

Full wwPDB X-ray Structure Validation Report (i)

Sep 6, 2023 – 02:09 PM EDT

PDB ID	:	4GZY
Title	:	Crystal structures of bacterial RNA Polymerase paused elongation complexes
Authors	:	Weixlbaumer, A.; Leon, K.; Landick, R.; Darst, S.A.
Deposited on	:	2012-09-06
Resolution	:	3.51 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
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 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 3.51 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))
Berry	130704	1659 (3 60-3 40)
Clashgeoro	1/161/	$\frac{1036}{1026} \left(2.58 \ 2.42 \right)$
Clashscore	141014	1030 (3.36-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559(3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

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	Quali	ty of chain		
1	А	315	43%	25%	•	29%
1	В	315	48%	22%	•	29%
2	С	1119	^{2%} 54%		38%	•••
3	D	1534	4% 51%	3	3%	• 11%



Mol	Chain	Length			Qu	ality of chain			
4	Е	99	5%		55%		31%	8%	6%
					69%		_	0,0	0,0
5	Ν	13			69%		15%	15%	
6	R	29	3% 10%	17%	•	69%			
7	Т	22		27%	64%		36%		_



4GZY

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 24400 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	<u> </u>	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	A	223	1759	1123	306	328	2	0	0	0
1	р	002	Total	С	Ν	0	S	0	0	0
	D	223	1759	1123	306	328	2	0	0	0

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

Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace
2	С	1083	Total 8548	C 5412	N 1524	O 1588	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	1358	Total 10714	C 6780	N 1900	O 2001	S 33	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1525	HIS	-	expression tag	UNP Q8RQE8
D	1526	HIS	-	expression tag	UNP Q8RQE8
D	1527	HIS	-	expression tag	UNP Q8RQE8
D	1528	HIS	-	expression tag	UNP Q8RQE8
D	1529	HIS	-	expression tag	UNP Q8RQE8
D	1530	HIS	-	expression tag	UNP Q8RQE8
D	1531	HIS	-	expression tag	UNP Q8RQE8
D	1532	HIS	-	expression tag	UNP Q8RQE8
D	1533	HIS	-	expression tag	UNP Q8RQE8
D	1534	HIS	-	expression tag	UNP Q8RQE8

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



Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
4	Е	93	Total 754	C 481	N 131	O 138	S 4	0	0	0

• Molecule 5 is a DNA chain called non-template DNA.

Mol	Chain	Residues		Ate	\mathbf{oms}			ZeroOcc	AltConf	Trace
Б	N	11	Total	С	Ν	Ο	Р	0	0	0
5		11	225	107	43	64	11	0	0	0

• Molecule 6 is a RNA chain called RNA transcript.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
6	R	9	Total 191	C 85	N 31	O 66	Р 9	0	0	0

• Molecule 7 is a DNA chain called template DNA.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
7	Т	22	Total 447	C 213	N 81	0 131	Р 22	0	0	0

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	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



54%



38%



4% Chain D: 51% 33% 11% .



MET	24 1	K/	K17 I18	G24	BC N	P29	E30 T31	132	L37	K38 D30	E40	R41 D42	G43	L44 F45	D46	149	F50	P52	153 K54	D55	Y56 E57	C58	C60	G61 K62	Y 63 K 64	R65	R67	F68	G70 K71	V72	C73 E74	R75	V78 E79	V80 T81 K82
284	R87	188 R89	193	A96		H101	1102 W103	F104	V108	P109	K111	1112 6113	T114	L115 L116	0	S119	L123 E124	1 770	L127 V128	F129	S130 K131	Y132 1133	V134	L135 D136	P137 K138	G139	L142	P146	V147 F148	K149	R150 Q151	L152 L153	T154	E157 E160
VIGS	G164	K165 Q166	E167 T168	Y169 P170	L171 D170		V175 D176	A177	L1/8 V179		6102 E183	E184	K187	L191	A192	P193 G194	V195	R198	L199 D200	G201	V202 A203	L204 V205		R209 R210	V211 R212	V213	F215	V216 LYS	LYS	ARG	ALA GLY	ARG	LEU PRO	LEU ALA ALA
TRP VAI	GLU	GLU	ALA TYR	LYS PRO	GLY	ILE	LEU ALA	GLU	LEU PRO	GLU	TYR	LEU	ARG	ALA GLU	GLU	GLY	VAL	GLU	LEU	GLU	GLU	GLU	ALA	PHE	VAL LEU	ARG	GLU	ASP GLU	PRO VAL	ALA	THR TYR	PHE	PRO VAL	GLY MET THR
PRO 1 EII	VAL	VAL HIS	GLU GLU	ILE VAL	GLU	GLY	GLN PRO	LEU	GLU	ALA	GLY	LEU	ARG	MET PRO	ARG	GLN VAL	ARG	ALA	GLN VAT.	GLU	GLU	GLU GLU	GLY	GLU THR	VAL TYR	LEU	TEU	PHE LEU	GLU TRP	T340	E341 P342	K343 D344	Y345 R346	V347 Q348 P349
H350	N352	V 353 V 354	V355 P356	A359	ц 1360	A363	G364 D365	K366	1367 V368	A369	I371	D372	E374	V377	1378	A379	E382	V384	V385	H388	E389 P390	A391 S392	1393	L394 V395	V396 K397	11 100		D405 D406	V407 F408		R414 V415	A416 P417	G418 D419	<mark>V420</mark> L421
G425 KA 26	V427	D430	V431 Y432	G433 R434	V435	R441	V447		7450 D451	1452 D/162	0454 A454	<u>4458</u>		I461	L473	L477	11 11 11 11 11 11 11 11 11 11 11 11 11	m481	K482 H483	P484	S485 R486	A487 R488	R489	K494	R495	V499 PEOO	A501	S505	FE 10	W511	M512 1513	V517	P518 V519	L520 P521 P522
р С J C J C J C J C J C J C J C J C J C J		0532 6532	G533	D539 L540	N541	L543	1548	N549	099N	R553	L004 K555	K556 1.667	L558	A559 Q560	G561	A562 P563	E564	1566 1566	1567 8568	N569	E570 K571	R572 M573	L574	0575	L581 L582	D583 ME84	1004	P590	P594 6595		L600 R601	S602 L603	T604 D605	1606 1607 8608
D613	F614	4615 Q616	N617	K621	D624 Vene	0701	R628 S629	V630	L637	0641	4041 C642	G643 1644	P645	K646 R647	M648	A649 L650	DOED		L658 K659	K660	M661	T677	1683	E686	A690	L691 E603	E693	V694 1695	H696	N7 00	L701 L702	N7 03 R7 04	A7 05	L708 H709 <mark>R710</mark>
L711	Q714	A/15 F716	Q717 P718	V719 L720	V721 E723	G723	0724 8725	1726	nr21	E734	A (33	D739 F740	D741	G742 D743	Q744	M745 A746	V747 174 0	n 140 V749	P750 1.751		F754 A755	0756 4757	E758	A759 R760	I761 0762	M763	L/04 S765	A766 H767	N768 1.769	L770	P777	K780	R783	D784 I785 I786
1707	1793	R796	K797 E798	K7 99 K800	G801	G803	L804 E805	F806	A807 T808	P809	E811	A812 1813	A814	A815 H816	E817	E820	V821	A022 L823	N824 ARD5	P826	1827 K828	V829 4830	G831	R832 E833	T834 S835	V836	V842	A849	L850	A852	V853	1857	L860 Q861	V864 T865
B 870	NOI 2	1/84	1880 L881	D892	WROF		K908	0917	A918 F919	L920	L922	T007	1701	K935	F939	1940 F941	S942	0561	T948 1949	G950	1951	V955 T956		K960	Y963 L964	E965 E066	E300 A967	D968 R969	K970 1.971		E975	Y978 E979	L983	T984 D985
R988	(1991	L995	N996	E1001 K1002	V1003		V1007 F1008		F1011 E1012	E1013	N1018	V1001	17011	G1027 A1028	R1029	G1030 N1031	P1032	41033 Q1034	11035 B1036	q 1037	L1038 C1039	G1040 L1041	R1042	G1043 L1044	V1055	P1056	R1058	E1063	E1060	Y1070	S1074	A1077	R1078 K1079	D1083
L1086	100 TVI	S1091	R1096	V1106	V1107 D1108	E1109	C1112		91111	1118 1118	ATTO	F1123	P1125	V1128	T1129	K1130 S1131	L1132	L1134	R1135 K1136		D1139 11140	G1 146	R1147	R1151	V1155	L1156	E1161	E1162 G1163	R1164 V1165		D1170		11183 Q1184	E1185
R1189	Q1195	R1196 R1197	Y1198 G1199	V1200	C1204 V1205	G1206	Y1207 D1208	L1209	S1210 M1211	A1212 B1212	C171V	G1218 F1219	A1220	P1232		41235 L1236	THR	ARG	THR PHE	HIS	THR GLY	GLY VAL	ALA	GLY ALA	ALA ASP	ILE	инк Q1254	R1258	F1 OG1	L1262	F1263 E1264	R1267	P1268 K1269	V1273







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	207.21Å 207.21Å 203.22Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	49.77 - 3.51	Depositor
Resolution (A)	49.77 - 3.51	EDS
% Data completeness	99.7 (49.77-3.51)	Depositor
(in resolution range)	87.9(49.77-3.51)	EDS
R _{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.76 (at 3.48 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.8_1069, CNS	Depositor
D D.	0.263 , 0.322	Depositor
Π, Π_{free}	0.266 , 0.324	DCC
R_{free} test set	3199 reflections $(5.04%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	95.9	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.27, 55.2	EDS
L-test for twinning ²	$< L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	24400	wwPDB-VP
Average B, all atoms $(Å^2)$	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.70% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities 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: ZN, MG

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

Mal	Chain	Bond	lengths	Bo	ond angles
MIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.28	0/1791	0.49	0/2436
1	В	0.29	0/1791	0.48	0/2436
2	С	0.30	0/8711	0.52	1/11784~(0.0%)
3	D	0.30	0/10897	0.50	1/14726~(0.0%)
4	Е	0.29	0/768	0.54	0/1035
5	N	0.43	0/252	1.11	0/386
6	R	0.22	0/212	0.77	0/328
7	Т	0.43	0/500	1.09	0/768
All	All	0.30	0/24922	0.54	2/33899~(0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	D	705	ALA	C-N-CD	5.90	140.78	128.40
2	С	853	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1759	0	1805	59	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	В	1759	0	1805	53	0
2	С	8548	0	8650	377	0
3	D	10714	0	10936	395	0
4	Е	754	0	769	24	0
5	Ν	225	0	124	1	0
6	R	191	0	95	7	0
7	Т	447	0	248	6	0
8	D	2	0	0	0	0
9	D	1	0	0	0	0
All	All	24400	0	24432	851	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 17.

