



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 12:57 am GMT

PDB ID : 4MQ9  
Title : Crystal structure of Thermus thermophilus RNA polymerase holoenzyme in complex with GE23077  
Authors : Ho, M.X.; Arnold, E.; Ebright, R.H.; Zhang, Y.; Tuske, S.  
Deposited on : 2013-09-16  
Resolution : 3.35 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](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

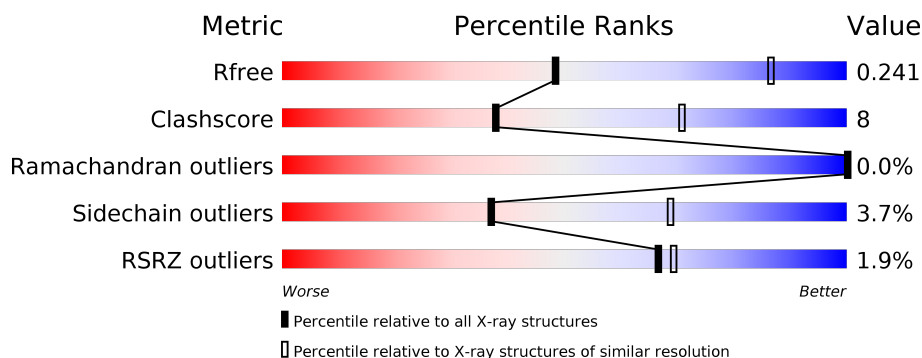
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.35 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))
$R_{free}$	111664	1314 (3.42-3.30)
Clashscore	122126	1380 (3.42-3.30)
Ramachandran outliers	120053	1359 (3.42-3.30)
Sidechain outliers	120020	1358 (3.42-3.30)
RSRZ outliers	108989	1272 (3.42-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	314	<div> <div style="width: 55%;"></div> <div style="width: 16%;"></div> <div style="width: 28%;"></div> </div>
1	B	314	<div> <div style="width: 53%;"></div> <div style="width: 18%;"></div> <div style="width: 29%;"></div> </div>
2	C	1119	<div> <div style="width: 75%;"></div> <div style="width: 23%;"></div> <div style="width: 2%;"></div> </div>
3	D	1524	<div> <div style="width: 68%;"></div> <div style="width: 20%;"></div> <div style="width: 10%;"></div> </div>
4	E	99	<div> <div style="width: 74%;"></div> <div style="width: 19%;"></div> <div style="width: 6%;"></div> </div>
5	F	443	<div> <div style="width: 62%;"></div> <div style="width: 13%;"></div> <div style="width: 23%;"></div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	I	7	<div><div></div><div>57%</div><div>43%</div></div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 26552 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
			1777	1135	309	331	2			
1	B	224	Total	C	N	O	S	0	0	0
			1750	1118	303	327	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1100	Total	C	N	O	S	0	0	0
			8677	5487	1552	1614	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1365	Total	C	N	O	S	0	0	0
			10781	6821	1912	2014	34			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	93	Total	C	N	O	S	0	0	0
			754	481	131	138	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	339	Total	C	N	O	S	0	0	0
			2754	1736	501	513	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	EXPRESSION TAG	UNP Q5SKW1
F	-18	GLY	-	EXPRESSION TAG	UNP Q5SKW1
F	-17	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	-16	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	-15	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-14	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-13	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-12	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-11	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-10	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-9	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	-8	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	-7	GLY	-	EXPRESSION TAG	UNP Q5SKW1
F	-6	LEU	-	EXPRESSION TAG	UNP Q5SKW1
F	-5	VAL	-	EXPRESSION TAG	UNP Q5SKW1
F	-4	PRO	-	EXPRESSION TAG	UNP Q5SKW1
F	-3	ARG	-	EXPRESSION TAG	UNP Q5SKW1
F	-2	GLY	-	EXPRESSION TAG	UNP Q5SKW1
F	-1	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	0	HIS	-	EXPRESSION TAG	UNP Q5SKW1

- Molecule 6 is a protein called GE23077.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	7	Total	C	N	O	0	0	0
			50	26	9	15			

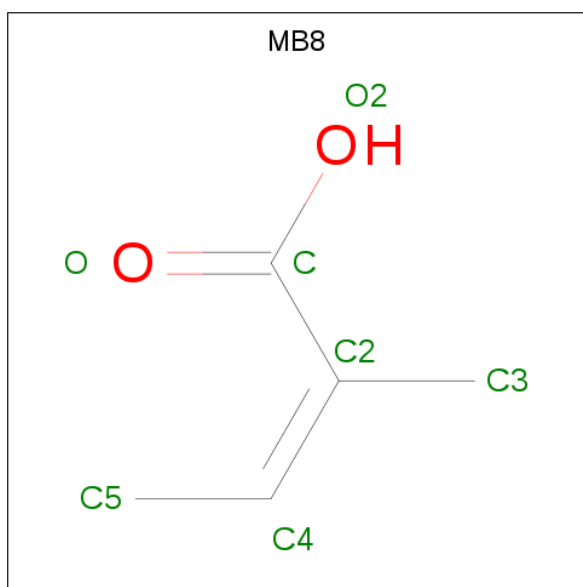
- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 9 is (2Z)-2-methylbut-2-enoic acid (three-letter code: MB8) (formula: C<sub>5</sub>H<sub>8</sub>O<sub>2</sub>).

