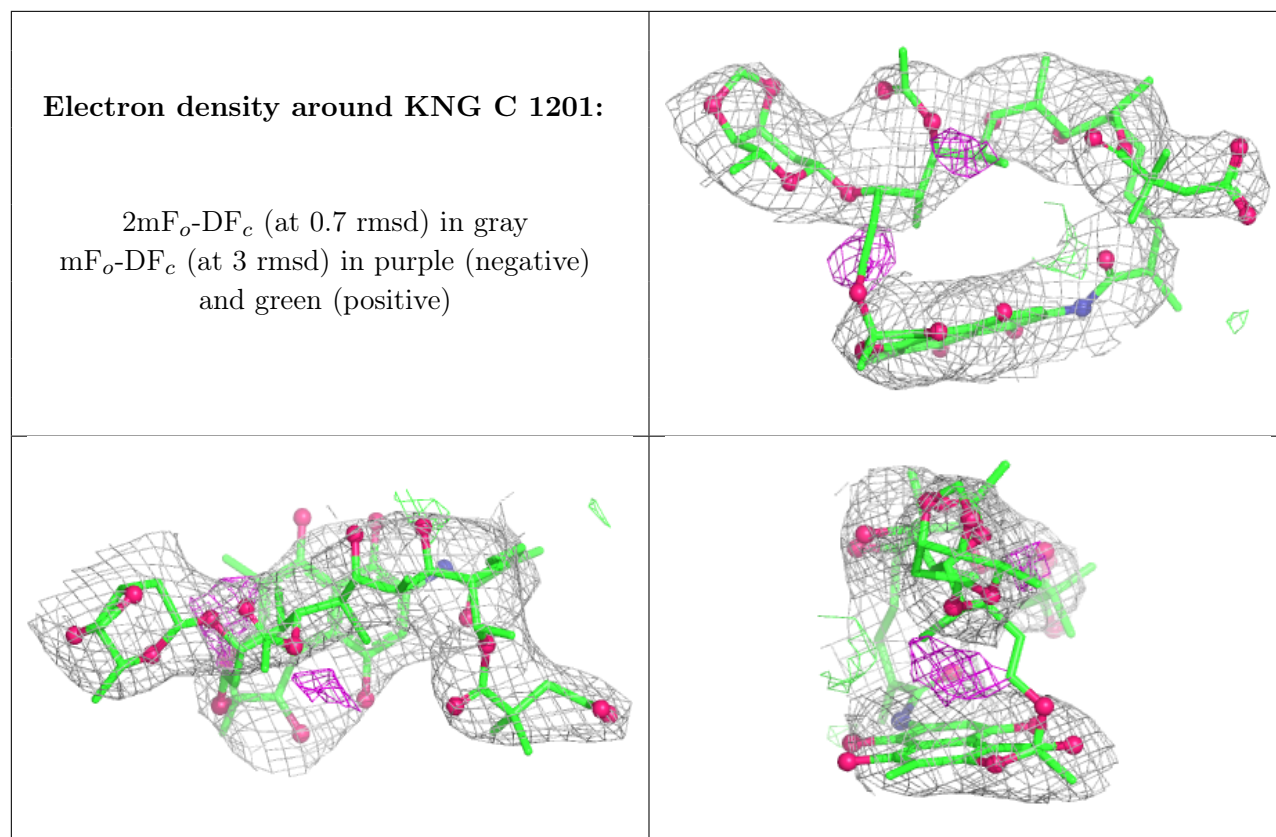
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
10	SO4	C	1203	5/5	0.52	0.11	176,177,184,205	0
10	SO4	F	501	5/5	0.66	0.13	120,120,137,146	0
10	SO4	D	2005	5/5	0.67	0.14	112,129,156,157	0
10	SO4	D	2007	5/5	0.68	0.07	180,186,220,337	0
14	EDO	F	504	4/4	0.69	0.09	84,105,126,126	0
13	GLU	D	2008	9/10	0.73	0.10	102,110,119,120	0
10	SO4	F	502	5/5	0.75	0.12	94,123,128,128	0
9	KNG	C	1201	70/70	0.82	0.11	99,127,142,159	0
12	MG	D	2003	1/1	0.82	0.07	151,151,151,151	0
10	SO4	C	1202	5/5	0.83	0.07	130,139,157,159	0
10	SO4	D	2004	5/5	0.85	0.11	117,122,130,130	0
10	SO4	C	1204	5/5	0.85	0.07	112,113,137,244	0
10	SO4	D	2006	5/5	0.86	0.17	120,134,161,165	0
14	EDO	F	503	4/4	0.94	0.19	83,100,114,121	0
11	ZN	D	2002	1/1	0.98	0.03	118,118,118,118	0
11	ZN	D	2001	1/1	0.99	0.03	89,89,89,89	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.