

# Full wwPDB X-ray Structure Validation Report (i)

#### Sep 25, 2023 – 05:42 AM EDT

PDB ID	:	5VOI
Title	:	X-ray crystal structure of bacterial RNA polymerase and pyrG promoter com-
		plex
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Deposited on	:	2017-05-02
Resolution	:	2.80  Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\;DIFFRACTION$ 

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive $(\#Entries)$	Similar resolution $(\#Entries, resolution range(Å))$
R <sub>free</sub>	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	А	315	54% 17%		28%	
			% *		2070	
1	В	315	55% 14%	•	30%	
2	$\mathbf{C}$	1119	73%		23%	••
3	D	1524	73%		22%	
		1021			2270	
4	Ε	99	84%		11%	5%



Mol	Chain	Length		Quality of chai	n	
5	F	423	3%	65%	16% ·	18%
6	G	22	23%	50%	9%	18%
7	Н	27	30%	22%	30%	19%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	ZN	D	2002	-	-	Х	-



# 2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 28432 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues		Ate	oms		ZeroOcc	AltConf	Trace	
1	Δ	226	Total	С	Ν	Ο	S	0	0	0
	A	220	1782	1138	310	332	2	0	0	0
1	р	າາາ	Total	С	Ν	0	S	0	0	0
	D		1750	1118	304	326	2	0	U	0

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

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

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

Mol	Chain	Residues		A	toms		ZeroOcc	AltConf	Trace	
3	D	1486	Total 11738	С 7440	N 2067	O 2195	S 36	0	0	0

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
4	Е	94	Total 761	C 486	N 132	O 139	$\frac{S}{4}$	0	0	0

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

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
5	F	346	Total 2807	C 1770	N 509	0 524	$\frac{S}{4}$	0	0	0

• Molecule 6 is a DNA chain called PyrG promoter.



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
6	G	18	Total 368	C 175	N 71	O 104	Р 18	0	0	0

• Molecule 7 is a DNA chain called PyrG promoter.

Mol	Chain	Residues		At	$\mathbf{oms}$			ZeroOcc	AltConf	Trace
7	Н	22	Total 451	C 216	N 84	O 130	Р 21	0	0	0

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

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

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

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



# 3 Residue-property plots (i)

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



• Molecule 1: DNA-directed RNA polymerase subunit alpha





PROTEIN DATA BANK





• Molecule 6: PyrG promoter







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	183.18Å 103.47Å 294.44Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $99.14^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{B}_{\mathrm{ascolution}}\left(\mathring{A}\right)$	29.74 - 2.80	Depositor
Resolution (A)	29.74 - 2.80	EDS
% Data completeness	98.2 (29.74-2.80)	Depositor
(in resolution range)	98.1 (29.74-2.80)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.30 (at 2.80 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
D D .	0.192 , $0.236$	Depositor
$n, n_{free}$	0.193 , $0.235$	DCC
$R_{free}$ test set	2000 reflections $(1.52%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	56.5	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , $49.6$	EDS
L-test for $twinning^2$	$<  L  > = 0.49, < L^2 > = 0.32$	Xtriage
	0.014  for  1/2 *h-3/2 *k,-1/2 *h-1/2 *k,-1/2 *h	
Estimated twinning fraction	+1/2*k-l	Xtriage
	0.014 for $1/2^{h+3}/2^{k}, 1/2^{h-1}/2^{k}, -1/2^{h-1}/2^{h-$	110110000
	1/2*k-1	EDC
$F_o, F_c$ correlation	0.94	EDS
'Iotal number of atoms	28432	wwPDB-VP
Average B, all atoms $(Å^2)$	72.0	wwPDB-VP

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

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: MG, ZN

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

Mal	Chain	Bo	ond lengths	B	ond angles
WIOI	Unain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.55	0/1814	0.78	0/2466
1	В	0.55	1/1782~(0.1%)	0.83	1/2424~(0.0%)
2	С	0.58	0/8937	0.82	5/12087~(0.0%)
3	D	0.59	1/11944~(0.0%)	0.81	6/16148~(0.0%)
4	Е	0.55	0/775	0.77	0/1045
5	F	0.51	0/2852	0.73	0/3837
6	G	1.62	7/413~(1.7%)	1.24	3/634~(0.5%)
7	Н	1.49	8/505~(1.6%)	1.45	8/776~(1.0%)
All	All	0.63	17/29022~(0.1%)	0.83	23/39417~(0.1%)

All (17) bond length outliers are listed below:

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



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

All (23) bond angle outliers are listed below:

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts (i)

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

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



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

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

All (520) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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