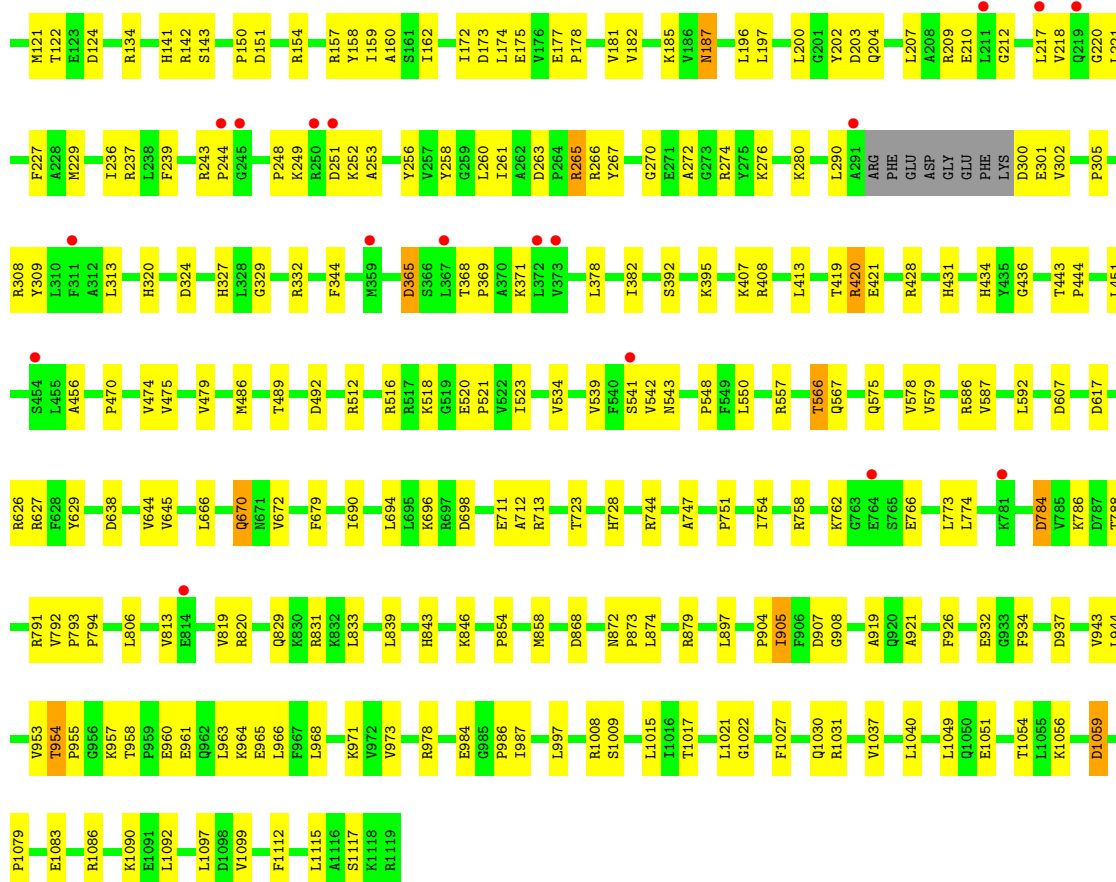


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	I	1	Total	C	O	0	0
			2	1	1		

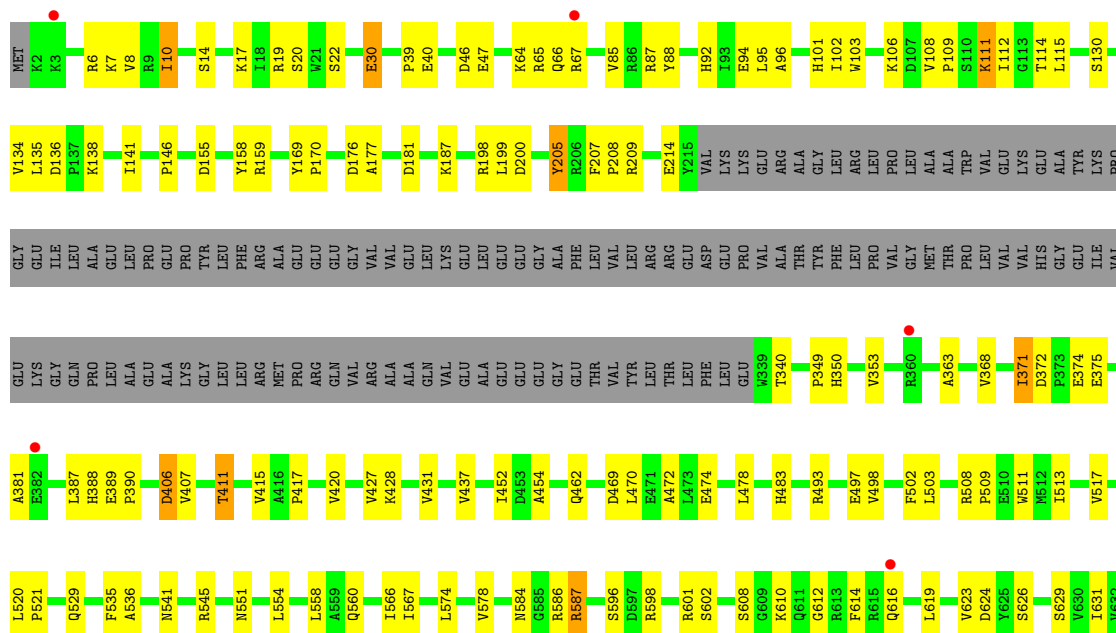
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	4	Total	O	0	0
			4	4		





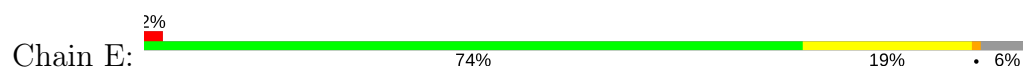
• Molecule 3: DNA-directed RNA polymerase subunit beta'



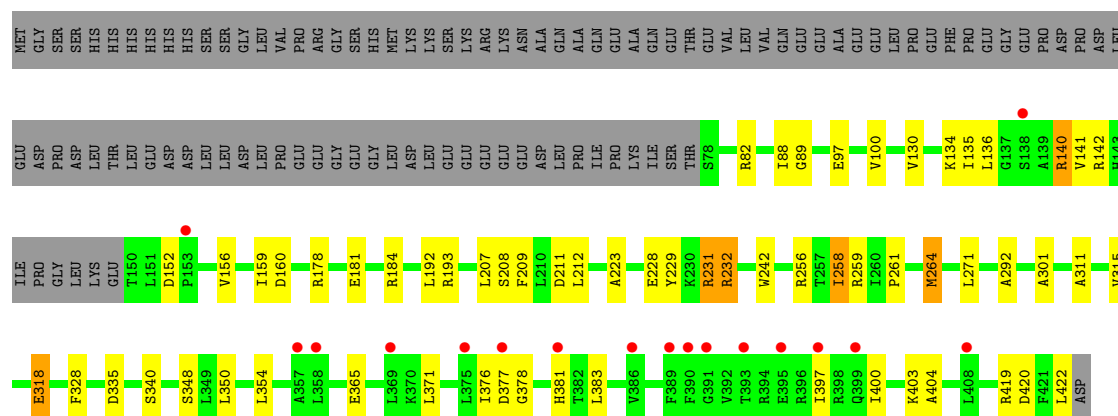




• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: RNA polymerase sigma factor



• Molecule 6: GE23077





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	236.57Å 236.57Å 252.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.97 – 3.35 38.97 – 3.35	Depositor EDS
% Data completeness (in resolution range)	98.9 (38.97-3.35) 98.9 (38.97-3.35)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 3.32Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, $R_{free}$	0.214 , 0.242 0.215 , 0.241	Depositor DCC
$R_{free}$ test set	2266 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	126.0	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 83.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.032 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	26552	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DSN, ZN, 2TL, DVA, MG, 2RA, FGL, MB8, 0QZ, R2T

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	0.24	0/1809	0.47	0/2461
1	B	0.23	0/1781	0.44	0/2426
2	C	0.25	0/8841	0.46	0/11956
3	D	0.25	0/10966	0.47	0/14820
4	E	0.23	0/768	0.41	0/1035
5	F	0.23	0/2797	0.41	0/3761
All	All	0.25	0/26962	0.46	0/36459

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
6	I	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	I	5	2TL	Peptide

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

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1777	0	1826	32	0
1	B	1750	0	1794	35	0
2	C	8677	0	8791	165	0
3	D	10781	0	10998	206	0
4	E	754	0	769	15	0
5	F	2754	0	2826	42	0
6	I	50	0	37	2	0
7	D	2	0	0	0	0
8	D	1	0	0	0	0
9	I	2	0	0	0	0
10	D	4	0	0	0	0
All	All	26552	0	27041	443	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 8.