All (851) 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)
2:C:610:ARG:HG3	2:C:610:ARG:HH11	1.16	1.08
3:D:346:ARG:NH1	3:D:347:VAL:O	1.89	1.05
2:C:405:ARG:NH1	2:C:442:GLU:OE2	1.90	1.04
2:C:274:ARG:NH1	2:C:284:ARG:HH12	1.54	1.03
3:D:550:ARG:HH11	3:D:573:MET:HB3	1.25	0.98
4:E:39:VAL:O	4:E:72:ARG:NH1	1.98	0.96
2:C:194:VAL:HG21	2:C:224:GLU:HG3	1.49	0.94
2:C:714:ASP:OD1	2:C:820:ARG:NH1	2.02	0.92
2:C:978:ARG:HG3	2:C:978:ARG:HH11	1.34	0.91
2:C:274:ARG:HH12	2:C:284:ARG:NH1	1.66	0.91
2:C:274:ARG:HH12	2:C:284:ARG:HH12	1.13	0.90
2:C:829:GLN:HE21	2:C:831:ARG:HH11	1.17	0.87
2:C:1103:ASP:HB3	2:C:1105:LYS:HZ1	1.40	0.86
3:D:1198:TYR:OH	3:D:1432:LYS:NZ	2.09	0.86
3:D:1106:VAL:HG12	3:D:1220:ALA:HA	1.57	0.83
2:C:290:LEU:HD11	2:C:301:GLU:H	1.43	0.82
2:C:239:PHE:HB2	2:C:251:ASP:HB3	1.62	0.81
3:D:486:ARG:HH21	3:D:489:ARG:HH11	1.29	0.80
1:B:56:VAL:HG21	1:B:82:LEU:HD13	1.63	0.80
1:B:91:ASN:ND2	1:B:119:ASP:OD2	2.14	0.80
2:C:512:ARG:HB3	2:C:523:ILE:HD11	1.64	0.80
2:C:288:ARG:H	2:C:288:ARG:HH11	1.30	0.79
3:D:1108:ARG:HH22	3:D:1460:ILE:HD11	1.47	0.79
1:B:188:GLN:O	3:D:646:LYS:NZ	2.14	0.78



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:738:ASP:HB2	2:C:744:ARG:HB3	1.66	0.78
3:D:770:LEU:HD12	3:D:1211:MET:HA	1.64	0.78
3:D:135:LEU:HD23	3:D:148:GLU:HB2	1.64	0.77
2:C:274:ARG:HH12	2:C:284:ARG:NH2	1.82	0.77
2:C:224:GLU:HB3	2:C:227:PHE:HB3	1.67	0.77
2:C:212:GLY:HA2	2:C:218:VAL:HG21	1.65	0.77
2:C:274:ARG:HH12	2:C:284:ARG:CZ	1.96	0.77
2:C:309:TYR:CZ	2:C:321:GLU:HB3	2.20	0.77
2:C:272:ALA:HB1	2:C:276:LYS:HZ1	1.50	0.76
3:D:1486:VAL:HG11	4:E:22:VAL:HG13	1.67	0.76
3:D:501:ALA:O	3:D:505:SER:OG	2.02	0.76
3:D:557:LEU:HD21	3:D:566:ILE:HG22	1.68	0.76
2:C:274:ARG:NH1	2:C:284:ARG:NH1	2.29	0.76
2:C:334:ARG:HH12	2:C:415:PRO:HG2	1.48	0.76
4:E:54:LEU:HG	4:E:58:PRO:HG2	1.66	0.75
2:C:1103:ASP:HB3	2:C:1105:LYS:NZ	2.01	0.75
2:C:274:ARG:HH21	2:C:278:GLU:HB2	1.51	0.74
2:C:437:ARG:NH1	2:C:491:GLU:OE1	2.14	0.74
3:D:700:VAL:HG12	3:D:749:VAL:HG12	1.70	0.74
3:D:960:LYS:NZ	3:D:1063:GLU:OE2	2.19	0.74
2:C:1008:ARG:HD2	2:C:1026:GLN:HB3	1.68	0.74
1:B:79:ILE:HA	1:B:82:LEU:HD12	1.68	0.74
2:C:584:GLU:HB3	2:C:666:LEU:H	1.52	0.74
2:C:274:ARG:HH12	2:C:284:ARG:HH22	1.35	0.74
3:D:983:LEU:HD13	3:D:988:ARG:HB2	1.69	0.74
2:C:185:LYS:HG2	2:C:190:LYS:HG2	1.67	0.73
2:C:462:ASP:OD2	2:C:468:ARG:NH1	2.17	0.73
2:C:205:GLU:HB2	2:C:209:ARG:HH12	1.54	0.73
3:D:213:VAL:HG11	3:D:385:VAL:HA	1.70	0.73
2:C:1105:LYS:HZ2	2:C:1105:LYS:H	1.35	0.73
4:E:46:PRO:HG3	4:E:66:LYS:HD3	1.71	0.72
1:A:58:ILE:HB	1:A:61:VAL:HB	1.71	0.72
2:C:204:GLN:NE2	2:C:222:MET:O	2.22	0.72
3:D:1147:ARG:HD3	3:D:1188:VAL:HG21	1.71	0.72
1:A:112:ARG:NH2	1:A:126:ASP:OD1	2.23	0.72
1:B:90:LEU:HB2	1:B:119:ASP:HB3	1.72	0.71
1:A:80:LEU:HD21	2:C:573:ARG:HH11	1.55	0.71
2:C:224:GLU:O	2:C:228:ALA:N	2.24	0.71
2:C:710:ILE:HD11	2:C:758:ARG:HH21	1.55	0.71
2:C:755:LEU:HD11	2:C:825:VAL:HG11	1.73	0.71
1:A:182:GLU:HB2	1:A:194:LYS:HD3	1.72	0.70



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:D:1273:VAL:HG12	3:D:1274:ILE:H	1.56	0.70
2:C:332:ARG:NH2	2:C:338:GLU:OE1	2.25	0.70
2:C:1005:MET:HB2	3:D:724:GLN:HE22	1.56	0.70
2:C:734:LEU:HG	2:C:737:LEU:HD12	1.73	0.70
3:D:362:GLU:O	3:D:364:GLY:N	2.23	0.70
1:B:185:ARG:NH1	3:D:692:GLU:OE1	2.24	0.70
2:C:610:ARG:HG3	2:C:610:ARG:NH1	1.90	0.70
3:D:1161:GLU:HB2	3:D:1164:ARG:HB2	1.74	0.69
3:D:1418:LYS:HD3	3:D:1419:PRO:HD2	1.74	0.69
3:D:112:ILE:HD11	3:D:461:ILE:HG21	1.73	0.69
3:D:136:ASP:HB2	3:D:137:PRO:HD2	1.74	0.69
1:A:104:GLU:OE1	1:A:137:ARG:NH1	2.25	0.69
4:E:40:LEU:HD21	4:E:67:GLU:HA	1.74	0.69
3:D:550:ARG:NH1	3:D:573:MET:HB3	2.03	0.69
2:C:442:GLU:HG2	2:C:454:SER:HB2	1.75	0.69
3:D:111:LYS:HD2	3:D:1452:ILE:HD13	1.73	0.69
3:D:133:ILE:HG23	3:D:454:ALA:HB1	1.75	0.69
3:D:501:ALA:HB1	3:D:1453:ALA:HB2	1.75	0.69
2:C:302:VAL:O	2:C:306:THR:OG1	2.11	0.68
3:D:691:LEU:HD23	3:D:720:LEU:HD21	1.74	0.68
3:D:1267:ARG:NH2	3:D:1331:ASP:OD2	2.25	0.68
2:C:670:GLN:NE2	2:C:699:PHE:O	2.27	0.68
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.75	0.68
2:C:829:GLN:NE2	2:C:831:ARG:HH11	1.89	0.68
3:D:486:ARG:HE	3:D:489:ARG:HD2	1.58	0.68
3:D:154:THR:HG23	3:D:157:GLU:H	1.59	0.67
3:D:1283:ILE:HD11	3:D:1290:LEU:HD12	1.76	0.67
2:C:978:ARG:HH11	2:C:978:ARG:CG	2.06	0.67
2:C:726:ILE:HD13	2:C:754:ILE:HD13	1.76	0.67
3:D:525:ARG:NH1	3:D:541:ASN:OD1	2.26	0.67
3:D:798:GLU:HB2	3:D:828:LYS:HE3	1.75	0.67
2:C:89:THR:HG22	2:C:129:ILE:HA	1.76	0.67
2:C:292:ARG:HB3	2:C:299:LYS:HB3	1.76	0.67
2:C:260:LEU:HD22	2:C:288:ARG:HH22	1.59	0.67
2:C:292:ARG:HG2	2:C:299:LYS:HE3	1.77	0.67
2:C:292:ARG:NH1	2:C:294:GLU:HB2	2.10	0.67
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.77	0.67
1:A:54:THR:HG21	1:A:158:ILE:HD12	1.77	0.66
1:B:101:LEU:HD21	1:B:109:VAL:HG11	1.77	0.66
1:A:67:THR:HG21	2:C:609:ASN:HD21	1.60	0.66
2:C:274:ARG:NH1	2:C:284:ARG:HH22	1.93	0.66