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



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:C:905:ILE:HG23	2:C:906:PHE:CD2	2.31	0.63
3:D:806:PHE:HB2	3:D:829:VAL:HG22	1.82	0.62
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.82	0.62
3:D:828:LYS:HG2	3:D:833:GLU:HB3	1.81	0.62
3:D:136:ASP:OD2	3:D:138:LYS:HE3	1.99	0.61
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.82	0.61
1:B:216:GLU:OE1	1:B:219:ARG:NH2	2.33	0.61
1:A:188:GLN:HG2	1:A:189:ARG:HG2	1.82	0.61
2:C:64:LEU:N	2:C:103:LYS:HE2	2.15	0.61
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.83	0.61
3:D:949:ILE:HD11	3:D:1023:MET:HE1	1.83	0.61
3:D:231:VAL:O	3:D:236:TYR:OH	2.19	0.60
3:D:1258:ARG:HH21	3:D:1351:GLU:CG	2.14	0.60
3:D:808:THR:O	3:D:811:GLU:HB2	2.01	0.60
2:C:221:LEU:HD11	2:C:307:LEU:HD21	1.81	0.60
2:C:1053:LEU:HA	3:D:621:LYS:HD2	1.84	0.59
3:D:828:LYS:HA	3:D:833:GLU:HA	1.84	0.59
3:D:841:TYR:HB2	3:D:864:VAL:HG22	1.85	0.59
1:A:228:PRO:HB3	1:B:13:VAL:HG21	1.84	0.59
2:C:591:SER:O	2:C:592:LEU:HB2	2.01	0.59
3:D:658:LEU:HD23	3:D:661:MET:HE1	1.84	0.59
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.83	0.59
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.28	0.58
3:D:1493:LYS:NZ	3:D:1496:GLU:HG3	2.18	0.58
1:A:11:PHE:O	1:B:228:PRO:HA	2.03	0.58
2:C:926:PHE:HE1	2:C:929:ARG:HH11	1.51	0.58
3:D:832:ARG:HD2	3:D:833:GLU:N	2.19	0.58
2:C:1001:VAL:HG13	3:D:630:VAL:HB	1.85	0.58
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.37	0.58
3:D:561:GLY:HA3	5:F:132:ARG:HD3	1.86	0.58
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.85	0.58
3:D:704:ARG:HB2	3:D:745:MET:HG2	1.84	0.58
1:A:220:GLU:O	1:A:223:THR:HB	2.04	0.58
2:C:405:ARG:HD2	2:C:442:GLU:OE2	2.04	0.58
3:D:805:GLU:HG3	3:D:828:LYS:HB2	1.85	0.58
3:D:832:ARG:NH2	3:D:833:GLU:O	2.36	0.58
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.86	0.57
3:D:1197:ARG:HB2	3:D:1398:TRP:CH2	2.39	0.57
3:D:1126:ASP:OD1	3:D:1128:VAL:HG13	2.03	0.57
1:A:226:SER:O	1:A:228:PRO:HD3	2.04	0.57
3:D:899:LEU:HD22	3:D:917:GLN:HB3	1.87	0.57



	A h o	Interatomic	Clash overlap (Å)	
Atom-1	Atom-2	distance $(\text{\AA})$		
3:D:1044:LEU:H	3:D:1044:LEU:HD12	1.68	0.57	
1:A:32:PHE:HA	1:A:35:THR:HB	1.85	0.57	
1:A:133:GLU:OE2	2:C:606:VAL:N	2.37	0.57	
3:D:960:LYS:NZ	3:D:1063:GLU:OE2	2.37	0.56	
3:D:73:CYS:CB	3:D:76:CYS:SG	2.93	0.56	
3:D:76:CYS:SG	8:D:2002:ZN:ZN	1.88	0.56	
3:D:657:LEU:HG	3:D:661:MET:HE2	1.86	0.56	
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.87	0.56	
3:D:262:LYS:HE2	3:D:341:GLU:OE1	2.04	0.56	
1:B:80:LEU:HG	3:D:844:ALA:HA	1.87	0.56	
2:C:627:ARG:NH1	2:C:638:ASP:OD2	2.39	0.56	
2:C:409:ARG:HD2	2:C:452:ILE:HG22	1.88	0.56	
2:C:853:LEU:HB2	2:C:858:MET:CE	2.35	0.56	
3:D:67:ARG:NH1	5:F:379:ARG:HD3	2.21	0.55	
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.89	0.55	
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.89	0.55	
2:C:210:GLU:HG2	2:C:304:LEU:HD21	1.89	0.55	
3:D:1211:MET:SD	4:E:16:LYS:HE3	2.46	0.55	
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.89	0.55	
3:D:892:ASP:OD1	3:D:894:LYS:HD2	2.06	0.55	
4:E:49:GLN:OE1	4:E:54:LEU:HD12	2.07	0.55	
5:F:188:ILE:HD13	5:F:221:ILE:HG12	1.89	0.55	
2:C:146:VAL:HG22	2:C:162:ILE:HG12	1.88	0.54	
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.21	0.54	
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.41	0.54	
3:D:371:ILE:HG13	5:F:232:ARG:NH1	2.22	0.54	
5:F:120:THR:HG21	5:F:122:LEU:HD22	1.89	0.54	
3:D:1310:ARG:HD2	3:D:1327:ARG:HD2	1.90	0.54	
3:D:271:VAL:HG22	3:D:281:THR:HG23	1.90	0.54	
2:C:3:ILE:HD13	2:C:900:ARG:HB2	1.89	0.54	
3:D:58:CYS:SG	3:D:76:CYS:SG	3.06	0.54	
1:B:80:LEU:HD11	3:D:842:VAL:HG12	1.88	0.54	
7:H:21:DA:H5'	7:H:21:DA:C8	2.43	0.54	
2:C:259:GLY:HA3	2:C:266:ARG:HH21	1.73	0.53	
7:H:22:DT:H2"	7:H:23:DG:C8	2.43	0.53	
1:A:70:GLY:HA3	1:A:136:GLY:HA2	1.90	0.53	
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.89	0.53	
3:D:180:LYS:NZ	3:D:357:GLU:OE1	2.37	0.53	
6:G:6:DA:H5"	6:G:6:DA:H8	1.73	0.53	
2:C:942:GLU:HG2	2:C:945:ARG:HH21	1.73	0.53	
3:D:141:ILE:HG23	3:D:450:TYR:OH	2.09	0.53	