All (443) 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:104:GLU:HB2	1:B:137:ARG:HA	1.60	0.82
2:C:102:HIS:HB3	2:C:105:THR:HB	1.65	0.77
3:D:508:ARG:HD3	3:D:509:PRO:HD2	1.66	0.77
2:C:904:PRO:HB2	2:C:907:ASP:HB3	1.69	0.73
3:D:95:LEU:HD11	3:D:517:VAL:HG23	1.70	0.73
3:D:693:GLU:HG2	4:E:48:MET:HE1	1.71	0.73
2:C:23:VAL:HA	2:C:121:MET:HE1	1.72	0.72
3:D:1087:ARG:NH1	3:D:1234:THR:O	2.22	0.72
2:C:1015:LEU:HA	5:F:335:ASP:HB2	1.72	0.71
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.73	0.71
3:D:1130:ARG:HH22	3:D:1313:VAL:HA	1.57	0.70
2:C:173:ASP:HB2	2:C:185:LYS:HB3	1.75	0.69
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.74	0.68
1:B:22:GLU:HG2	1:B:198:ARG:HG2	1.75	0.68
5:F:136:LEU:HB3	5:F:140:ARG:HD3	1.74	0.68
3:D:889:ALA:O	3:D:929:ARG:NH1	2.27	0.68
2:C:162:ILE:HB	2:C:172:ILE:HB	1.77	0.67
5:F:261:PRO:HG2	5:F:264:MET:HG3	1.76	0.67
3:D:711:LEU:HD22	3:D:778:LEU:HD23	1.76	0.67
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.77	0.66
5:F:397:ILE:HD12	5:F:400:ILE:HD11	1.76	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:19:ARG:NH1	3:D:94:GLU:OE2	2.28	0.66
1:A:215:VAL:HG13	1:B:222:LEU:HD22	1.78	0.66
5:F:135:ILE:HD11	5:F:178:ARG:HB3	1.78	0.65
2:C:428:ARG:HH21	2:C:451:LEU:HD11	1.61	0.65
3:D:1101:VAL:HG23	3:D:1102:THR:HG23	1.78	0.65
3:D:1219:GLU:HG2	3:D:1221:VAL:HG23	1.80	0.64
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.79	0.64
2:C:53:PRO:O	2:C:265:ARG:NH2	2.29	0.64
3:D:612:GLY:O	3:D:616:GLN:N	2.28	0.64
3:D:875:THR:HG21	3:D:902:LEU:HG	1.80	0.63
1:B:58:ILE:HB	1:B:61:VAL:HB	1.80	0.63
4:E:83:ASP:OD1	4:E:83:ASP:N	2.32	0.63
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.79	0.62
3:D:828:LYS:HG2	3:D:833:GLU:HG2	1.81	0.62
1:B:44:LEU:HA	1:B:48:ILE:HD13	1.80	0.62
2:C:1008:ARG:NH1	2:C:1027:PHE:O	2.31	0.62
2:C:22:GLN:HG3	2:C:407:LYS:HB3	1.82	0.62
2:C:711:GLU:O	2:C:758:ARG:NH1	2.31	0.62
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.82	0.62
3:D:349:PRO:HB3	5:F:97:GLU:HG2	1.81	0.61
3:D:1498:ALA:HB1	4:E:84:ARG:HH11	1.63	0.61
2:C:305:PRO:HA	2:C:308:ARG:HG2	1.82	0.61
2:C:280:LYS:HE3	2:C:309:TYR:HE2	1.66	0.61
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.81	0.61
2:C:143:SER:HB3	2:C:332:ARG:HB2	1.82	0.61
1:B:206:THR:HG22	1:B:209:GLU:H	1.66	0.61
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.83	0.60
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.36	0.60
3:D:844:ALA:HB1	3:D:867:ARG:HH21	1.65	0.60
2:C:21:ILE:HD12	2:C:21:ILE:H	1.67	0.60
2:C:1083:GLU:OE2	3:D:87:ARG:NH1	2.35	0.60
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.83	0.59
2:C:263:ASP:OD2	2:C:266:ARG:N	2.20	0.59
1:A:58:ILE:HG12	1:A:140:MET:HG2	1.85	0.58
3:D:7:LYS:HG2	3:D:1458:GLU:HG3	1.85	0.58
1:A:198:ARG:NH2	2:C:932:GLU:OE1	2.36	0.57
5:F:232:ARG:HB2	5:F:232:ARG:HH11	1.69	0.57
2:C:15:LEU:O	2:C:586:ARG:NH2	2.37	0.57
3:D:94:GLU:O	3:D:551:ASN:ND2	2.37	0.57
1:B:216:GLU:OE1	1:B:219:ARG:NH2	2.29	0.57
3:D:363:ALA:HA	3:D:381:ALA:HA	1.87	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:160:ASP:OD1	5:F:178:ARG:NH2	2.37	0.57
3:D:890:VAL:HG23	3:D:892:ASP:H	1.70	0.56
3:D:838:ARG:NH1	3:D:874:GLU:OE1	2.39	0.56
2:C:758:ARG:HH21	2:C:788:THR:HB	1.69	0.56
2:C:1115:LEU:HB3	3:D:85:VAL:HG12	1.88	0.56
2:C:151:ASP:HB2	2:C:159:ILE:HG13	1.88	0.55
3:D:102:ILE:HD11	3:D:587:ARG:HB3	1.87	0.55
3:D:411:THR:HB	3:D:437:VAL:H	1.71	0.55
1:A:83:LYS:NZ	2:C:698:ASP:OD2	2.40	0.55
2:C:958:THR:HG23	2:C:961:GLU:H	1.71	0.55
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.88	0.55
2:C:644:VAL:HG22	2:C:645:VAL:H	1.71	0.55
3:D:536:ALA:HA	5:F:315:VAL:O	2.06	0.55
2:C:512:ARG:HB3	2:C:523:ILE:HD11	1.89	0.55
3:D:1372:VAL:HG22	3:D:1375:MET:HE3	1.87	0.55
3:D:558:LEU:HD23	3:D:567:ILE:HD12	1.90	0.54
3:D:899:LEU:HD22	3:D:917:GLN:HB3	1.88	0.54
2:C:141:HIS:ND1	2:C:142:ARG:O	2.41	0.54
2:C:207:LEU:HD23	2:C:221:LEU:HD13	1.88	0.54
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.90	0.54
1:B:176:ARG:NH2	3:D:888:GLU:OE2	2.40	0.54
3:D:208:PRO:HA	3:D:389:GLU:O	2.08	0.54
2:C:203:ASP:OD2	2:C:204:GLN:N	2.41	0.54
3:D:770:LEU:HA	3:D:777:PRO:HA	1.90	0.54
3:D:808:THR:HB	3:D:811:GLU:HG3	1.89	0.53
1:A:128:HIS:CE1	1:A:131:THR:HG23	2.43	0.53
3:D:39:PRO:HG3	3:D:47:GLU:HG3	1.91	0.53
3:D:634:GLY:HA3	3:D:637:LEU:HD12	1.89	0.53
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.90	0.53
4:E:46:PRO:HG3	4:E:66:LYS:HD3	1.90	0.53
3:D:835:SER:HB3	3:D:838:ARG:HB2	1.90	0.53
2:C:32:ALA:HB2	2:C:73:LEU:HD12	1.91	0.53
2:C:987:ILE:HD11	3:D:946:GLY:HA2	1.90	0.53
2:C:270:GLY:O	2:C:274:ARG:N	2.38	0.53
2:C:124:ASP:HA	2:C:592:LEU:HD21	1.90	0.53
2:C:784:ASP:N	2:C:784:ASP:OD1	2.42	0.53
3:D:65:ARG:HG2	5:F:376:ILE:HD12	1.90	0.53
5:F:256:ARG:NH1	5:F:311:ALA:O	2.35	0.53
5:F:130:VAL:HG21	5:F:159:ILE:HG21	1.91	0.52
2:C:365:ASP:N	2:C:365:ASP:OD1	2.41	0.52
2:C:1030:GLN:HB2	3:D:626:SER:HB2	1.92	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:614:PHE:HB3	3:D:1439:SER:HA	1.90	0.52
3:D:709:HIS:HD2	3:D:711:LEU:H	1.56	0.52
5:F:181:GLU:OE2	5:F:184:ARG:NH1	2.35	0.52
2:C:202:TYR:OH	2:C:300:ASP:O	2.25	0.52
2:C:236:ILE:HG23	2:C:248:PRO:HB3	1.91	0.52
4:E:39:VAL:O	4:E:72:ARG:NH1	2.42	0.52
2:C:187:ASN:OD1	2:C:187:ASN:N	2.43	0.52
3:D:907:GLU:HB2	3:D:1026:SER:HA	1.92	0.52
2:C:239:PHE:CZ	2:C:256:TYR:HB3	2.45	0.52
2:C:751:PRO:HB3	2:C:794:PRO:HA	1.91	0.52
3:D:809:PRO:HB3	3:D:839:LEU:HD13	1.93	0.51
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.93	0.51
2:C:550:LEU:HB3	2:C:905:ILE:HG22	1.91	0.51
2:C:17:PRO:HB2	2:C:20:GLU:HB2	1.92	0.51
3:D:1310:ARG:HD2	3:D:1327:ARG:HD2	1.92	0.51
3:D:684:LYS:HB3	3:D:687:VAL:HG23	1.92	0.51
2:C:984:GLU:O	3:D:946:GLY:HA3	2.10	0.51
3:D:989:TYR:CZ	3:D:993:LEU:HD11	2.46	0.51
1:A:55:SER:HB3	1:A:143:ARG:HB3	1.92	0.51
1:A:89:PHE:HB2	1:A:146:ARG:HH21	1.74	0.51
2:C:474:VAL:HG12	2:C:479:VAL:HG13	1.93	0.51
4:E:52:GLU:OE1	4:E:52:GLU:N	2.44	0.51
2:C:1054:THR:HG21	2:C:1079:PRO:CB	2.41	0.50
2:C:105:THR:HG22	2:C:107:LEU:HD13	1.93	0.50
2:C:134:ARG:NH2	2:C:392:SER:O	2.44	0.50
3:D:469:ASP:HB3	3:D:472:ALA:HB3	1.91	0.50
3:D:709:HIS:CD2	3:D:711:LEU:HB2	2.45	0.50
3:D:834:THR:HG23	3:D:838:ARG:HD2	1.93	0.50
3:D:67:ARG:NH2	5:F:377:ASP:OD1	2.31	0.50
2:C:368:THR:H	2:C:371:LYS:HD2	1.77	0.50
2:C:41:ASN:HD21	2:C:49:ARG:HG2	1.77	0.50
5:F:136:LEU:HB3	5:F:140:ARG:CD	2.42	0.50
2:C:944:LEU:HD11	2:C:963:LEU:HG	1.92	0.50
3:D:808:THR:HG22	3:D:810:GLU:H	1.76	0.50
3:D:1084:THR:HG22	3:D:1087:ARG:NH2	2.27	0.50
2:C:197:LEU:HD13	2:C:207:LEU:HD21	1.93	0.50