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:D:1453:ALA:O	3:D:1455:LYS:N	2.29	0.66
3:D:114:THR:O	3:D:495:ARG:NH1	2.29	0.66
2:C:267:TYR:HB2	2:C:272:ALA:HB3	1.78	0.65
2:C:388:ARG:NH1	7:T:22:DT:OP1	2.29	0.65
2:C:829:GLN:HE21	2:C:831:ARG:NH1	1.91	0.65
2:C:808:ARG:HD3	2:C:820:ARG:HD2	1.78	0.65
2:C:56:GLU:HA	2:C:356:ARG:HH12	1.61	0.65
2:C:292:ARG:HG3	2:C:292:ARG:HH11	1.62	0.65
3:D:1495:ILE:HG23	4:E:84:ARG:HD3	1.78	0.65
2:C:1031:ARG:HB3	7:T:16:DC:OP1	1.97	0.65
2:C:144:PRO:HA	2:C:163:ILE:HG23	1.79	0.64
2:C:953:VAL:HG13	2:C:966:LEU:HD13	1.78	0.64
2:C:1008:ARG:HH12	2:C:1011:GLY:N	1.95	0.64
2:C:1008:ARG:NH2	3:D:624:ASP:OD1	2.30	0.64
2:C:230:ARG:HB3	2:C:233:GLU:HB2	1.79	0.64
2:C:720:GLU:O	2:C:820:ARG:NH2	2.31	0.64
3:D:165:LYS:HE3	3:D:200:ASP:HB2	1.80	0.64
2:C:48:PHE:HB3	2:C:52:PHE:HD2	1.63	0.64
2:C:428:ARG:NH1	3:D:1086:LEU:HD11	2.12	0.64
3:D:18:ILE:HG23	3:D:518:PRO:HG3	1.78	0.64
3:D:808:THR:H	3:D:809:PRO:HD2	1.63	0.64
3:D:629:SER:HB3	3:D:726:ILE:HG12	1.79	0.63
2:C:292:ARG:HH12	2:C:294:GLU:HB2	1.63	0.63
3:D:100:ALA:HB2	3:D:513:ILE:HG13	1.81	0.63
3:D:813:LEU:HD12	3:D:814:ALA:H	1.64	0.63
2:C:205:GLU:HB2	2:C:209:ARG:NH1	2.14	0.63
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.81	0.63
2:C:680:ASP:H	3:D:943:THR:HG21	1.63	0.62
2:C:845:ASN:HD22	2:C:884:GLN:HE22	1.46	0.62
1:A:221:HIS:HB3	1:B:36:LEU:HD11	1.81	0.62
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.82	0.62
2:C:395:LYS:HD3	2:C:397:GLU:OE2	1.99	0.62
1:A:70:GLY:HA2	1:A:133:GLU:HB3	1.80	0.62
2:C:473:ARG:HA	2:C:531:PHE:HA	1.82	0.62
3:D:148:GLU:HB3	3:D:151:GLN:HB2	1.80	0.62
3:D:1296:SER:HB3	3:D:1299:PHE:HD2	1.64	0.62
3:D:368:VAL:HB	3:D:377:VAL:HG12	1.81	0.62
3:D:764:LEU:O	3:D:768:ASN:ND2	2.32	0.62
4:E:38:THR:HG23	4:E:41:GLU:HG2	1.80	0.62
1:A:85:LEU:HA	1:A:124:ASN:HD22	1.63	0.62
2:C:146:VAL:HG22	2:C:162:ILE:HG12	1.82	0.61



	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:290:LEU:HD21	2:C:300:ASP:HB2	1.83	0.61
1:B:216:GLU:OE2	1:B:219:ARG:NH2	2.32	0.61
2:C:336:VAL:HA	2:C:339:LEU:HD12	1.82	0.61
3:D:1273:VAL:HG21	3:D:1305:LEU:HD12	1.82	0.61
3:D:553:ARG:NH2	3:D:570:GLU:OE2	2.34	0.61
2:C:428:ARG:HB3	2:C:450:GLY:HA3	1.82	0.61
3:D:808:THR:H	3:D:809:PRO:CD	2.13	0.61
2:C:22:GLN:HG3	2:C:407:LYS:HB3	1.82	0.61
2:C:384:GLU:HA	2:C:388:ARG:HH21	1.66	0.61
3:D:477:LEU:HA	3:D:480:GLU:HB3	1.82	0.61
3:D:1174:LEU:HD22	3:D:1183:ILE:HD11	1.83	0.61
1:B:175:ARG:N	1:B:200:TRP:O	2.33	0.61
3:D:1274:ILE:HG21	3:D:1334:GLN:HB3	1.83	0.61
2:C:326:ASP:HB2	2:C:331:ARG:NH1	2.16	0.61
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.82	0.61
3:D:1057:VAL:HG13	3:D:1069:GLU:HB3	1.83	0.60
1:A:176:ARG:NH2	2:C:863:ASP:OD1	2.34	0.60
2:C:185:LYS:NZ	2:C:190:LYS:HE2	2.16	0.60
2:C:437:ARG:HD3	2:C:467:ILE:HB	1.82	0.60
2:C:642:ARG:NE	2:C:657:ASP:OD2	2.35	0.60
2:C:1008:ARG:HH12	2:C:1010:THR:C	2.05	0.60
3:D:1319:VAL:HG23	3:D:1323:GLN:HE21	1.67	0.60
3:D:852:ALA:HB1	3:D:857:ILE:HD11	1.83	0.60
2:C:292:ARG:NH1	2:C:292:ARG:HG3	2.17	0.60
1:A:108:GLU:HG2	1:A:131:THR:HG22	1.84	0.59
2:C:987:ILE:HA	3:D:948:THR:HG21	1.83	0.59
2:C:7:GLY:HA3	2:C:904:PRO:HG2	1.85	0.59
1:A:151:VAL:HB	1:A:169:ALA:HB3	1.85	0.59
2:C:540:PHE:O	2:C:545:ASN:ND2	2.36	0.59
2:C:787:ASP:OD1	2:C:791:ARG:NH2	2.35	0.59
2:C:824:ARG:NH2	2:C:826:TYR:OH	2.35	0.59
3:D:164:GLY:HA3	3:D:397:LYS:HE3	1.85	0.59
3:D:629:SER:OG	3:D:630:VAL:N	2.34	0.59
3:D:1108:ARG:HH12	3:D:1460:ILE:CG1	2.16	0.59
2:C:744:ARG:HG3	2:C:747:ALA:HB2	1.84	0.59
2:C:971:LYS:HA	2:C:988:VAL:HA	1.85	0.58
3:D:734:GLU:OE2	3:D:780:LYS:NZ	2.32	0.58
3:D:1258:ARG:NH1	3:D:1262:LEU:HD11	2.17	0.58
2:C:101:ILE:HD12	2:C:107:LEU:HD22	1.86	0.58
3:D:820:GLU:HB2	3:D:836:VAL:HG21	1.86	0.58
1:A:71:VAL:HG11	1:A:78:ILE:HD11	1.84	0.58