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



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
3:D:230:TRP:CZ2	3:D:232:GLU:HG2	2.46	0.51	
3:D:1083:ASP:OD1	3:D:1238:MET:HB3	2.11	0.51	
2:C:74:GLY:HA3	2:C:93:PRO:HG2	1.93	0.50	
3:D:474:GLU:OE2	3:D:500:ARG:NE	2.42	0.50	
1:A:106:PRO:HG3	1:A:134:GLU:HG2	1.91	0.50	
1:A:186:LEU:HB3	1:A:188:GLN:OE1	2.11	0.50	
1:B:49:PRO:HA	1:B:148:VAL:HG12	1.93	0.50	
1:B:57:TYR:CD1	1:B:161:ARG:HD2	2.46	0.50	
2:C:212:GLY:HA2	2:C:218:VAL:HG21	1.93	0.50	
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.93	0.50	
3:D:963:TYR:CE2	3:D:1002:LYS:HD3	2.47	0.50	
3:D:798:GLU:OE2	3:D:824:ASN:HB2	2.12	0.50	
3:D:1288:GLU:O	3:D:1307:LYS:HE3	2.12	0.50	
2:C:197:LEU:HD12	2:C:221:LEU:HD21	1.93	0.49	
2:C:478:VAL:HG13	2:C:506:ASN:HB3	1.93	0.49	
2:C:587:VAL:O	2:C:591:SER:HB3	2.12	0.49	
1:B:56:VAL:HG21	1:B:82:LEU:HD13	1.94	0.49	
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.52	0.49	
2:C:513:VAL:HG22	2:C:524:VAL:HG12	1.94	0.49	
2:C:577:PRO:HB3	2:C:993:PHE:CG	2.48	0.49	
3:D:1093:TYR:OH	3:D:1441:GLN:OE1	2.18	0.49	
1:B:94:LEU:HD12	1:B:96:THR:H	1.77	0.49	
2:C:679:PHE:HA	3:D:943:THR:HB	1.95	0.49	
3:D:34:TYR:CZ	3:D:35:ARG:HG3	2.47	0.49	
3:D:44:LEU:HB3	3:D:525:ARG:NH2	2.27	0.49	
1:B:32:PHE:HA	1:B:35:THR:HB	1.94	0.49	
1:B:179:PHE:HB3	1:B:197:LEU:HD23	1.93	0.49	
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.94	0.49	
1:A:206:THR:HB	1:A:209:GLU:HG3	1.94	0.49	
2:C:1006:HIS:HB2	2:C:1024:LYS:HG3	1.94	0.49	
3:D:1219:GLU:HG2	3:D:1221:VAL:HG23	1.95	0.49	
3:D:1263:PHE:HD2	3:D:1375:MET:HE2	1.78	0.49	
5:F:392:VAL:HB	5:F:396:ARG:HG2	1.94	0.49	
2:C:614:ARG:CZ	2:C:620:LEU:HD13	2.42	0.49	
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.95	0.49	
2:C:374:ASN:OD1	2:C:376:ARG:HG2	2.13	0.48	
3:D:573:MET:SD	5:F:210:LEU:HB3	2.53	0.48	
2:C:135:VAL:HG23	2:C:395:LYS:HG3	1.94	0.48	
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.46	0.48	
2:C:35:PRO:HG2	2:C:38:LYS:HD3	1.96	0.48	
2:C:758:ARG:HH21	2:C:788:THR:HB	1.77	0.48	