2:C:261:ILE:HG23	2:C:290:LEU:HB2	1.93	0.50
1:B:74:ASP:OD1	1:B:74:ASP:N	2.40	0.50
2:C:408:ARG:NH2	2:C:456:ALA:O	2.45	0.50
3:D:1306:PRO:HG2	3:D:1309:ALA:HB2	1.94	0.50
3:D:879:ARG:HD3	3:D:902:LEU:O	2.12	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:872:ASN:OD1	2:C:873:PRO:HD2	2.11	0.50
2:C:897:LEU:HG	2:C:921:ALA:HB2	1.94	0.50
2:C:68:PHE:HA	2:C:98:LEU:HG	1.93	0.50
3:D:1479:ASP:OD2	3:D:1482:ARG:NH2	2.40	0.50
3:D:141:ILE:HA	3:D:146:PRO:HA	1.94	0.49
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.93	0.49
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.95	0.49
2:C:239:PHE:HZ	2:C:256:TYR:HB3	1.77	0.49
1:A:186:LEU:HD23	1:A:188:GLN:H	1.77	0.49
3:D:1312:LEU:HD13	3:D:1327:ARG:HG2	1.94	0.49
2:C:1086:ARG:NH1	3:D:88:TYR:OH	2.40	0.49
3:D:138:LYS:HB2	3:D:452:ILE:HA	1.94	0.49
3:D:30:GLU:OE2	5:F:259:ARG:NH1	2.44	0.49
1:A:150:TYR:CD1	2:C:696:LYS:HG2	2.48	0.49
2:C:212:GLY:HA2	2:C:218:VAL:HB	1.95	0.49
2:C:762:LYS:HD3	2:C:786:LYS:HD3	1.93	0.49
2:C:806:LEU:HB3	2:C:813:VAL:HG21	1.94	0.49
3:D:847:ASP:OD1	3:D:847:ASP:N	2.45	0.49
3:D:1459:LEU:HB2	3:D:1470:ARG:HH21	1.77	0.49
4:E:40:LEU:HG	4:E:67:GLU:HG2	1.93	0.49
2:C:879:ARG:HH11	3:D:1029:ARG:HH21	1.60	0.49
3:D:1045:MET:HB2	3:D:1072:ILE:HG22	1.95	0.49
3:D:198:ARG:HD2	3:D:199:LEU:HG	1.95	0.49
3:D:1000:THR:HA	3:D:1041:LEU:HD21	1.95	0.49
2:C:229:MET:HE1	2:C:237:ARG:HH21	1.77	0.48
3:D:1378:TYR:CE2	3:D:1396:GLU:HG2	2.48	0.48
3:D:350:HIS:HD2	5:F:100:VAL:HG21	1.77	0.48
3:D:699:VAL:HG12	3:D:717:GLN:HB3	1.94	0.48
3:D:574:LEU:O	3:D:578:VAL:HG23	2.13	0.48
3:D:1192:LEU:HD22	3:D:1345:GLU:OE2	2.13	0.48
3:D:64:LYS:HB2	5:F:378:GLY:HA3	1.95	0.48
2:C:954:THR:OG1	2:C:965:GLU:OE2	2.31	0.48
2:C:239:PHE:CZ	2:C:253:ALA:HA	2.48	0.48
2:C:679:PHE:HA	3:D:943:THR:HG23	1.96	0.48
1:B:68:ILE:HB	1:B:71:VAL:HB	1.96	0.48
2:C:290:LEU:HD22	2:C:302:VAL:HG11	1.95	0.48
3:D:353:VAL:HG12	3:D:368:VAL:HG22	1.96	0.48
3:D:39:PRO:HB2	3:D:46:ASP:HA	1.96	0.48
2:C:713:ARG:HA	2:C:819:VAL:HA	1.96	0.48
2:C:774:LEU:HD22	5:F:350:LEU:HD11	1.94	0.48
1:A:213:GLN:O	1:A:217:ILE:HG13	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1031:ARG:HD3	3:D:619:LEU:HG	1.96	0.47
3:D:1440:PHE:HE2	3:D:1463:LYS:HZ2	1.62	0.47
3:D:474:GLU:O	3:D:478:LEU:HB2	2.14	0.47
2:C:919:ALA:HB2	2:C:968:LEU:HD21	1.95	0.47
2:C:971:LYS:HB3	2:C:986:PRO:HB2	1.96	0.47
2:C:1051:GLU:OE1	3:D:752:SER:OG	2.27	0.47
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	1.95	0.47
3:D:1106:VAL:O	3:D:1108:ARG:HG3	2.14	0.47
3:D:1112:CYS:HB3	3:D:1201:CYS:HB3	1.97	0.47
3:D:1434:TRP:CD1	3:D:1457:ASP:HB2	2.49	0.47
3:D:1460:ILE:HG13	3:D:1460:ILE:H	1.56	0.47
3:D:560:GLN:O	5:F:184:ARG:NH2	2.38	0.47
3:D:959:GLU:HB3	3:D:963:TYR:CE2	2.50	0.47
2:C:150:PRO:HB3	2:C:158:TYR:HD1	1.79	0.47
2:C:313:LEU:HG	2:C:320:HIS:HB3	1.96	0.47
2:C:492:ASP:HB3	2:C:518:LYS:HD3	1.96	0.47
2:C:249:LYS:HG3	2:C:251:ASP:OD2	2.14	0.47
3:D:187:LYS:HB2	3:D:200:ASP:HB2	1.97	0.47
3:D:709:HIS:ND1	3:D:1231:GLU:HG3	2.30	0.47
3:D:111:LYS:HA	3:D:114:THR:HB	1.96	0.47
3:D:629:SER:HB3	3:D:726:ILE:HG13	1.96	0.47
3:D:639:LEU:HA	3:D:729:HIS:CD2	2.50	0.47
3:D:684:LYS:HG3	3:D:686:GLU:H	1.80	0.47
3:D:801:GLY:HA2	3:D:821:VAL:HG13	1.95	0.47
2:C:100:LEU:HB2	2:C:369:PRO:HG3	1.96	0.47
2:C:754:ILE:HG13	2:C:791:ARG:HG2	1.97	0.47
2:C:833:LEU:HD21	2:C:839:LEU:HD11	1.97	0.47
5:F:228:GLU:HG3	5:F:231:ARG:HH21	1.79	0.47
1:A:211:LEU:O	1:A:215:VAL:HG23	2.15	0.47
1:A:14:ARG:HG2	1:B:231:ALA:HB3	1.97	0.47
1:B:24:VAL:HG22	1:B:196:THR:HG23	1.96	0.47
3:D:114:THR:HG21	3:D:498:VAL:HG21	1.96	0.47
5:F:89:GLY:HA2	5:F:193:ARG:HH21	1.80	0.47
2:C:516:ARG:HA	2:C:520:GLU:O	2.14	0.46
3:D:1139:ASP:N	3:D:1139:ASP:OD1	2.49	0.46
1:A:63:HIS:O	1:A:66:SER:OG	2.30	0.46
1:B:138:LEU:HD11	1:B:140:MET:HE3	1.97	0.46
3:D:181:ASP:CG	3:D:205:TYR:HB3	2.36	0.46
4:E:46:PRO:HD2	4:E:63:TRP:CZ2	2.50	0.46
3:D:1429:LEU:HD21	3:D:1441:GLN:NE2	2.30	0.46
3:D:374:GLU:HG3	3:D:375:GLU:H	1.81	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.50	0.46
3:D:860:LEU:HA	3:D:877:PRO:HB2	1.97	0.46
1:A:209:GLU:O	1:A:213:GLN:HG2	2.16	0.46
2:C:567:GLN:HB2	2:C:997:LEU:HD22	1.98	0.46
2:C:690:ILE:HB	2:C:694:LEU:HD12	1.97	0.46
2:C:1054:THR:HG21	2:C:1079:PRO:HB2	1.98	0.46
2:C:258:TYR:O	2:C:263:ASP:N	2.48	0.46
2:C:672:VAL:HB	2:C:868:ASP:HB2	1.98	0.46
3:D:1198:TYR:OH	3:D:1396:GLU:OE1	2.23	0.46
3:D:155:ASP:O	3:D:159:ARG:HB2	2.16	0.46
1:B:64:GLU:HG2	1:B:76:VAL:HG22	1.97	0.46
2:C:943:VAL:HG11	2:C:973:VAL:HG22	1.98	0.46
3:D:964:LEU:HD21	3:D:1058:ARG:HD2	1.98	0.46
3:D:1368:ILE:HD12	3:D:1368:ILE:H	1.80	0.46
3:D:900:ILE:HD13	3:D:902:LEU:HD13	1.98	0.46
5:F:208:SER:HB3	5:F:211:ASP:OD2	2.15	0.46
5:F:371:LEU:O	5:F:381:HIS:ND1	2.44	0.46
2:C:1090:LYS:HE2	2:C:1112:PHE:CZ	2.51	0.46
3:D:1353:GLN:O	3:D:1357:ARG:HG3	2.16	0.45
3:D:65:ARG:HG3	3:D:67:ARG:H	1.81	0.45
2:C:926:PHE:HE2	2:C:960:GLU:HG2	1.81	0.45
3:D:350:HIS:CD2	5:F:100:VAL:HG21	2.51	0.45
2:C:267:TYR:CE2	2:C:290:LEU:HG	2.52	0.45
2:C:344:PHE:HD2	2:C:382:ILE:HD11	1.81	0.45
1:B:153:ALA:HB1	1:B:166:PRO:HB2	1.99	0.45
2:C:773:LEU:HD11	5:F:354:LEU:HD22	1.99	0.45
2:C:744:ARG:HG3	2:C:747:ALA:HB2	1.99	0.45
3:D:1383:ASP:HB3	3:D:1416:ALA:HB3	1.99	0.45
3:D:529:GLN:HB3	3:D:535:PHE:CE2	2.52	0.45
3:D:1057:VAL:HG13	3:D:1069:GLU:CD	2.37	0.45
3:D:584:ASN:HB2	3:D:602:SER:HB3	1.99	0.45
2:C:157:ARG:HA	2:C:157:ARG:HD3	1.66	0.45
2:C:124:ASP:HB3	2:C:592:LEU:HD11	1.97	0.45
3:D:1217:ILE:HD12	3:D:1217:ILE:H	1.82	0.45
4:E:47:LYS:NZ	4:E:56:ASP:OD1	2.47	0.45
2:C:1056:LYS:HA	3:D:624:ASP:HB2	1.98	0.45
2:C:954:THR:HA	2:C:955:PRO:HD3	1.87	0.45
3:D:10:ILE:O	3:D:1454:GLY:HA2	2.16	0.45
3:D:417:PRO:HG3	3:D:431:VAL:HA	1.99	0.45
2:C:548:PRO:O	2:C:843:HIS:HE1	2.00	0.45
3:D:1498:ALA:O	4:E:84:ARG:NH1	2.50	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:13:VAL:HG21	4:E:19:LEU:HB2	1.98	0.45
2:C:728:HIS:ND1	5:F:422:LEU:HG	2.32	0.45
3:D:134:VAL:HG12	3:D:454:ALA:HB2	1.99	0.45
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.98	0.45
1:A:115:LEU:HA	1:A:116:PRO:HD3	1.81	0.44
2:C:541:SER:OG	2:C:542:VAL:N	2.50	0.44
3:D:567:ILE:HG13	5:F:140:ARG:NH2	2.33	0.44
2:C:428:ARG:O	3:D:1078:ARG:NH1	2.50	0.44
2:C:431:HIS:H	2:C:434:HIS:CE1	2.36	0.44
2:C:944:LEU:HD21	2:C:963:LEU:HD23	1.98	0.44
3:D:1049:SER:OG	3:D:1051:GLU:HG2	2.17	0.44
2:C:1009:SER:HB3	3:D:651:GLU:O	2.18	0.44
2:C:712:ALA:O	2:C:820:ARG:N	2.51	0.44
3:D:1130:ARG:NH2	3:D:1317:ASP:OD2	2.50	0.44
3:D:8:VAL:HG12	3:D:1434:TRP:HZ2	1.82	0.44
3:D:790:TYR:CD2	3:D:1022:VAL:HG13	2.53	0.44
4:E:46:PRO:HD2	4:E:63:TRP:CE2	2.52	0.44