	t i i i i i i i i i i i i i i i i i i i	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:D:135:LEU:HD22	3:D:153:LEU:HD23	1.85	0.58
2:C:115:LEU:HA	2:C:375:SER:HB2	1.85	0.58
2:C:674:VAL:HG22	2:C:869:VAL:HB	1.86	0.58
2:C:1009:SER:HA	3:D:625:TYR:HA	1.86	0.58
3:D:32:ILE:HG21	3:D:37:LEU:HD13	1.86	0.58
2:C:863:ASP:OD1	2:C:864:GLY:N	2.37	0.58
1:A:7:LYS:HD3	1:A:186:LEU:HD22	1.86	0.57
2:C:324:ASP:O	2:C:330:ASN:ND2	2.32	0.57
6:R:22:U:H2'	6:R:23:G:C8	2.39	0.57
2:C:122:THR:HB	2:C:124:ASP:OD2	2.04	0.57
2:C:145:GLY:H	2:C:163:ILE:HG23	1.69	0.57
2:C:64:LEU:HD13	2:C:359:MET:SD	2.44	0.57
2:C:1082:PRO:HB2	2:C:1085:PHE:HB3	1.86	0.57
2:C:158:TYR:HD1	2:C:314:THR:HG22	1.69	0.57
2:C:193:LEU:HD21	2:C:307:LEU:HD21	1.87	0.57
3:D:210:ARG:HB3	3:D:388:HIS:HB2	1.85	0.57
2:C:246:ASP:OD1	2:C:246:ASP:N	2.38	0.57
2:C:576:ALA:N	2:C:662:GLU:OE1	2.37	0.57
3:D:860:LEU:HD23	3:D:877:PRO:HB2	1.87	0.57
4:E:27:ALA:HB1	4:E:60:ALA:HB1	1.87	0.57
2:C:243:ARG:HE	2:C:254:VAL:HG21	1.70	0.56
2:C:1008:ARG:HH21	2:C:1020:PRO:HB3	1.69	0.56
2:C:1008:ARG:HD3	2:C:1028:GLY:H	1.70	0.56
3:D:169:TYR:HB3	3:D:195:VAL:HG11	1.85	0.56
2:C:1050:GLN:HG3	3:D:1469:GLY:O	2.05	0.56
2:C:111:ASP:HB3	2:C:112:GLU:OE2	2.05	0.56
2:C:1051:GLU:HG3	2:C:1055:LEU:HD23	1.87	0.56
3:D:1458:GLU:O	3:D:1460:ILE:HG22	2.05	0.56
2:C:284:ARG:HG3	2:C:285:LEU:N	2.21	0.56
3:D:1283:ILE:HD13	3:D:1311:LEU:HD22	1.87	0.56
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.86	0.56
3:D:978:TYR:HB2	3:D:988:ARG:HD3	1.86	0.56
3:D:1289:LYS:HZ3	3:D:1304:LYS:HB2	1.70	0.56
1:A:59:GLU:HB2	1:A:139:ASN:HB3	1.88	0.56
3:D:1165:TYR:HB3	3:D:1207:TYR:HE1	1.70	0.55
3:D:1289:LYS:NZ	3:D:1304:LYS:HB2	2.21	0.55
2:C:194:VAL:HG12	2:C:221:LEU:HB2	1.86	0.55
1:A:132:LEU:HD21	1:A:138:LEU:HD23	1.89	0.55
3:D:96:ALA:HB2	3:D:555:LYS:HG3	1.86	0.55
3:D:1281:VAL:HG11	3:D:1313:VAL:HG22	1.89	0.55
2:C:54:ILE:HG22	2:C:66:LEU:HD23	1.89	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:537:LYS:HG2	2:C:905:ILE:HG12	1.89	0.55
2:C:846:LYS:NZ	6:R:29:U:OP1	2.35	0.55
3:D:827:ILE:HG23	3:D:828:LYS:HG3	1.89	0.55
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.87	0.55
1:A:25:LEU:HD23	1:A:28:LEU:HD11	1.88	0.55
2:C:1105:LYS:HZ2	2:C:1105:LYS:N	2.03	0.55
3:D:53:ILE:HA	3:D:86:ARG:HD3	1.89	0.55
2:C:462:ASP:O	2:C:464:LEU:N	2.38	0.55
2:C:571:LEU:HD13	2:C:670:GLN:HE21	1.72	0.55
3:D:616:GLN:OE1	3:D:621:LYS:NZ	2.38	0.55
1:B:32:PHE:HA	1:B:35:THR:HB	1.89	0.55
2:C:140:ILE:HG12	2:C:333:ILE:HG12	1.89	0.55
2:C:468:ARG:HB3	2:C:485:TYR:HB3	1.88	0.55
3:D:119:SER:HB2	3:D:123:LEU:HB2	1.89	0.55
3:D:165:LYS:HG2	3:D:199:LEU:HB3	1.88	0.55
3:D:1379:VAL:HG12	3:D:1419:PRO:HA	1.89	0.55
3:D:660:LYS:HG3	3:D:694:VAL:HG12	1.89	0.55
3:D:770:LEU:HD23	3:D:777:PRO:HA	1.89	0.55
3:D:130:SER:OG	3:D:131:LYS:N	2.40	0.54
1:B:76:VAL:HG13	3:D:872:ARG:HH21	1.72	0.54
2:C:2:GLU:HG3	2:C:899:GLN:HB3	1.88	0.54
3:D:1128:VAL:HG12	3:D:1129:THR:H	1.72	0.54
3:D:1286:THR:OG1	3:D:1287:GLU:N	2.39	0.54
3:D:187:LYS:HG3	3:D:199:LEU:HA	1.88	0.54
1:B:163:ASN:OD1	1:B:163:ASN:N	2.41	0.54
3:D:1282:ARG:HB2	3:D:1293:PHE:O	2.06	0.54
1:B:86:VAL:HG21	1:B:204:SER:HB2	1.90	0.54
1:B:149:GLY:HA2	1:B:172:SER:HB2	1.90	0.54
2:C:52:PHE:HE1	2:C:98:LEU:HD13	1.72	0.54
2:C:54:ILE:CG2	2:C:66:LEU:HD23	2.37	0.54
3:D:345:TYR:CZ	3:D:377:VAL:HB	2.43	0.54
3:D:1283:ILE:HG13	3:D:1292:VAL:HG22	1.90	0.54
6:R:26:U:H2'	6:R:27:G:C8	2.43	0.54
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.88	0.54
3:D:608:SER:HB3	3:D:1443:THR:HB	1.89	0.54
3:D:1018:ASN:HB3	3:D:1021:TYR:HB3	1.90	0.54
1:A:7:LYS:NZ	1:A:7:LYS:HB3	2.23	0.54
2:C:18:LEU:HD22	2:C:404:LEU:HD21	1.89	0.54
2:C:949:LYS:HD3	3:D:796:ARG:NH1	2.23	0.54
3:D:171:LEU:N	3:D:391:ALA:O	2.36	0.54
3:D:783:ARG:HD3	3:D:1029:ARG:HG2	1.90	0.54



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:D:955:VAL:HB	3:D:1011:PHE:HE1	1.72	0.54
3:D:1434:TRP:NE1	3:D:1457:ASP:HB2	2.23	0.54
2:C:390:GLN:HB3	6:R:25:G:H5'	1.90	0.53
3:D:24:GLY:HA3	3:D:49:ILE:HG12	1.90	0.53
3:D:100:ALA:HB3	3:D:128:TYR:CE1	2.42	0.53
3:D:658:LEU:HA	3:D:661:MET:HE2	1.89	0.53
3:D:1106:VAL:HG11	3:D:1474:ALA:HB2	1.90	0.53
2:C:351:LEU:HD11	2:C:373:VAL:HG13	1.88	0.53
2:C:1082:PRO:HB3	3:D:1469:GLY:HA3	1.89	0.53
2:C:1101:THR:HG21	2:C:1111:ILE:HD11	1.89	0.53
2:C:1105:LYS:HZ1	2:C:1107:ASN:HB2	1.73	0.53
3:D:908:LYS:HB2	3:D:1027:GLY:HA3	1.89	0.53
2:C:272:ALA:C	2:C:276:LYS:HZ2	2.11	0.53
2:C:1085:PHE:HD1	3:D:1468:LEU:HD22	1.74	0.53
3:D:52:PRO:HG2	3:D:80:VAL:HG13	1.88	0.53
3:D:568:ARG:NH1	3:D:571:LYS:HE3	2.22	0.53
3:D:1155:VAL:HG23	3:D:1156:LEU:H	1.73	0.53
2:C:334:ARG:NH1	2:C:415:PRO:HG2	2.21	0.53
3:D:1435:LEU:HD21	3:D:1468:LEU:HD21	1.91	0.53
1:A:133:GLU:HG2	1:A:134:GLU:H	1.73	0.53
3:D:172:PRO:HG2	3:D:175:VAL:HG21	1.89	0.53
3:D:458:ALA:HB2	3:D:575:GLN:HE22	1.73	0.53
2:C:185:LYS:HZ2	2:C:190:LYS:HE2	1.73	0.53
2:C:1034:GLU:OE2	3:D:1096:ARG:NH2	2.42	0.53
3:D:87:ARG:HD2	3:D:88:TYR:CE1	2.44	0.53
2:C:284:ARG:NH1	2:C:285:LEU:H	2.05	0.53
3:D:1232:PRO:HB3	3:D:1361:VAL:HG21	1.89	0.53
3:D:1275:SER:OG	3:D:1322:GLY:N	2.42	0.53
1:B:64:GLU:HA	1:B:165:ILE:HD13	1.90	0.53
2:C:1007:ALA:HB2	3:D:648:MET:HG2	1.90	0.53
3:D:614:PHE:HB3	3:D:1439:SER:HA	1.90	0.53
1:B:149:GLY:H	1:B:171:PHE:HB2	1.74	0.53
3:D:176:ASP:O	3:D:390:PRO:HD2	2.08	0.53
3:D:784:ASP:HB3	3:D:939:PHE:CE1	2.44	0.53
3:D:554:LEU:HD13	3:D:570:GLU:HB3	1.91	0.52
2:C:300:ASP:OD2	2:C:303:PHE:HB2	2.10	0.52
3:D:165:LYS:H	3:D:199:LEU:HD13	1.74	0.52
1:B:205:VAL:HG13	1:B:209:GLU:HB2	1.90	0.52
2:C:91:GLN:HA	2:C:119:PRO:HA	1.90	0.52
2:C:184:MET:HB2	2:C:193:LEU:HB2	1.91	0.52
2:C:1034:GLU:OE2	3:D:1096:ARG:NH1	2.39	0.52