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	1.95	0.48	
2:C:368:THR:H	2:C:371:LYS:HD2	1.78	0.48	
2:C:767:PRO:CB	2:C:771:GLU:HG2	2.44	0.48	
2:C:118:ILE:HD11	2:C:344:PHE:CE2	2.49	0.48	
2:C:211:LEU:HD21	2:C:307:LEU:HG	1.95	0.48	
2:C:224:GLU:CD	2:C:224:GLU:H	2.16	0.48	
2:C:911:GLU:O	2:C:915:LYS:HG2	2.14	0.48	
3:D:658:LEU:HD23	3:D:661:MET:CE	2.43	0.48	
3:D:957:PRO:HG3	3:D:1007:VAL:HA	1.95	0.48	
6:G:18:DA:H2'	6:G:19:DA:C8	2.49	0.48	
2:C:563:ASN:O	2:C:566:THR:HB	2.14	0.48	
3:D:1493:LYS:HZ2	3:D:1496:GLU:HG3	1.79	0.48	
3:D:780:LYS:HE3	3:D:912:LYS:HD3	1.96	0.48	
3:D:1053:PHE:CZ	3:D:1072:ILE:HD12	2.49	0.48	
3:D:1237:THR:HG22	3:D:1238:MET:H	1.78	0.48	
1:B:111:ALA:HB3	1:B:125:PRO:HA	1.95	0.48	
2:C:286:SER:OG	2:C:301:GLU:OE2	2.19	0.48	
2:C:580:MET:HB3	2:C:584:GLU:CD	2.34	0.48	
3:D:1277:ILE:HG22	3:D:1278:ASP:H	1.78	0.48	
7:H:23:DG:O5'	7:H:23:DG:H2'	2.14	0.48	
2:C:6:PHE:CD2	2:C:909:ALA:HB2	2.48	0.47	
3:D:432:TYR:O	3:D:448:GLU:HA	2.14	0.47	
3:D:939:PHE:O	3:D:943:THR:HG22	2.14	0.47	
3:D:1087:ARG:HG3	3:D:1256:LEU:HD23	1.96	0.47	
3:D:1290:LEU:HD13	3:D:1291:SER:N	2.29	0.47	
1:A:206:THR:HG22	1:A:208:LEU:N	2.29	0.47	
3:D:801:GLY:HA2	3:D:821:VAL:HG22	1.96	0.47	
3:D:1149:LEU:HG	3:D:1166:LEU:HD21	1.96	0.47	
2:C:499:ALA:HB2	2:C:533:ASP:HB2	1.96	0.47	
3:D:1237:THR:HG22	3:D:1238:MET:N	2.29	0.47	
3:D:134:VAL:HG22	3:D:151:GLN:H	1.80	0.47	
3:D:835:SER:OG	3:D:838:ARG:HG3	2.14	0.47	
3:D:1386:ASP:HB3	3:D:1412:LYS:HD2	1.97	0.47	
5:F:370:LYS:HB3	5:F:376:ILE:HG13	1.95	0.47	
1:A:112:ARG:HG2	1:A:112:ARG:HH21	1.79	0.47	
1:B:188:GLN:HG2	1:B:189:ARG:N	2.30	0.47	
2:C:683:ASN:HB3	2:C:872:ASN:HB2	1.97	0.47	
3:D:156:GLU:CD	3:D:156:GLU:H	2.17	0.47	
3:D:664:LYS:NZ	3:D:693:GLU:OE1	2.24	0.47	
1:B:188:GLN:HE21	1:B:189:ARG:HG3	1.80	0.47	
2:C:285:LEU:HD13	2:C:301:GLU:OE1	2.15	0.47	



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
2:C:617:ASP:OD1	2:C:617:ASP:N	2.47	0.47	
2:C:926:PHE:HE1	2:C:929:ARG:NH1	2.10	0.47	
3:D:44:LEU:HB3	3:D:525:ARG:HH21	1.80	0.47	
3:D:167:GLU:O	3:D:394:LEU:HD12	2.15	0.47	
3:D:258:VAL:HG12	3:D:273:ARG:O	2.15	0.47	
3:D:557:LEU:HD13	3:D:566:ILE:HG22	1.96	0.47	
3:D:816:HIS:CG	3:D:836:VAL:HG11	2.50	0.47	
1:A:6:LEU:HB2	1:A:29:GLU:OE2	2.15	0.47	
3:D:792:ILE:HD13	3:D:941:PHE:CE1	2.49	0.47	
3:D:1046:GLN:OE1	3:D:1046:GLN:N	2.45	0.47	
5:F:172:ARG:HG3	5:F:173:TYR:N	2.30	0.47	
1:B:150:TYR:HB3	3:D:855:HIS:ND1	2.30	0.46	
2:C:1057:SER:HB3	2:C:1058:ASP:H	1.49	0.46	
3:D:840:LYS:HE3	3:D:841:TYR:OH	2.16	0.46	
4:E:70:THR:OG1	4:E:72:ARG:HG3	2.15	0.46	
2:C:11:GLU:OE1	2:C:537:LYS:HE2	2.16	0.46	
2:C:168:ARG:O	2:C:267:TYR:HA	2.14	0.46	
4:E:52:GLU:OE1	4:E:52:GLU:N	2.43	0.46	
3:D:879:ARG:HD3	3:D:902:LEU:O	2.15	0.46	
5:F:166:LEU:O	5:F:171:LYS:HD2	2.15	0.46	
1:A:94:LEU:HD21	1:A:97:VAL:CG2	2.45	0.46	
3:D:242:LEU:HD23	3:D:285:PRO:HG3	1.97	0.46	
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.15	0.46	
3:D:1319:VAL:HG12	3:D:1323:GLN:NE2	2.31	0.46	
1:B:24:VAL:HA	1:B:195:LEU:O	2.15	0.46	
1:B:161:ARG:HG3	1:B:162:ILE:O	2.15	0.46	
2:C:157:ARG:HA	2:C:157:ARG:HD3	1.78	0.46	
3:D:534:ARG:HE	3:D:534:ARG:HB3	1.47	0.46	
5:F:193:ARG:HB3	7:H:7:DG:H5"	1.98	0.46	
2:C:797:GLY:O	2:C:829:GLN:NE2	2.49	0.46	
2:C:776:SER:CB	5:F:373:LYS:NZ	2.79	0.46	
3:D:103:TRP:HB3	3:D:1448:THR:HG21	1.97	0.46	
3:D:711:LEU:HD13	3:D:778:LEU:CD1	2.46	0.46	
1:A:70:GLY:N	2:C:607:ASP:OD1	2.49	0.46	
1:B:176:ARG:HG2	1:B:200:TRP:CZ3	2.51	0.46	
2:C:598:GLU:O	2:C:651:LYS:HG3	2.16	0.46	
3:D:273:ARG:HB3	3:D:278:PRO:HA	1.98	0.46	
6:G:8:DC:H2"	6:G:9:DA:C8	2.51	0.46	
2:C:948:GLU:HB3	2:C:953:VAL:HG23	1.97	0.45	
2:C:999:HIS:ND1	2:C:1004:LYS:NZ	2.61	0.45	
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.98	0.45	