1:A:57:TYR:CD1	1:A:161:ARG:HD3	2.53	0.44
2:C:251:ASP:OD2	2:C:251:ASP:N	2.51	0.44
3:D:108:VAL:HB	3:D:109:PRO:HD3	1.98	0.44
3:D:1372:VAL:HA	3:D:1375:MET:HG3	1.99	0.44
3:D:785:ILE:HD13	3:D:935:LYS:HA	2.00	0.44
1:A:222:LEU:HD22	1:B:215:VAL:HG13	1.98	0.44
3:D:1253:THR:HG23	3:D:1269:LYS:HG3	1.98	0.44
3:D:1489:GLN:HG2	3:D:1492:LEU:HD13	1.99	0.44
3:D:631:ILE:HG22	3:D:726:ILE:HB	1.98	0.44
2:C:874:LEU:HD11	3:D:787:LEU:HD22	1.98	0.44
1:A:42:ARG:NH2	1:B:34:VAL:HB	2.33	0.44
1:B:13:VAL:HG22	1:B:23:PHE:HD1	1.83	0.44
2:C:470:PRO:HB2	2:C:534:VAL:HG21	1.99	0.44
2:C:521:PRO:HB2	3:D:1055:VAL:HG11	2.00	0.44
3:D:861:GLN:N	3:D:861:GLN:OE1	2.48	0.44
4:E:57:ASP:HA	4:E:58:PRO:HD3	1.90	0.44
5:F:318:GLU:HA	5:F:328:PHE:HB3	2.00	0.44
1:A:196:THR:HG21	2:C:934:PHE:HE1	1.83	0.44
3:D:1463:LYS:HE3	3:D:1463:LYS:HB2	1.88	0.44
1:B:110:LYS:HD3	1:B:126:ASP:HA	2.00	0.43
1:B:220:GLU:O	1:B:223:THR:OG1	2.20	0.43
2:C:626:ARG:HD3	2:C:629:TYR:CD2	2.53	0.43
2:C:846:LYS:NZ	6:I:4:R2T:HG2	2.33	0.43
3:D:1459:LEU:HD12	3:D:1470:ARG:HH21	1.83	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:575:GLN:HG3	2:C:670:GLN:NE2	2.32	0.43
3:D:1286:THR:HG22	3:D:1287:GLU:H	1.82	0.43
3:D:1462:LEU:HD22	3:D:1472:ILE:HB	2.00	0.43
2:C:587:VAL:HG11	2:C:666:LEU:HD22	2.01	0.43
3:D:864:VAL:HG22	3:D:877:PRO:HD3	2.01	0.43
3:D:22:SER:HB3	3:D:92:HIS:HB3	2.00	0.43
1:A:218:LEU:HD23	1:B:222:LEU:HD21	2.00	0.43
1:B:30:ARG:NH2	2:C:854:PRO:HB3	2.34	0.43
3:D:1114:THR:OG1	3:D:1116:ASN:OD1	2.31	0.43
3:D:1231:GLU:HB3	3:D:1232:PRO:HD3	2.01	0.43
3:D:1370:ILE:O	3:D:1374:GLN:HG2	2.18	0.43
3:D:1384:PRO:HB3	3:D:1389:LEU:O	2.19	0.43
1:B:99:LEU:HD23	1:B:114:PHE:HB3	2.00	0.43
1:B:226:SER:O	1:B:228:PRO:HD3	2.19	0.43
1:B:91:ASN:HA	1:B:92:PRO:HD3	1.88	0.43
2:C:1054:THR:O	2:C:1059:ASP:HB3	2.19	0.43
2:C:557:ARG:CZ	2:C:879:ARG:HD2	2.48	0.43
1:B:43:ILE:HG23	1:B:47:SER:HB2	2.01	0.43
2:C:792:VAL:HA	2:C:793:PRO:HD3	1.90	0.43
3:D:17:LYS:O	3:D:20:SER:OG	2.34	0.43
3:D:899:LEU:HD21	3:D:921:ARG:HG3	2.00	0.43
1:B:91:ASN:HB3	1:B:94:LEU:HG	2.01	0.43
2:C:177:GLU:HB3	2:C:178:PRO:HD2	2.00	0.43
2:C:627:ARG:NH1	2:C:638:ASP:OD2	2.52	0.43
3:D:1281:VAL:HG21	3:D:1313:VAL:HG21	1.99	0.43
3:D:176:ASP:OD1	3:D:177:ALA:N	2.51	0.43
3:D:209:ARG:HH12	3:D:349:PRO:HD3	1.83	0.43
2:C:35:PRO:HA	2:C:36:PRO:HD3	1.88	0.43
1:A:72:LYS:HA	2:C:607:ASP:HA	2.01	0.43
3:D:115:LEU:HD23	3:D:115:LEU:HA	1.81	0.43
3:D:67:ARG:HD3	5:F:376:ILE:HD11	2.00	0.43
2:C:70:GLU:HG2	2:C:97:ARG:HB2	2.00	0.43
1:A:174:VAL:HA	1:A:201:THR:HG22	2.01	0.42
3:D:757:ALA:O	3:D:761:ILE:HG12	2.18	0.42
2:C:1090:LYS:HD3	2:C:1090:LYS:HA	1.83	0.42
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.54	0.42
3:D:1350:GLU:O	3:D:1354:LYS:HG3	2.20	0.42
3:D:207:PHE:O	3:D:390:PRO:HA	2.18	0.42
3:D:65:ARG:HD3	3:D:66:GLN:H	1.84	0.42
5:F:223:ALA:HB2	5:F:242:TRP:HB2	2.01	0.42
2:C:1021:LEU:HD12	2:C:1022:GLY:H	1.84	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:209:ARG:HG3	2:C:210:GLU:H	1.83	0.42
1:B:51:THR:OG1	1:B:87:VAL:O	2.25	0.42
5:F:152:ASP:OD1	5:F:152:ASP:N	2.53	0.42
3:D:633:VAL:HG22	3:D:635:PRO:HD3	2.01	0.42
3:D:761:ILE:H	3:D:761:ILE:HG12	1.73	0.42
1:A:99:LEU:HD23	1:A:114:PHE:CG	2.54	0.42
1:B:213:GLN:O	1:B:217:ILE:HG13	2.19	0.42
2:C:124:ASP:OD2	2:C:395:LYS:NZ	2.45	0.42
2:C:329:GLY:HA3	2:C:489:THR:HG23	2.01	0.42
2:C:829:GLN:NE2	2:C:831:ARG:HH21	2.17	0.42
3:D:1116:ASN:OD1	3:D:1116:ASN:N	2.52	0.42
3:D:1273:VAL:H	3:D:1326:THR:HG1	1.67	0.42
3:D:601:ARG:HH11	3:D:610:LYS:HD2	1.85	0.42
1:B:34:VAL:HG11	2:C:978:ARG:HB3	2.02	0.42
2:C:122:THR:OG1	2:C:124:ASP:OD1	2.33	0.42
3:D:95:LEU:HA	3:D:551:ASN:HD21	1.84	0.42
5:F:292:ALA:HB2	5:F:301:ALA:HA	2.01	0.42
3:D:964:LEU:HD11	3:D:1058:ARG:HD2	2.00	0.42
1:A:85:LEU:HD22	1:A:87:VAL:HG23	2.02	0.42
2:C:272:ALA:O	2:C:276:LYS:HG2	2.19	0.42
2:C:344:PHE:CD2	2:C:378:LEU:HD11	2.55	0.42
2:C:420:ARG:HG2	2:C:420:ARG:H	1.54	0.42
3:D:1047:LYS:HG2	3:D:1053:PHE:CD1	2.55	0.42
3:D:106:LYS:O	3:D:586:ARG:NH1	2.52	0.42
4:E:45:ARG:HA	4:E:46:PRO:HD3	1.93	0.42
1:B:8:ALA:HA	1:B:9:PRO:HD3	1.84	0.42
3:D:1083:ASP:O	3:D:1087:ARG:HG3	2.20	0.42
3:D:30:GLU:HB3	3:D:40:GLU:HG3	2.01	0.42
2:C:444:PRO:HB3	6:I:1:2RA:HA	2.02	0.42
1:A:83:LYS:HE2	1:A:168:ASP:HB2	2.02	0.41
2:C:436:GLY:H	2:C:539:VAL:HG23	1.85	0.41
2:C:578:VAL:HG23	2:C:579:VAL:HG23	2.01	0.41
2:C:966:LEU:HD22	2:C:986:PRO:HG3	2.01	0.41
3:D:1047:LYS:HD2	3:D:1051:GLU:HG3	2.02	0.41
3:D:637:LEU:O	3:D:935:LYS:NZ	2.53	0.41
1:B:86:VAL:HB	1:B:123:MET:HB2	2.01	0.41
2:C:1097:LEU:HD11	3:D:103:TRP:CZ3	2.55	0.41
2:C:243:ARG:HA	2:C:244:PRO:HD3	1.78	0.41
3:D:371:ILE:HG13	3:D:372:ASP:H	1.85	0.41
3:D:692:GLU:HG2	3:D:720:LEU:HD12	2.01	0.41
3:D:1125:PRO:HA	3:D:1131:SER:O	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:205:TYR:HD2	3:D:205:TYR:H	1.62	0.41
3:D:566:ILE:HD11	5:F:192:LEU:HD21	2.02	0.41
5:F:258:ILE:HG13	5:F:258:ILE:H	1.52	0.41
1:B:105:GLY:O	1:B:107:LYS:N	2.53	0.41
2:C:1040:LEU:HA	2:C:1040:LEU:HD23	1.93	0.41
2:C:966:LEU:HD13	2:C:986:PRO:HB3	2.01	0.41
3:D:1443:THR:HG23	3:D:1443:THR:H	1.55	0.41
3:D:169:TYR:HA	3:D:170:PRO:HD3	1.87	0.41
2:C:543:ASN:ND2	2:C:566:THR:HG22	2.35	0.41
3:D:1267:ARG:HA	3:D:1268:PRO:HD3	1.84	0.41
3:D:541:ASN:O	3:D:545:ARG:HG3	2.21	0.41
3:D:596:SER:OG	3:D:598:ARG:HG2	2.21	0.41
2:C:1056:LYS:HB3	3:D:623:VAL:HG13	2.02	0.41
3:D:1084:THR:HG22	3:D:1087:ARG:HH21	1.86	0.41
3:D:214:GLU:HB3	3:D:340:THR:HB	2.01	0.41
1:A:206:THR:HG22	1:A:208:LEU:H	1.86	0.41
1:B:70:GLY:HA3	1:B:136:GLY:HA2	2.03	0.41
2:C:954:THR:OG1	2:C:957:LYS:HD3	2.21	0.41
3:D:845:ASN:HB2	3:D:848:GLU:HB2	2.01	0.41
2:C:159:ILE:HG12	2:C:175:GLU:HG3	2.03	0.41
2:C:258:TYR:CD1	2:C:263:ASP:HB2	2.56	0.41
2:C:953:VAL:HG12	2:C:965:GLU:HB2	2.02	0.41
3:D:1282:ARG:NH2	3:D:1295:GLU:OE2	2.37	0.41
3:D:845:ASN:HB3	3:D:847:ASP:OD1	2.21	0.41
3:D:462:GLN:HB2	3:D:513:ILE:HG21	2.03	0.41
2:C:520:GLU:HA	2:C:521:PRO:HD3	1.86	0.41
3:D:493:ARG:O	3:D:497:GLU:HG3	2.21	0.41
3:D:470:LEU:HB3	3:D:503:LEU:HD23	2.03	0.41
3:D:6:ARG:HH11	3:D:6:ARG:HB2	1.86	0.41
4:E:35:PHE:HE2	4:E:63:TRP:CG	2.39	0.41
5:F:207:LEU:HA	5:F:207:LEU:HD23	1.86	0.41
1:A:111:ALA:HB3	1:A:125:PRO:HA	2.02	0.40
2:C:486:MET:HB2	2:C:486:MET:HE2	1.94	0.40
2:C:943:VAL:HG21	2:C:973:VAL:HG13	2.03	0.40
3:D:1295:GLU:HG2	3:D:1300:SER:OG	2.22	0.40
3:D:428:LYS:HB3	3:D:428:LYS:HE2	1.88	0.40
1:A:183:ASP:N	1:A:183:ASP:OD1	2.54	0.40
2:C:964:LYS:O	2:C:968:LEU:HG	2.22	0.40
3:D:1102:THR:HG21	3:D:1371:VAL:HG22	2.03	0.40
3:D:704:ARG:HD2	3:D:738:ALA:HB2	2.04	0.40
3:D:752:SER:HB2	3:D:755:ALA:H	1.85	0.40