	A + O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:D:39:PRO:HD3	3:D:53:ILE:HG21	1.91	0.52
3:D:792:ILE:HG13	3:D:793:THR:HG23	1.92	0.52
3:D:802:ALA:HB3	3:D:824:ASN:HB3	1.92	0.52
3:D:964:LEU:HD13	3:D:1058:ARG:HH12	1.74	0.52
3:D:1128:VAL:HB	3:D:1131:SER:OG	2.10	0.52
2:C:236:ILE:HA	2:C:251:ASP:OD2	2.09	0.52
2:C:66:LEU:HD12	2:C:98:LEU:HD11	1.90	0.52
3:D:800:LYS:NZ	3:D:804:LEU:HD13	2.24	0.52
3:D:805:GLU:HG2	3:D:809:PRO:HG2	1.91	0.52
2:C:1:MET:O	2:C:899:GLN:HA	2.10	0.52
3:D:832:ARG:NE	3:D:833:GLU:OE2	2.43	0.52
3:D:1112:CYS:HB2	3:D:1195:GLN:HG2	1.91	0.52
2:C:408:ARG:NH2	2:C:456:ALA:O	2.43	0.52
2:C:437:ARG:HG2	2:C:469:THR:HG23	1.92	0.52
2:C:806:LEU:HB2	2:C:822:VAL:HG22	1.91	0.52
3:D:421:LEU:HB2	3:D:427:VAL:HG12	1.92	0.52
3:D:543:LEU:HD13	3:D:581:LEU:HA	1.91	0.52
1:A:80:LEU:HD21	2:C:573:ARG:HD2	1.92	0.52
2:C:165:LEU:HG	2:C:166:PRO:HA	1.91	0.52
2:C:756:VAL:O	2:C:789:SER:HB3	2.10	0.52
3:D:50:PHE:CD1	3:D:522:PRO:HD3	2.45	0.52
3:D:367:ILE:HG13	3:D:377:VAL:HG13	1.91	0.52
2:C:756:VAL:HB	2:C:790:LEU:HB3	1.91	0.52
2:C:841:ASN:HD21	2:C:884:GLN:HE21	1.56	0.52
2:C:842:ARG:HH11	2:C:842:ARG:HB3	1.75	0.52
2:C:1008:ARG:HH12	2:C:1010:THR:CA	2.23	0.52
3:D:806:PHE:CD1	3:D:812:ALA:HB3	2.45	0.52
1:B:73:GLU:OE2	1:B:128:HIS:NE2	2.40	0.51
2:C:205:GLU:CB	2:C:209:ARG:HH12	2.22	0.51
3:D:560:GLN:HG3	3:D:561:GLY:H	1.74	0.51
1:A:34:VAL:HG21	2:C:939:ARG:HE	1.75	0.51
2:C:288:ARG:H	2:C:288:ARG:NH1	2.04	0.51
2:C:425:PHE:H	2:C:428:ARG:HD2	1.75	0.51
2:C:458:TYR:HB3	2:C:470:PRO:HG3	1.92	0.51
2:C:733:ALA:HB1	2:C:754:ILE:HD12	1.91	0.51
3:D:522:PRO:O	3:D:525:ARG:N	2.30	0.51
3:D:988:ARG:HA	3:D:991:GLN:HB2	1.92	0.51
3:D:1108:ARG:NH2	3:D:1460:ILE:HD11	2.19	0.51
2:C:679:PHE:CE2	2:C:853:LEU:HD21	2.45	0.51
3:D:1107:VAL:O	3:D:1218:GLY:N	2.42	0.51
2:C:95:TYR:HD1	2:C:112:GLU:HB3	1.74	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:D:842:VAL:HG12	3:D:865:THR:HB	1.93	0.51
3:D:1396:GLU:HA	3:D:1399:ASP:OD2	2.11	0.51
1:A:44:LEU:HD23	1:A:48:ILE:HD11	1.90	0.51
1:B:56:VAL:HG22	1:B:142:VAL:HG22	1.92	0.51
1:B:185:ARG:NH2	1:B:187:GLY:HA2	2.26	0.51
3:D:100:ALA:HB3	3:D:128:TYR:HE1	1.76	0.51
3:D:1036:ARG:HH21	3:D:1042:ARG:HA	1.75	0.51
2:C:468:ARG:NE	2:C:485:TYR:O	2.41	0.51
3:D:800:LYS:HZ3	3:D:804:LEU:HD22	1.76	0.51
1:B:185:ARG:HB3	1:B:190:THR:HG23	1.92	0.51
3:D:61:GLY:HA3	3:D:64:LYS:NZ	2.26	0.51
3:D:484:PRO:HB3	3:D:488:ARG:NE	2.25	0.51
3:D:1425:THR:O	3:D:1429:LEU:HB2	2.10	0.51
2:C:890:LEU:HB2	2:C:914:ILE:HD12	1.91	0.51
3:D:139:GLY:HA2	3:D:452:ILE:HG12	1.93	0.51
3:D:827:ILE:O	3:D:835:SER:OG	2.23	0.51
1:A:100:LEU:HD22	1:A:141:GLU:HG3	1.92	0.51
1:B:59:GLU:HB3	1:B:137:ARG:HH12	1.75	0.51
2:C:42:VAL:HA	2:C:46:ALA:HB2	1.92	0.51
4:E:48:MET:HB2	4:E:54:LEU:HB2	1.93	0.51
1:A:178:ALA:HB2	2:C:864:GLY:HA2	1.92	0.51
2:C:19:THR:HG21	2:C:124:ASP:O	2.11	0.51
2:C:140:ILE:HG13	2:C:410:ILE:HG21	1.93	0.51
3:D:54:LYS:HG3	3:D:55:ASP:H	1.76	0.51
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.46	0.51
4:E:48:MET:HG2	4:E:49:GLN:H	1.75	0.51
1:A:24:VAL:HG22	1:A:196:THR:HG22	1.94	0.50
3:D:101:HIS:ND1	3:D:582:LEU:HD13	2.25	0.50
3:D:584:ASN:OD1	3:D:590:PRO:HD2	2.11	0.50
6:R:22:U:H2'	6:R:23:G:H8	1.75	0.50
3:D:160:GLU:HA	3:D:163:TYR:CZ	2.46	0.50
3:D:414:ARG:HG3	3:D:433:GLY:H	1.75	0.50
3:D:800:LYS:NZ	3:D:804:LEU:HD22	2.27	0.50
3:D:832:ARG:O	3:D:834:THR:N	2.42	0.50
1:A:9:PRO:HG2	1:B:224:TYR:CE2	2.47	0.50
2:C:184:MET:HE2	2:C:193:LEU:HD12	1.94	0.50
3:D:52:PRO:HG3	3:D:78:VAL:HG13	1.94	0.50
3:D:637:LEU:HB2	3:D:641:GLN:HG3	1.94	0.50
3:D:917:GLN:HB3	3:D:921:ARG:NH1	2.26	0.50
3:D:1294:VAL:O	3:D:1295:GLU:HB2	2.11	0.50
1:B:59:GLU:HG3	1:B:139:ASN:HB3	1.94	0.50