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.99	0.45	
3:D:418:GLY:N	3:D:429:SER:O	2.33	0.45	
3:D:1462:LEU:HD22	3:D:1472:ILE:HB	1.98	0.45	
3:D:1290:LEU:HD22	3:D:1290:LEU:HA	1.71	0.45	
1:B:188:GLN:CD	1:B:188:GLN:H	2.20	0.45	
2:C:425:PHE:CE2	3:D:1086:LEU:HD12	2.51	0.45	
2:C:937:ASP:OD1	2:C:939:ARG:HG2	2.16	0.45	
3:D:411:THR:HB	3:D:437:VAL:H	1.82	0.45	
5:F:154:LYS:O	5:F:158:GLU:HG3	2.16	0.45	
5:F:202:TYR:O	5:F:205:ARG:HG3	2.16	0.45	
2:C:99:GLN:OE1	2:C:101:ILE:HD11	2.16	0.45	
2:C:118:ILE:HG12	2:C:382:ILE:HD13	1.99	0.45	
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.64	0.45	
3:D:103:TRP:CZ2	3:D:1444:THR:HG22	2.52	0.45	
3:D:844:ALA:O	3:D:867:ARG:HB3	2.17	0.45	
3:D:1275:SER:OG	3:D:1294:VAL:HG21	2.16	0.45	
2:C:243:ARG:NH2	7:H:9:DG:O6	2.48	0.45	
2:C:838:LYS:HE3	3:D:741:ASP:O	2.16	0.45	
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.96	0.45	
7:H:17:DT:H2"	7:H:18:DC:H5'	1.99	0.45	
2:C:203:ASP:OD2	2:C:204:GLN:N	2.50	0.45	
2:C:356:ARG:HA	2:C:359:MET:HE2	1.99	0.45	
2:C:557:ARG:HG3	2:C:844:GLY:HA3	1.99	0.45	
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.52	0.45	
5:F:89:GLY:HA3	7:H:7:DG:C6	2.52	0.45	
1:A:57:TYR:CG	1:A:161:ARG:HD2	2.51	0.45	
2:C:260:LEU:O	2:C:261:ILE:HD12	2.17	0.45	
2:C:678:PRO:HA	2:C:683:ASN:HD22	1.82	0.45	
2:C:911:GLU:OE1	3:D:1062:ARG:NH1	2.50	0.45	
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.99	0.45	
2:C:150:PRO:HG3	2:C:322:VAL:HG11	1.99	0.44	
2:C:617:ASP:HB2	2:C:619:ARG:HG2	1.98	0.44	
3:D:15:PRO:0	3:D:19:ARG:HG3	2.18	0.44	
3:D:1342:GLU:CD	3:D:1342:GLU:H	2.21	0.44	
3:D:214:GLU:HB3	3:D:340:THR:HB	1.98	0.44	
2:C:775:ARG:HG3	2:C:780:GLU:O	2.18	0.44	
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.98	0.44	
4:E:14:ASP:OD2	4:E:14:ASP:N	2.50	0.44	
2:C:983:ILE:HG21	2:C:987:ILE:CD1	2.47	0.44	
2:C:290:LEU:O	2:C:301:GLU:HB2	2.17	0.44	
2:C:1001:VAL:CG1	3:D:630:VAL:HB	2.46	0.44	