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:209:PHE:HA	5:F:212:LEU:HD12	2.03	0.40
2:C:1097:LEU:HD13	3:D:10:ILE:HD11	2.03	0.40
3:D:478:LEU:HA	3:D:478:LEU:HD12	1.90	0.40
5:F:134:LYS:HD3	5:F:134:LYS:HA	1.78	0.40
3:D:669:ASN:HD21	5:F:420:ASP:CG	2.24	0.40
1:A:97:VAL:HG12	1:A:99:LEU:HD12	2.03	0.40
2:C:249:LYS:O	2:C:252:LYS:N	2.54	0.40
2:C:154:ARG:NH1	2:C:177:GLU:HA	2.36	0.40
2:C:181:VAL:HA	2:C:220:GLY:O	2.22	0.40
2:C:2:GLU:N	2:C:2:GLU:OE1	2.54	0.40
3:D:608:SER:HA	3:D:612:GLY:HA3	2.04	0.40
5:F:383:LEU:HD22	5:F:397:ILE:HG23	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	224/314 (71%)	223 (100%)	1 (0%)	0	100	100
1	B	220/314 (70%)	217 (99%)	3 (1%)	0	100	100
2	C	1094/1119 (98%)	1059 (97%)	35 (3%)	0	100	100
3	D	1359/1524 (89%)	1317 (97%)	41 (3%)	1 (0%)	53	85
4	E	91/99 (92%)	90 (99%)	1 (1%)	0	100	100
5	F	335/443 (76%)	328 (98%)	7 (2%)	0	100	100
All	All	3323/3813 (87%)	3234 (97%)	88 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	406	ASP