	A	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:D:191:LEU:HD11	3:D:395:VAL:HG13	1.94	0.50
3:D:483:HIS:HB2	3:D:484:PRO:HD3	1.93	0.50
7:T:13:DC:H2"	7:T:14:DA:OP2	2.12	0.50
2:C:210:GLU:HG2	2:C:304:LEU:HD21	1.94	0.50
2:C:471:TYR:CE2	2:C:496:ILE:HG21	2.46	0.50
3:D:584:ASN:HB2	3:D:602:SER:HB3	1.94	0.50
1:B:14:ARG:HG3	1:B:14:ARG:HH11	1.77	0.49
2:C:108:ILE:HG13	2:C:366:SER:HB2	1.94	0.49
6:R:26:U:H2'	6:R:27:G:H8	1.76	0.49
1:A:18:ARG:HG3	1:A:206:THR:HG22	1.94	0.49
2:C:251:ASP:OD1	2:C:252:LYS:N	2.45	0.49
2:C:442:GLU:HG2	2:C:454:SER:CB	2.41	0.49
2:C:1094:ALA:HB2	3:D:520:LEU:HD12	1.92	0.49
1:A:153:ALA:HA	1:A:156:HIS:CE1	2.47	0.49
3:D:119:SER:H	3:D:123:LEU:HD22	1.76	0.49
2:C:1046:ALA:HB2	3:D:1472:ILE:HG13	1.94	0.49
2:C:1103:ASP:H	2:C:1107:ASN:H	1.59	0.49
3:D:1261:GLU:OE2	3:D:1269:LYS:HG3	2.12	0.49
3:D:1383:ASP:HB2	3:D:1416:ALA:HB3	1.94	0.49
1:A:89:PHE:HE1	1:A:97:VAL:HB	1.78	0.49
2:C:44:ILE:HG23	2:C:344:PHE:CE2	2.47	0.49
2:C:338:GLU:HA	2:C:341:THR:HG22	1.94	0.49
3:D:1108:ARG:HH12	3:D:1460:ILE:HG13	1.76	0.49
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.45	0.49
3:D:1301:LYS:HD2	3:D:1303:TYR:CE1	2.48	0.49
1:B:128:HIS:CE1	1:B:131:THR:HG23	2.48	0.49
2:C:428:ARG:NH1	3:D:1086:LEU:HD21	2.27	0.49
3:D:31:THR:OG1	3:D:32:ILE:N	2.45	0.49
3:D:473:LEU:HD23	3:D:499:VAL:HG21	1.95	0.49
3:D:1074:SER:HA	3:D:1077:ALA:HB3	1.95	0.49
2:C:689:VAL:HB	2:C:870:ILE:HB	1.94	0.49
3:D:800:LYS:HZ3	3:D:804:LEU:HD13	1.78	0.49
2:C:604:ALA:HB3	2:C:612:VAL:HB	1.95	0.49
2:C:1006:HIS:HB2	3:D:628:ARG:HG2	1.95	0.49
2:C:474:VAL:HG12	2:C:479:VAL:HA	1.95	0.49
3:D:1258:ARG:NH1	3:D:1262:LEU:HD21	2.28	0.49
1:B:185:ARG:HD3	3:D:692:GLU:OE2	2.13	0.49
2:C:327:HIS:HA	2:C:431:HIS:NE2	2.28	0.48
2:C:739:GLU:HB2	2:C:742:VAL:HB	1.95	0.48
3:D:179:VAL:HG13	3:D:183:GLU:HB3	1.95	0.48
1:A:98:THR:HG22	1:A:143:ARG:HG3	1.94	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:228:PRO:HB3	1:B:13:VAL:HG23	1.95	0.48
1:B:85:LEU:HB3	1:B:127:LEU:HD23	1.95	0.48
2:C:858:MET:HG3	2:C:859:PRO:HD2	1.93	0.48
2:C:1034:GLU:CD	3:D:1096:ARG:HH12	2.17	0.48
3:D:690:ALA:O	3:D:694:VAL:HG13	2.13	0.48
3:D:695:ILE:HG13	3:D:696:HIS:H	1.77	0.48
3:D:820:GLU:HB3	3:D:836:VAL:HG11	1.95	0.48
2:C:472:ARG:O	2:C:532:MET:N	2.46	0.48
2:C:1008:ARG:HD3	2:C:1028:GLY:N	2.29	0.48
3:D:7:LYS:HA	3:D:1459:LEU:HD13	1.94	0.48
3:D:539:ASP:HB3	3:D:600:LEU:HB3	1.94	0.48
3:D:1146:GLY:HA3	3:D:1207:TYR:HB2	1.96	0.48
2:C:97:ARG:HG2	2:C:112:GLU:OE2	2.13	0.48
2:C:424:GLY:O	2:C:426:ASP:N	2.41	0.48
3:D:353:VAL:HG22	3:D:368:VAL:HG22	1.94	0.48
3:D:153:LEU:HB2	3:D:157:GLU:HG2	1.95	0.48
3:D:739:ASP:OD1	3:D:739:ASP:N	2.47	0.48
3:D:850:LEU:HD22	3:D:881:LEU:HD12	1.95	0.48
2:C:540:PHE:HB3	2:C:544:THR:HB	1.95	0.48
2:C:810:ASP:HB2	2:C:813:VAL:HG13	1.96	0.48
3:D:101:HIS:HE1	3:D:582:LEU:HD22	1.77	0.48
3:D:1189:ARG:HD2	3:D:1204:CYS:SG	2.54	0.48
3:D:50:PHE:O	3:D:89:ARG:HD2	2.14	0.48
2:C:680:ASP:N	3:D:943:THR:HG21	2.27	0.48
3:D:415:VAL:O	3:D:432:TYR:HA	2.14	0.48
3:D:702:LEU:HB3	3:D:745:MET:CE	2.44	0.48
3:D:1284:GLU:HB2	3:D:1291:SER:O	2.14	0.48
1:A:133:GLU:HG2	1:A:134:GLU:N	2.29	0.47
2:C:45:GLN:O	2:C:48:PHE:HB2	2.14	0.47
1:B:75:VAL:O	1:B:79:ILE:HG13	2.14	0.47
2:C:1056:LYS:O	3:D:624:ASP:HB2	2.14	0.47
2:C:198:ARG:NH1	2:C:202:TYR:O	2.39	0.47
2:C:919:ALA:HB2	2:C:968:LEU:HD21	1.95	0.47
3:D:123:LEU:HG	3:D:152:LEU:HD13	1.96	0.47
3:D:1031:ASN:HB3	3:D:1034:GLN:HB2	1.96	0.47
2:C:198:ARG:NH1	2:C:203:ASP:HA	2.30	0.47
2:C:713:ARG:HA	2:C:819:VAL:HA	1.97	0.47
2:C:1008:ARG:NH1	2:C:1011:GLY:N	2.61	0.47
3:D:365:ASP:O	3:D:379:ALA:HB2	2.13	0.47
3:D:1264:GLU:OE2	3:D:1425:THR:HG22	2.15	0.47
2:C:47:ALA:CB	2:C:345:ARG:HG2	2.43	0.47



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:602:GLU:H	2:C:614:ARG:HB3	1.80	0.47
2:C:865:THR:HA	2:C:866:PRO:HD3	1.78	0.47
3:D:61:GLY:HA3	3:D:64:LYS:HZ3	1.79	0.47
3:D:165:LYS:O	3:D:167:GLU:N	2.48	0.47
3:D:829:VAL:O	3:D:831:GLY:N	2.43	0.47
3:D:1354:LYS:HA	3:D:1357:ARG:HD2	1.96	0.47
3:D:1394:VAL:HG21	3:D:1432:LYS:NZ	2.30	0.47
2:C:891:GLY:O	2:C:991:GLN:HG2	2.15	0.47
2:C:978:ARG:CG	2:C:978:ARG:NH1	2.73	0.47
3:D:348:GLN:HB3	3:D:350:HIS:CE1	2.50	0.47
3:D:565:ILE:O	3:D:569:ASN:HB2	2.15	0.47
5:N:3:DA:H2"	5:N:4:DA:C8	2.50	0.47
3:D:956:ILE:HA	3:D:1039:CYS:HB3	1.97	0.47
2:C:216:GLU:O	2:C:218:VAL:N	2.48	0.47
1:A:150:TYR:CD1	2:C:696:LYS:HG2	2.50	0.46
2:C:976:ASP:OD2	2:C:978:ARG:NH1	2.48	0.46
1:A:165:ILE:HA	1:A:166:PRO:HD3	1.83	0.46
2:C:397:GLU:HG2	2:C:403:SER:OG	2.15	0.46
2:C:759:THR:HG22	2:C:787:ASP:HA	1.98	0.46
2:C:910:LYS:O	2:C:914:ILE:HG12	2.15	0.46
2:C:946:ARG:HH11	2:C:946:ARG:HG2	1.80	0.46
3:D:29:PRO:HB3	3:D:548:ILE:HB	1.97	0.46
3:D:607:LEU:HD23	3:D:614:PHE:CE1	2.49	0.46
2:C:1051:GLU:OE2	3:D:751:LEU:HB2	2.16	0.46
3:D:786:ILE:HG21	3:D:1027:GLY:H	1.81	0.46
1:A:97:VAL:HG21	1:A:120:VAL:HG21	1.97	0.46
3:D:1107:VAL:HA	3:D:1200:VAL:O	2.16	0.46
1:B:58:ILE:HB	1:B:61:VAL:HB	1.98	0.46
3:D:1458:GLU:O	3:D:1460:ILE:N	2.49	0.46
2:C:98:LEU:HD21	2:C:373:VAL:HG21	1.98	0.46
2:C:290:LEU:HD13	2:C:302:VAL:HG12	1.97	0.46
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.97	0.46
3:D:1135:ARG:NH1	3:D:1139:ASP:HB3	2.31	0.46
3:D:1197:ARG:HB3	3:D:1396:GLU:CD	2.36	0.46
1:A:169:ALA:HB1	1:A:171:PHE:CE2	2.51	0.46
2:C:100:LEU:HB3	2:C:368:THR:OG1	2.15	0.46
2:C:478:VAL:HG22	2:C:507:ARG:HG2	1.97	0.46
1:A:67:THR:HB	2:C:627:ARG:HD3	1.98	0.46
1:B:94:LEU:HD11	1:B:119:ASP:HB2	1.97	0.46
2:C:198:ARG:HH12	2:C:203:ASP:HA	1.81	0.46
2:C:851:LYS:HG3	2:C:853:LEU:HD12	1.98	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:D:1041:LEU:HD12	3:D:1058:ARG:HA	1.98	0.46
1:B:201:THR:HG22	1:B:202:ASP:H	1.81	0.46
2:C:288:ARG:HH11	2:C:288:ARG:N	2.07	0.46
2:C:861:LEU:HD12	2:C:865:THR:HG23	1.97	0.46
3:D:1044:LEU:HA	3:D:1056:PRO:HA	1.97	0.46
1:A:13:VAL:HG21	1:B:228:PRO:HB3	1.98	0.45
1:A:174:VAL:HA	1:A:201:THR:HG22	1.97	0.45
2:C:3:ILE:HD11	2:C:665:PHE:CE2	2.50	0.45
2:C:165:LEU:HD12	2:C:165:LEU:HA	1.87	0.45
2:C:966:LEU:HD12	2:C:966:LEU:HA	1.77	0.45
3:D:182:GLY:HA2	3:D:203:ALA:O	2.16	0.45
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.98	0.45
3:D:792:ILE:HD13	3:D:941:PHE:CD2	2.51	0.45
3:D:792:ILE:HD13	3:D:941:PHE:HD2	1.81	0.45
2:C:86:LYS:HD3	2:C:813:VAL:HG12	1.98	0.45
2:C:335:THR:O	2:C:339:LEU:HG	2.16	0.45
2:C:586:ARG:NH1	2:C:590:ASP:OD2	2.49	0.45
2:C:136:ILE:HB	2:C:336:VAL:HG13	1.98	0.45
2:C:146:VAL:HB	2:C:281:LEU:HD11	1.99	0.45
2:C:602:GLU:HA	2:C:648:ARG:HA	1.99	0.45
3:D:30:GLU:HB3	3:D:40:GLU:HB3	1.97	0.45
3:D:805:GLU:HA	3:D:832:ARG:HB3	1.98	0.45
3:D:908:LYS:HB2	3:D:1027:GLY:CA	2.47	0.45
3:D:1369:GLU:HA	3:D:1372:VAL:HG12	1.98	0.45
2:C:97:ARG:HG2	2:C:111:ASP:HB3	1.97	0.45
2:C:327:HIS:C	2:C:329:GLY:H	2.20	0.45
2:C:1009:SER:HB2	3:D:625:TYR:CD1	2.51	0.45
2:C:1040:LEU:HD23	2:C:1049:LEU:HA	1.99	0.45
3:D:165:LYS:NZ	3:D:199:LEU:HD22	2.31	0.45
3:D:613:ARG:NH1	3:D:616:GLN:HG2	2.32	0.45
3:D:826:PRO:HD2	3:D:829:VAL:HG21	1.98	0.45
3:D:939:PHE:O	3:D:943:THR:HG23	2.17	0.45
4:E:72:ARG:HB2	4:E:73:LEU:HD12	1.97	0.45
1:B:109:VAL:HA	1:B:113:ASP:OD2	2.16	0.45
2:C:134:ARG:NH2	2:C:392:SER:O	2.50	0.45
2:C:976:ASP:OD1	2:C:978:ARG:NH1	2.50	0.45
1:A:30:ARG:HH21	1:A:191:ASP:HB3	1.82	0.45
1:A:85:LEU:HD12	1:A:124:ASN:HB3	1.98	0.45
2:C:290:LEU:HD12	2:C:290:LEU:HA	1.60	0.45
2:C:344:PHE:CE1	2:C:378:LEU:HD11	2.52	0.45
3:D:58:CYS:HA	3:D:78:VAL:HG11	1.98	0.45