A 4 1	A 4 0	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
3:D:172:PRO:HA	3:D:173:PRO:HD3	1.91	0.44	
3:D:236:TYR:CZ	3:D:242:LEU:HD12	2.52	0.44	
5:F:88:ILE:HG23	5:F:193:ARG:HG2	1.98	0.44	
1:A:201:THR:HG22	1:A:202:ASP:N	2.32	0.44	
2:C:194:VAL:HG22	2:C:221:LEU:HD23	1.99	0.44	
3:D:141:ILE:HD11	3:D:144:GLY:HA2	2.00	0.44	
2:C:683:ASN:HB3	2:C:872:ASN:ND2	2.25	0.44	
3:D:530:VAL:HG22	3:D:534:ARG:O	2.17	0.44	
3:D:658:LEU:HD11	3:D:674:ARG:HH11	1.83	0.44	
3:D:660:LYS:HD3	3:D:663:GLU:OE1	2.18	0.44	
3:D:29:PRO:HG3	3:D:549:ASN:OD1	2.17	0.44	
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.99	0.44	
3:D:1280:VAL:HG12	3:D:1295:GLU:O	2.17	0.44	
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.17	0.44	
1:A:94:LEU:HD21	1:A:97:VAL:HG23	1.99	0.43	
1:B:94:LEU:HD11	1:B:97:VAL:HG23	2.00	0.43	
1:B:206:THR:HG22	1:B:209:GLU:N	2.13	0.43	
2:C:281:LEU:HD11	2:C:306:THR:HG22	1.99	0.43	
2:C:676:ILE:HA	2:C:871:LEU:O	2.18	0.43	
2:C:858:MET:HE3	2:C:858:MET:HB2	1.84	0.43	
3:D:418:GLY:O	3:D:428:LYS:HD3	2.18	0.43	
3:D:1053:PHE:CE1	3:D:1072:ILE:HG23	2.52	0.43	
3:D:1386:ASP:CB	3:D:1412:LYS:HD2	2.48	0.43	
2:C:805:ARG:NH2	2:C:821:GLU:OE1	2.49	0.43	
3:D:171:LEU:HD22	3:D:390:PRO:HG2	1.99	0.43	
3:D:192:ALA:HB3	3:D:195:VAL:HB	2.01	0.43	
3:D:683:ILE:HG23	3:D:687:VAL:HG21	2.00	0.43	
3:D:827:ILE:O	3:D:833:GLU:HA	2.18	0.43	
7:H:21:DA:H5'	7:H:21:DA:H8	1.82	0.43	
2:C:757:GLY:HA2	2:C:789:SER:OG	2.18	0.43	
3:D:256:GLU:OE2	3:D:300:LYS:HE2	2.17	0.43	
3:D:553:ARG:HD2	3:D:570:GLU:OE2	2.17	0.43	
3:D:893:GLU:H	3:D:894:LYS:HZ3	1.65	0.43	
5:F:162:LYS:HB2	5:F:162:LYS:HE3	1.75	0.43	
2:C:144:PRO:HG2	2:C:165:LEU:HD23	2.00	0.43	
2:C:677:MET:HB3	2:C:987:ILE:HD13	1.99	0.43	
2:C:936:VAL:HG11	2:C:959:PRO:CB	2.46	0.43	
3:D:128:TYR:CZ	3:D:587:ARG:HD3	2.53	0.43	
3:D:988:ARG:HH22	3:D:1054:GLU:CD	2.22	0.43	
7:H:20:DG:H2"	7:H:21:DA:C8	2.54	0.43	
1:B:85:LEU:HG	1:B:87:VAL:HG23	1.99	0.43	



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



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
5:F:387:GLY:HA2	5:F:397:ILE:HD13	2.02	0.42	
1:A:39:PRO:HG3	1:B:39:PRO:CG	2.50	0.42	
1:A:97:VAL:HG12	1:A:99:LEU:HD12	2.01	0.42	
2:C:304:LEU:HB3	2:C:305:PRO:HD3	2.02	0.42	
3:D:236:TYR:H	3:D:319:ALA:HB3	1.84	0.42	
3:D:367:ILE:HB	3:D:377:VAL:HG12	2.01	0.42	
5:F:408:LEU:HD23	5:F:408:LEU:HA	1.83	0.42	
2:C:17:PRO:HB2	2:C:20:GLU:HB3	2.01	0.42	
2:C:482:GLU:HG3	2:C:482:GLU:O	2.20	0.42	
2:C:719:PRO:HB3	2:C:820:ARG:NE	2.34	0.42	
3:D:1065:LEU:HD23	3:D:1069:GLU:HB3	2.01	0.42	
1:A:36:LEU:HD23	1:A:36:LEU:HA	1.83	0.42	
2:C:83:CYS:HA	2:C:88:LEU:HB2	2.02	0.42	
2:C:540:PHE:HB3	2:C:544:THR:HB	2.02	0.42	
3:D:58:CYS:CB	3:D:76:CYS:SG	3.07	0.42	
1:A:64:GLU:HG2	1:A:76:VAL:HG22	2.02	0.42	
2:C:367:LEU:HA	2:C:371:LYS:HD2	2.01	0.42	
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	2.02	0.42	
1:A:228:PRO:HB3	1:B:13:VAL:CG2	2.48	0.41	
2:C:575:GLN:HG3	2:C:670:GLN:HA	2.01	0.41	
3:D:945:SER:OG	3:D:947:ILE:HG12	2.20	0.41	
5:F:80:PRO:HB2	5:F:210:LEU:HD11	2.01	0.41	
2:C:261:ILE:HG22	2:C:262:ALA:N	2.35	0.41	
3:D:462:GLN:HB2	3:D:513:ILE:HG21	2.02	0.41	
3:D:607:LEU:HA	3:D:607:LEU:HD23	1.79	0.41	
2:C:269:LEU:HB2	2:C:288:ARG:O	2.19	0.41	
2:C:792:VAL:HA	2:C:793:PRO:HD3	1.93	0.41	
3:D:876:SER:OG	3:D:879:ARG:HG3	2.20	0.41	
1:B:197:LEU:HD13	1:B:199:ILE:HD11	2.02	0.41	
2:C:355:VAL:O	2:C:359:MET:HG3	2.20	0.41	
2:C:561:GLY:O	2:C:565:GLN:HG3	2.20	0.41	
2:C:595:LEU:HD12	2:C:595:LEU:HA	1.89	0.41	
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.55	0.41	
3:D:97:THR:OG1	3:D:571:LYS:HE2	2.19	0.41	
3:D:566:ILE:HD11	5:F:192:LEU:HD21	2.03	0.41	
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.75	0.41	
2:C:170:PRO:HD2	2:C:267:TYR:CE1	2.55	0.41	
3:D:1014:ASN:OD1	3:D:1014:ASN:N	2.53	0.41	
2:C:15:LEU:HA	2:C:16:PRO:HD3	1.97	0.41	
2:C:1023:GLY:HA2	6:G:18:DA:OP2	2.21	0.41	
2:C:6:PHE:CE2	2:C:909:ALA:HB2	2.56	0.41	