### 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	197/272 (72%)	188 (95%)	9 (5%)	29	64
1	B	193/272 (71%)	187 (97%)	6 (3%)	43	74
2	C	926/941 (98%)	895 (97%)	31 (3%)	41	72
3	D	1155/1279 (90%)	1115 (96%)	40 (4%)	39	71
4	E	82/88 (93%)	80 (98%)	2 (2%)	52	78
5	F	295/388 (76%)	279 (95%)	16 (5%)	24	59
All	All	2848/3240 (88%)	2744 (96%)	104 (4%)	37	69

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	41	ARG
1	A	66	SER
1	A	67	THR
1	A	74	ASP
1	A	85	LEU
1	A	86	VAL
1	A	162	ILE
1	A	186	LEU
1	B	12	THR
1	B	74	ASP
1	B	104	GLU
1	B	107	LYS
1	B	204	SER
1	B	206	THR
2	C	26	TYR
2	C	42	VAL
2	C	104	ASP
2	C	182	VAL
2	C	187	ASN
2	C	196	LEU
2	C	200	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	C	217	LEU
2	C	227	PHE
2	C	260	LEU
2	C	265	ARG
2	C	301	GLU
2	C	365	ASP
2	C	419	THR
2	C	420	ARG
2	C	421	GLU
2	C	443	THR
2	C	475	VAL
2	C	566	THR
2	C	617	ASP
2	C	670	GLN
2	C	723	THR
2	C	766	GLU
2	C	784	ASP
2	C	858	MET
2	C	905	ILE
2	C	937	ASP
2	C	954	THR
2	C	1017	THR
2	C	1059	ASP
2	C	1117	SER
3	D	10	ILE
3	D	30	GLU
3	D	101	HIS
3	D	111	LYS
3	D	112	ILE
3	D	130	SER
3	D	135	LEU
3	D	136	ASP
3	D	205	TYR
3	D	371	ILE
3	D	387	LEU
3	D	388	HIS
3	D	406	ASP
3	D	407	VAL
3	D	411	THR
3	D	415	VAL
3	D	420	VAL
3	D	427	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	D	483	HIS
3	D	502	PHE
3	D	587	ARG
3	D	707	THR
3	D	754	PHE
3	D	761	ILE
3	D	778	LEU
3	D	783	ARG
3	D	784	ASP
3	D	907	GLU
3	D	994	GLN
3	D	1041	LEU
3	D	1061	PHE
3	D	1127	GLU
3	D	1129	THR
3	D	1131	SER
3	D	1188	VAL
3	D	1190	SER
3	D	1286	THR
3	D	1427	SER
3	D	1443	THR
3	D	1444	THR
4	E	50	THR
4	E	83	ASP
5	F	82	ARG
5	F	88	ILE
5	F	140	ARG
5	F	141	VAL
5	F	142	ARG
5	F	156	VAL
5	F	229	TYR
5	F	231	ARG
5	F	232	ARG
5	F	258	ILE
5	F	264	MET
5	F	271	LEU
5	F	318	GLU
5	F	340	SER
5	F	348	SER
5	F	419	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	HIS
2	C	204	GLN
2	C	829	GLN
3	D	709	HIS
3	D	1441	GLN
3	D	1442	ASN
5	F	217	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