	h h h o	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:D:1381:VAL:HB	3:D:1389:LEU:HA	1.98	0.45
4:E:47:LYS:HA	4:E:54:LEU:HB3	1.98	0.45
1:A:49:PRO:HA	1:A:148:VAL:HG22	1.99	0.45
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.97	0.45
2:C:235:LEU:HD11	2:C:298:PHE:HE2	1.81	0.45
2:C:503:LEU:HD23	2:C:508:ILE:HA	1.97	0.45
3:D:558:LEU:HD23	3:D:567:ILE:HD13	1.99	0.45
3:D:963:TYR:CE1	3:D:1002:LYS:HB3	2.51	0.45
1:A:56:VAL:HG21	1:A:82:LEU:HD13	1.99	0.45
2:C:288:ARG:H	2:C:288:ARG:HD3	1.81	0.45
2:C:1089:VAL:HA	2:C:1099:VAL:HG21	1.99	0.45
3:D:123:LEU:O	3:D:127:LEU:HG	2.16	0.45
3:D:805:GLU:OE2	3:D:816:HIS:NE2	2.49	0.45
3:D:209:ARG:HB2	3:D:389:GLU:HG3	1.99	0.45
3:D:346:ARG:HH22	3:D:349:PRO:HD3	1.82	0.45
3:D:553:ARG:O	3:D:557:LEU:HB2	2.17	0.45
3:D:721:VAL:HG12	3:D:722:GLU:O	2.17	0.45
3:D:784:ASP:HB3	3:D:939:PHE:HE1	1.82	0.45
3:D:1462:LEU:HG	3:D:1472:ILE:HB	1.99	0.45
1:A:183:ASP:OD1	1:A:183:ASP:N	2.50	0.45
1:B:143:ARG:HD2	1:B:160:ASP:HB2	1.98	0.45
2:C:139:GLN:HA	2:C:411:SER:O	2.17	0.45
2:C:272:ALA:C	2:C:276:LYS:NZ	2.71	0.45
2:C:716:LYS:HA	2:C:716:LYS:HD3	1.83	0.45
2:C:953:VAL:HB	2:C:962:GLN:OE1	2.17	0.45
3:D:179:VAL:HG11	3:D:203:ALA:HB3	1.99	0.45
3:D:800:LYS:HG2	3:D:804:LEU:HD22	1.99	0.45
1:B:74:ASP:HB2	3:D:872:ARG:HH22	1.83	0.44
2:C:428:ARG:HH11	3:D:1086:LEU:HD11	1.81	0.44
2:C:473:ARG:HG3	2:C:480:THR:HB	1.99	0.44
2:C:1053:LEU:HD13	3:D:617:ASN:HB3	1.99	0.44
3:D:701:LEU:O	3:D:747:VAL:HA	2.17	0.44
3:D:758:GLU:O	3:D:762:GLN:HG2	2.18	0.44
3:D:1481:VAL:HG13	4:E:18:ARG:HA	1.99	0.44
2:C:200:LEU:HA	2:C:298:PHE:HB2	1.99	0.44
2:C:223:ASP:HB2	2:C:224:GLU:H	1.36	0.44
2:C:341:THR:O	2:C:345:ARG:HG3	2.18	0.44
2:C:1043:TYR:CD1	3:D:763:MET:HG2	2.52	0.44
3:D:176:ASP:HB3	3:D:177:ALA:H	1.56	0.44
3:D:510:GLU:HG3	3:D:511:TRP:HD1	1.82	0.44
3:D:764:LEU:HD23	3:D:766:ALA:H	1.83	0.44



	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:42:ARG:O	1:A:46:SER:HB3	2.18	0.44
2:C:1036:GLU:OE1	2:C:1036:GLU:N	2.47	0.44
2:C:1055:LEU:HD11	2:C:1066:ALA:HB2	1.99	0.44
3:D:708:LEU:HD21	3:D:1091:SER:HB2	1.99	0.44
3:D:709:HIS:CD2	3:D:711:LEU:HB2	2.52	0.44
2:C:290:LEU:HD22	2:C:302:VAL:HG12	2.00	0.44
2:C:858:MET:HE3	2:C:858:MET:HB2	1.91	0.44
3:D:486:ARG:HH21	3:D:489:ARG:NH1	2.04	0.44
2:C:146:VAL:HB	2:C:281:LEU:HD21	1.99	0.44
3:D:101:HIS:HD2	3:D:104:PHE:CE2	2.35	0.44
3:D:602:SER:O	3:D:606:ILE:HG12	2.17	0.44
3:D:1136:LYS:HB3	3:D:1139:ASP:OD2	2.17	0.44
3:D:1213:ARG:NH2	4:E:10:PHE:O	2.51	0.44
2:C:9:ILE:HG12	2:C:907:ASP:CG	2.38	0.44
2:C:673:LEU:HA	2:C:991:GLN:HA	1.99	0.44
2:C:710:ILE:HG22	2:C:823:VAL:HB	1.99	0.44
3:D:108:VAL:HB	3:D:109:PRO:HD3	1.99	0.44
3:D:714:GLN:HB2	3:D:716:PHE:CE2	2.53	0.44
2:C:78:PHE:HA	2:C:79:PRO:HD3	1.90	0.44
2:C:695:LEU:HD21	2:C:833:LEU:HB3	2.00	0.44
3:D:42:ASP:HA	3:D:46:ASP:HB2	2.00	0.44
3:D:165:LYS:HZ2	3:D:199:LEU:HD22	1.81	0.44
3:D:967:ALA:HB1	3:D:995:LEU:HD21	2.00	0.44
3:D:1294:VAL:HG12	3:D:1295:GLU:N	2.32	0.44
3:D:1307:LYS:HB3	3:D:1308:GLU:OE2	2.18	0.44
2:C:48:PHE:HB3	2:C:52:PHE:CD2	2.49	0.44
2:C:71:TYR:HA	2:C:96:ALA:HA	2.00	0.44
2:C:246:ASP:HA	2:C:247:PRO:HD3	1.72	0.44
2:C:1070:ILE:HD11	2:C:1076:VAL:HG22	2.00	0.44
3:D:1422:MET:HB2	3:D:1426:LYS:HD3	2.00	0.44
3:D:65:ARG:HD2	3:D:65:ARG:HA	1.69	0.44
3:D:355:VAL:HG11	3:D:385:VAL:HG11	2.00	0.44
3:D:1311:LEU:HA	3:D:1325:LEU:O	2.18	0.44
1:B:57:TYR:CD2	1:B:161:ARG:HG3	2.53	0.43
2:C:136:ILE:HD11	2:C:386:PHE:CE1	2.53	0.43
2:C:358:ARG:HD3	2:C:371:LYS:O	2.17	0.43
3:D:136:ASP:CB	3:D:137:PRO:HD2	2.45	0.43
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.53	0.43
1:A:79:ILE:HA	1:A:82:LEU:HD12	2.00	0.43
2:C:585:GLU:O	2:C:589:ARG:HG2	2.19	0.43
3:D:408:GLU:H	3:D:408:GLU:HG2	1.59	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:D:650:LEU:HD21	3:D:677:LEU:HD23	2.00	0.43
3:D:1131:SER:OG	3:D:1133:ARG:NH2	2.51	0.43
1:B:62:LEU:HD23	1:B:163:ASN:HD22	1.83	0.43
2:C:124:ASP:HB3	2:C:592:LEU:HD12	2.01	0.43
2:C:184:MET:O	2:C:190:LYS:HA	2.18	0.43
2:C:666:LEU:HG	2:C:668:LEU:HG	2.00	0.43
2:C:21:ILE:HD11	2:C:455:LEU:HD22	2.00	0.43
2:C:47:ALA:HB2	2:C:345:ARG:HG2	2.00	0.43
2:C:233:GLU:OE1	2:C:233:GLU:N	2.41	0.43
2:C:627:ARG:HG3	2:C:628:PHE:CD2	2.54	0.43
2:C:722:ILE:HD12	2:C:823:VAL:HG21	2.00	0.43
3:D:798:GLU:HG2	3:D:799:LYS:H	1.83	0.43
3:D:919:PHE:HA	3:D:927:THR:OG1	2.19	0.43
3:D:1280:VAL:O	3:D:1294:VAL:HG13	2.17	0.43
1:A:102:LYS:HA	1:A:138:LEU:O	2.19	0.43
1:A:218:LEU:HD23	1:B:222:LEU:HD21	2.01	0.43
2:C:853:LEU:HB2	2:C:858:MET:CE	2.49	0.43
3:D:563:PRO:HG2	3:D:566:ILE:HG13	2.01	0.43
3:D:568:ARG:HH11	3:D:571:LYS:HE3	1.83	0.43
3:D:739:ASP:OD2	3:D:741:ASP:OD2	2.36	0.43
3:D:1118:ILE:HD12	3:D:1118:ILE:HA	1.84	0.43
1:B:221:HIS:HA	1:B:224:TYR:CD2	2.53	0.43
2:C:13:ILE:HD13	2:C:483:VAL:HG11	2.00	0.43
2:C:1075:ASP:OD1	2:C:1076:VAL:N	2.52	0.43
3:D:1123:PHE:HB3	3:D:1132:LEU:HG	2.00	0.43
2:C:18:LEU:HB3	2:C:408:ARG:HD2	2.00	0.43
2:C:147:TYR:HA	2:C:323:ASP:OD2	2.18	0.43
2:C:429:ASP:OD1	3:D:1079:LYS:HD3	2.19	0.43
2:C:715:THR:OG1	2:C:718:GLY:O	2.36	0.43
2:C:810:ASP:O	2:C:812:GLY:N	2.50	0.43
3:D:975:GLU:HG3	3:D:979:GLU:OE2	2.18	0.43
3:D:1135:ARG:HB3	3:D:1140:ILE:HD11	2.00	0.43
3:D:1274:ILE:HA	3:D:1325:LEU:HD21	2.00	0.43
2:C:501:THR:HA	2:C:502:PRO:HD3	1.88	0.43
2:C:759:THR:HB	2:C:785:VAL:HG22	2.01	0.43
1:A:38:ASN:O	1:A:42:ARG:HG2	2.18	0.43
1:B:14:ARG:HG3	1:B:14:ARG:NH1	2.34	0.43
2:C:219:GLN:O	2:C:223:ASP:OD2	2.37	0.43
2:C:334:ARG:HH22	2:C:415:PRO:HG2	1.84	0.43
3:D:165:LYS:HD2	3:D:397:LYS:HB2	2.00	0.43
3:D:486:ARG:HA	3:D:489:ARG:HB3	2.00	0.43