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
2:C:351:LEU:HD12	2:C:375:SER:HA	2.03	0.41	
2:C:1101:THR:OG1	2:C:1109:VAL:O	2.39	0.41	
3:D:134:VAL:HG23	3:D:149:LYS:HA	2.03	0.41	
3:D:241:ILE:HG12	3:D:312:ARG:NH1	2.35	0.41	
3:D:983:LEU:HD13	3:D:988:ARG:HB2	2.03	0.41	
2:C:548:PRO:O	2:C:843:HIS:HE1	2.03	0.41	
1:B:115:LEU:HD23	1:B:115:LEU:HA	1.80	0.41	
2:C:1070:ILE:CG2	3:D:655:PRO:HB2	2.51	0.41	
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.87	0.41	
3:D:731:LEU:HD23	3:D:731:LEU:HA	1.77	0.41	
3:D:940:THR:O	3:D:943:THR:HG23	2.21	0.41	
3:D:949:ILE:HD11	3:D:1023:MET:CE	2.49	0.41	
3:D:1487:VAL:HG11	3:D:1492:LEU:HD23	2.03	0.41	
5:F:317:LEU:HD23	5:F:317:LEU:HA	1.85	0.41	
3:D:988:ARG:NH2	3:D:1054:GLU:OE2	2.53	0.41	
6:G:3:DT:H2"	6:G:4:DG:C8	2.56	0.41	
7:H:20:DG:H2"	7:H:21:DA:H5'	2.03	0.41	
2:C:598:GLU:HG3	2:C:623:TYR:OH	2.21	0.40	
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.56	0.40	
1:A:106:PRO:CG	1:A:134:GLU:HG2	2.51	0.40	
1:B:7:LYS:NZ	1:B:7:LYS:HB3	2.35	0.40	
2:C:118:ILE:HA	2:C:119:PRO:HD3	1.96	0.40	
3:D:154:THR:OG1	3:D:157:GLU:HG3	2.21	0.40	
3:D:586:ARG:HH11	3:D:586:ARG:HD3	1.70	0.40	
3:D:1197:ARG:HB2	3:D:1398:TRP:CZ2	2.56	0.40	
3:D:1493:LYS:HZ1	3:D:1496:GLU:HG3	1.86	0.40	
5:F:270:LYS:HE2	5:F:295:MET:HE2	2.03	0.40	
1:A:42:ARG:NH2	1:B:34:VAL:HG22	2.36	0.40	
2:C:181:VAL:HG23	2:C:220:GLY:O	2.22	0.40	
3:D:770:LEU:HB2	3:D:1210:SER:HA	2.03	0.40	
3:D:895:VAL:HG11	3:D:922:LEU:HD21	2.04	0.40	
3:D:961:LYS:HE3	3:D:961:LYS:HB2	1.86	0.40	
3:D:1208:ASP:OD1	3:D:1208:ASP:C	2.60	0.40	
5:F:393:THR:HG22	5:F:395:GLU:N	2.30	0.40	
1:A:111:ALA:HB3	1:A:125:PRO:HA	2.03	0.40	
3:D:850:LEU:HD23	3:D:850:LEU:HA	1.85	0.40	
3:D:999:THR:O	3:D:1003:VAL:HG13	2.21	0.40	
3:D:1106:VAL:O	3:D:1108:ARG:HG3	2.21	0.40	
3:D:1312:LEU:HD12	3:D:1324:PRO:HB2	2.03	0.40	
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.90	0.40	
2:C:954:THR:HG23	2:C:965:GLU:OE2	2.21	0.40	



2.57

Clash overlap (Å)

0.40

Continuea from previo	bus page	
Atom-1	Atom 2	Interatomic
	Atom-2	distance (Å)

3:D:1378:TYR:CZ

There are no symmetry-related clashes.

### 5.3 Torsion angles (i)

Continued former constructions of

3:D:1377:LYS:HE3

#### 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	Perce	ntiles
1	А	224/315~(71%)	222 (99%)	2(1%)	0	100	100
1	В	220/315~(70%)	215~(98%)	5 (2%)	0	100	100
2	С	1107/1119 (99%)	1084 (98%)	23~(2%)	0	100	100
3	D	1482/1524~(97%)	1457 (98%)	24 (2%)	1 (0%)	51	81
4	Е	92/99~(93%)	89 (97%)	2(2%)	1 (1%)	14	41
5	F	344/423~(81%)	341 (99%)	3 (1%)	0	100	100
All	All	3469/3795~(91%)	3408 (98%)	59 (2%)	2(0%)	51	81

All (2) Ramachandran outliers are listed below:

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

#### 5.3.2 Protein sidechains (i)

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

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



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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	199/273~(73%)	189~(95%)	10 (5%)	24	56
1	В	195/273~(71%)	186 (95%)	9~(5%)	27	60
2	С	936/941~(100%)	872 (93%)	64 (7%)	16	42
3	D	1253/1279~(98%)	1167 (93%)	86 (7%)	15	41
4	Ε	83/88~(94%)	82~(99%)	1 (1%)	71	92
5	F	301/371~(81%)	286~(95%)	15 (5%)	24	56
All	All	2967/3225~(92%)	2782 (94%)	185~(6%)	18	47

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

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



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



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



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



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

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

Mol	Chain	Res	Type
1	А	128	HIS
1	В	81	ASN
2	С	204	GLN
3	D	1195	GLN
3	D	1359	GLN
5	F	279	GLN



#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis. There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

#### 5.7 Other polymers (i)

There are no such residues in this entry.