7 non-standard protein/DNA/RNA residues are modelled in this entry.

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
6	2RA	I	1	9,6	4,5,6	1.23	1 (25%)	2,5,7	1.63	1 (50%)
6	DSN	I	2	6	5,5,6	1.77	1 (20%)	2,5,7	1.56	1 (50%)
6	DVA	I	3	6	6,6,7	1.43	1 (16%)	6,7,9	1.35	1 (16%)
6	R2T	I	4	6	10,10,11	2.00	3 (30%)	8,13,15	0.96	0
6	2TL	I	5	6	6,6,7	1.02	0	6,7,9	1.02	1 (16%)
6	0QZ	I	6	6	5,5,6	1.41	1 (20%)	4,5,7	1.45	1 (25%)
6	FGL	I	7	6	1,6,7	0.72	0	2,7,9	2.48	1 (50%)

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
6	2RA	I	1	9,6	-	0/2/4/6	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	DSN	I	2	6	-	0/2/4/6	0/0/0/0
6	DVA	I	3	6	-	0/4/6/8	0/0/0/0
6	R2T	I	4	6	-	0/11/14/16	0/0/0/0
6	2TL	I	5	6	-	0/4/6/8	0/0/0/0
6	0QZ	I	6	6	-	0/2/4/6	0/0/0/0
6	FGL	I	7	6	-	0/0/6/8	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	6	0QZ	OB-CA	-2.91	1.38	1.43
6	I	4	R2T	OB1-CB	-2.13	1.37	1.43
6	I	1	2RA	CA-C	2.25	1.53	1.50
6	I	3	DVA	CA-C	3.22	1.54	1.50
6	I	4	R2T	CA-C	3.72	1.55	1.50
6	I	2	DSN	CA-C	3.77	1.55	1.50
6	I	4	R2T	CD-NE2	4.07	1.43	1.32

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	7	FGL	O-C-CA	-3.40	119.42	124.40
6	I	3	DVA	O-C-CA	-2.76	118.66	125.09
6	I	6	0QZ	O-C-CA	-2.41	119.25	125.00
6	I	1	2RA	O-C-CA	-2.29	118.67	124.96
6	I	2	DSN	O-C-CA	-2.21	118.91	124.96
6	I	5	2TL	O-C-CA	-2.11	120.17	125.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	1	2RA	1	0
6	I	4	R2T	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\# Z  > 2$
9	MB8	I	101	6	0,1,6	0.00	-	0,0,7	0.00	-

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
9	MB8	I	101	6	-	0/0/0/6	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	226/314 (71%)	-0.24	3 (1%) 77 79	84, 110, 169, 199	0
1	B	224/314 (71%)	0.13	4 (1%) 68 70	97, 165, 233, 259	0
2	C	1100/1119 (98%)	0.01	24 (2%) 62 64	67, 135, 240, 281	0
3	D	1365/1524 (89%)	-0.07	13 (0%) 82 85	68, 114, 213, 249	0
4	E	93/99 (93%)	-0.08	2 (2%) 62 64	96, 142, 212, 216	0
5	F	339/443 (76%)	0.06	17 (5%) 29 31	89, 153, 249, 267	0
6	I	0/7	-	-	-	-
All	All	3347/3820 (87%)	-0.03	63 (1%) 66 69	67, 129, 230, 281	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	372	LEU	4.6
2	C	217	LEU	4.4
2	C	98	LEU	4.4
2	C	250	ARG	4.2
2	C	99	GLN	4.1
3	D	360	ARG	4.1
2	C	245	GLY	3.8
1	A	231	ALA	3.8
2	C	211	LEU	3.8
5	F	138	SER	3.7
3	D	1251	ASP	3.6
5	F	390	PHE	3.5
2	C	367	LEU	3.4
5	F	397	ILE	3.4
5	F	375	LEU	3.3
5	F	393	THR	3.2
2	C	251	ASP	3.2
1	B	97	VAL	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	D	1239	ARG	3.2
5	F	389	PHE	3.2
3	D	1240	THR	3.0
2	C	100	LEU	3.0
2	C	781	LYS	3.0
2	C	541	SER	2.9
2	C	373	VAL	2.9
3	D	616	GLN	2.9
5	F	408	LEU	2.8
2	C	454	SER	2.7
5	F	399	GLN	2.7
3	D	382	GLU	2.7
2	C	359	MET	2.7
5	F	381	HIS	2.7
3	D	1431	THR	2.6
2	C	111	ASP	2.6
5	F	377	ASP	2.6
2	C	109	LYS	2.5
2	C	764	GLU	2.5
5	F	386	VAL	2.5
3	D	821	VAL	2.5
5	F	153	PRO	2.5
5	F	358	LEU	2.4
1	A	6	LEU	2.4
3	D	831	GLY	2.4
3	D	1409	ALA	2.4
5	F	395	GLU	2.3
2	C	291	ALA	2.3
2	C	244	PRO	2.3
3	D	1130	ARG	2.3
3	D	3	LYS	2.3
4	E	92	LEU	2.2
1	B	137	ARG	2.2
3	D	67	ARG	2.2
2	C	219	GLN	2.2
1	A	230	ALA	2.1
2	C	311	PHE	2.1
1	B	130	ALA	2.1
5	F	369	LEU	2.1
5	F	391	GLY	2.1
5	F	357	ALA	2.1
2	C	814	GLU	2.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	C	67	ASP	2.1
1	B	98	THR	2.1
4	E	89	MET	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	DVA	I	3	7/8	0.95	0.26	81,85,91,93	0
6	FGL	I	7	7/8	0.96	0.15	82,93,106,108	0
6	2RA	I	1	6/7	0.96	0.17	85,96,99,111	0
6	DSN	I	2	6/7	0.97	0.11	80,85,93,97	0
6	2TL	I	5	7/8	0.98	0.20	78,84,91,93	0
6	R2T	I	4	11/12	0.98	0.17	77,87,94,97	0
6	0QZ	I	6	6/7	0.99	0.19	75,79,86,87	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
9	MB8	I	101	2/7	0.82	0.36	102,102,102,107	0
7	ZN	D	1601	1/1	0.97	0.07	159,159,159,159	0
7	ZN	D	1602	1/1	0.99	0.19	105,105,105,105	0
8	MG	D	1603	1/1	0.99	0.11	75,75,75,75	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.