### 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Fit of model and data (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,  $95^{th}$  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	$\mathbf{OWAB}(\mathbf{A}^2)$	Q < 0.9
1	А	226/315~(71%)	-0.51	1 (0%) 92 91	43, 64, 95, 117	0
1	В	222/315~(70%)	-0.35	4 (1%) 68 61	43, 76, 114, 141	0
2	С	1111/1119 (99%)	-0.34	20 (1%) 68 61	23, 56, 125, 169	0
3	D	1486/1524~(97%)	-0.16	47 (3%) 47 37	23, 64, 127, 154	0
4	Ε	94/99~(94%)	-0.53	0 100 100	31, 58, 96, 129	0
5	F	346/423~(81%)	-0.10	13 (3%) 40 30	38, 86, 133, 171	0
6	G	18/22~(81%)	0.03	0 100 100	46, 75, 164, 175	0
7	Н	22/27~(81%)	-0.06	2 (9%) 9 5	58, 91, 140, 171	0
All	All	3525/3844 (91%)	-0.25	87 (2%) 57 47	23, 65, 125, 175	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1128	VAL	5.4
3	D	1297	GLU	5.1
5	F	147	LEU	4.8
3	D	144	GLY	4.7
5	F	149	GLU	4.6
5	F	150	THR	4.5
5	F	148	LYS	4.3
3	D	422	ALA	4.3
2	С	296	GLY	3.9
2	С	219	GLN	3.8
3	D	406	ASP	3.7
3	D	1499	ARG	3.6
3	D	427	VAL	3.6
5	F	414	ARG	3.4
2	С	188	LYS	3.4
3	D	1287	GLU	3.4



5	V	Ο	Ι

Mol	Chain	Res	Type	RSRZ	
2	С	1	MET	3.3	
5	F	145	PRO	3.3	
2	С	295	ASP	3.3	
3	D	310	LEU	3.3	
5	F	141	VAL	3.1	
2	С	811	PRO	3.1	
2	С	365	ASP	3.0	
3	D	320	ALA	3.0	
1	А	187	GLY	3.0	
2	С	362	GLY	3.0	
2	С	104	ASP	3.0	
3	D	1497	GLU	2.9	
3	D	1502	ALA	2.9	
3	D	1500	LYS	2.8	
3	D	216	VAL	2.8	
1	В	188	GLN	2.7	
3	D	241	ILE	2.7	
3	D	1127	GLU	2.7	
3	D	197	SER	2.7	
3	D	350	HIS	2.6	
2	С	203	ASP	2.6	
3	D	360	ARG	2.6	
2	С	293	PHE	2.6	
3	D	1129	THR	2.6	
3	D	404	GLU	2.5	
7	Н	24	DC	2.5	
5	F	146	GLY	2.5	
5	F	423	ASP	2.5	
2	С	232	GLU	2.5	
2	С	249	LYS	2.5	
3	D	345	TYR	2.5	
7	H	25	DA	2.4	
1	В	189	ARG	2.4	
1	В	190	THR	2.4	
3	D	362	GLU	2.4	
3	D	193	PRO	2.4	
1	В	93	SER	2.4	
5	F	153	PRO	2.4	
2	С	103	LYS	2.4	
3	D	1126	ASP	2.3	
3	D	174	GLY	2.3	
3	D	165	LYS	2.3	



Mol	Chain	Res	Type	RSRZ	
3	D	976	GLN	2.3	
3	D	1501	GLU	2.3	
3	D	1299	PHE	2.3	
3	D	1281	VAL	2.2	
3	D	175	VAL	2.2	
5	F	142	ARG	2.2	
3	D	1315	ASP	2.2	
3	D	1283	ILE	2.2	
3	D	380	GLU	2.2	
5	F	377	ASP	2.2	
3	D	1130	ARG	2.2	
2	С	775	ARG	2.2	
3	D	1284	GLU	2.2	
3	D	346	ARG	2.2	
3	D	1282	ARG	2.2	
2	С	247	PRO	2.2	
3	D	384	VAL	2.2	
2	С	764	GLU	2.1	
3	D	201	GLY	2.1	
3	D	316	GLN	2.1	
3	D	372	ASP	2.1	
2	С	766	GLU	2.1	
3	D	1292	VAL	2.1	
5	F	297	PRO	2.1	
2	С	254	VAL	2.1	
3	D	191	LEU	2.1	
2	С	194	VAL	2.1	
3	D	363	ALA	2.0	
3	D	429	SER	2.0	

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### 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 monosaccharides 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,  $95^{th}$  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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
9	MG	G	101	1/1	0.86	0.58	91,91,91,91	0
9	MG	D	2004	1/1	0.93	0.48	52,52,52,52	0
8	ZN	D	2002	1/1	0.94	0.33	238,238,238,238	0
9	MG	D	2003	1/1	0.97	0.19	44,44,44,44	0
8	ZN	D	2001	1/1	0.98	0.18	77,77,77,77	0

### 6.5 Other polymers (i)

There are no such residues in this entry.