		Interatomic	Clash
Atom-1	Atom-1 Atom-2		overlap (Å)
3:D:645:PRO:HA	3:D:721:VAL:O	2.19	0.43
3:D:1003:VAL:O	3:D:1007:VAL:HG23	2.19	0.43
4:E:45:ARG:HH21	4:E:63:TRP:HH2	1.66	0.43
2:C:238:LEU:HD21	2:C:242:LEU:HD13	2.01	0.43
2:C:676:ILE:HG23	2:C:988:VAL:HG13	1.99	0.43
2:C:749:VAL:HB	2:C:792:VAL:HG21	2.00	0.43
3:D:1366:LYS:O	3:D:1370:ILE:HG13	2.19	0.43
1:B:143:ARG:CZ	1:B:158:ILE:HG21	2.49	0.42
3:D:531:ASP:C	3:D:533:GLY:H	2.23	0.42
3:D:625:TYR:CD2	3:D:751:LEU:HD11	2.54	0.42
3:D:628:ARG:NH1	7:T:16:DC:H2"	2.34	0.42
2:C:34:VAL:HB	2:C:38:LYS:HZ2	1.84	0.42
2:C:87:ASP:HA	2:C:131:GLY:HA3	2.00	0.42
2:C:876:VAL:HG11	3:D:949:ILE:HG21	2.01	0.42
3:D:895:VAL:HG21	3:D:922:LEU:HD21	2.00	0.42
4:E:54:LEU:HG	4:E:58:PRO:CG	2.44	0.42
1:B:92:PRO:HA	1:B:146:ARG:HH12	1.85	0.42
2:C:37:GLU:OE2	2:C:38:LYS:HG2	2.20	0.42
2:C:52:PHE:CE1	2:C:98:LEU:HD13	2.53	0.42
2:C:274:ARG:HH22	2:C:284:ARG:HA	1.84	0.42
2:C:334:ARG:HE	2:C:339:LEU:HD23	1.85	0.42
2:C:512:ARG:HA	2:C:512:ARG:HD3	1.84	0.42
3:D:520:LEU:HG	3:D:521:PRO:HD2	2.01	0.42
3:D:630:VAL:O	3:D:725:SER:HB3	2.18	0.42
3:D:1018:ASN:O	3:D:1021:TYR:N	2.51	0.42
3:D:1037:GLN:HG2	3:D:1042:ARG:HG2	2.00	0.42
3:D:1124:GLN:HA	3:D:1125:PRO:HD3	1.85	0.42
3:D:1277:ILE:H	3:D:1277:ILE:HG13	1.68	0.42
3:D:1435:LEU:HB2	3:D:1457:ASP:OD1	2.20	0.42
2:C:379:GLU:O	2:C:383:ARG:HB3	2.19	0.42
2:C:893:ALA:HB2	2:C:918:LEU:HD23	2.00	0.42
3:D:205:TYR:CE1	3:D:390:PRO:HG3	2.54	0.42
3:D:500:ARG:HG2	3:D:1388:ARG:NH1	2.35	0.42
3:D:966:GLU:HA	3:D:969:ARG:HG2	2.01	0.42
3:D:1128:VAL:HG12	3:D:1129:THR:N	2.33	0.42
2:C:700:TYR:HB2	2:C:833:LEU:HB2	2.01	0.42
2:C:718:GLY:HA3	2:C:761:PHE:CG	2.54	0.42
3:D:93:ILE:HB	3:D:517:VAL:HB	2.01	0.42
3:D:864:VAL:HG22	3:D:877:PRO:HD3	2.01	0.42
3:D:1209:LEU:HD11	4:E:16:LYS:HD2	2.01	0.42
3:D:1296:SER:HB3	3:D:1299:PHE:CD2	2.49	0.42



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:202:TYR:CE1	2:C:304:LEU:HD22	2.55	0.42
2:C:211:LEU:HD13	2:C:221:LEU:HD21	2.01	0.42
2:C:889:HIS:CE1	3:D:951:ILE:H	2.37	0.42
2:C:1085:PHE:HB2	3:D:1468:LEU:HB3	2.01	0.42
3:D:212:ARG:HB3	3:D:388:HIS:CD2	2.54	0.42
3:D:1008:PHE:CZ	3:D:1032:PRO:HA	2.55	0.42
3:D:1312:LEU:HD21	3:D:1327:ARG:HH21	1.85	0.42
4:E:3:GLU:O	4:E:5:GLY:N	2.52	0.42
2:C:113:VAL:O	2:C:115:LEU:N	2.49	0.42
2:C:313:LEU:HD22	2:C:321:GLU:O	2.20	0.42
2:C:393:GLN:HG2	6:R:25:G:O2'	2.20	0.42
2:C:475:VAL:HG23	2:C:480:THR:OG1	2.19	0.42
2:C:678:PRO:HA	2:C:683:ASN:HD21	1.84	0.42
2:C:905:ILE:HG22	2:C:906:PHE:CD2	2.54	0.42
2:C:1019:GLN:HA	2:C:1020:PRO:HD3	1.70	0.42
3:D:167:GLU:OE1	3:D:198:ARG:NH2	2.53	0.42
3:D:171:LEU:HD23	3:D:171:LEU:HA	1.91	0.42
3:D:458:ALA:HB2	3:D:575:GLN:NE2	2.33	0.42
3:D:583:ASP:OD2	3:D:604:THR:HG21	2.19	0.42
4:E:24:ALA:O	4:E:28:GLN:HG3	2.20	0.42
1:A:180:GLN:HB2	1:A:196:THR:OG1	2.19	0.42
2:C:469:THR:O	2:C:485:TYR:HA	2.20	0.42
2:C:1014:SER:HB3	2:C:1017:THR:O	2.19	0.42
1:A:228:PRO:HB3	1:B:13:VAL:CG2	2.50	0.42
2:C:127:PHE:O	2:C:129:ILE:HD12	2.20	0.42
3:D:719:VAL:O	3:D:721:VAL:HG23	2.20	0.42
3:D:877:PRO:O	3:D:880:ILE:HG22	2.20	0.42
2:C:295:ASP:C	2:C:297:GLU:H	2.23	0.42
2:C:350:ARG:HB3	2:C:377:PRO:HB3	2.00	0.42
2:C:521:PRO:HB2	3:D:1055:VAL:HG21	2.02	0.42
3:D:352:ASN:HB2	3:D:369:ALA:O	2.20	0.42
3:D:1401:GLU:OE2	3:D:1402:ALA:N	2.53	0.42
2:C:127:PHE:HB2	2:C:129:ILE:HD11	2.01	0.41
2:C:906:PHE:HZ	3:D:1070:TYR:HD1	1.67	0.41
2:C:1071:ILE:HD13	2:C:1071:ILE:HA	1.91	0.41
3:D:28:LYS:C	3:D:548:ILE:HG21	2.40	0.41
3:D:212:ARG:H	3:D:388:HIS:HD2	1.68	0.41
3:D:494:LYS:HB2	3:D:494:LYS:NZ	2.35	0.41
3:D:1263:PHE:CZ	3:D:1352:ILE:HD13	2.55	0.41
1:B:101:LEU:HD23	1:B:140:MET:HG2	2.02	0.41
2:C:48:PHE:O	2:C:52:PHE:HB2	2.20	0.41



Atom-1	Atom-2	Interatomic	Clash
	1100111 2	distance (Å)	overlap (Å)
2:C:205:GLU:H	2:C:205:GLU:HG3	1.43	0.41
2:C:223:ASP:OD1	2:C:224:GLU:HG2	2.20	0.41
3:D:433:GLY:HA3	3:D:447:VAL:O	2.19	0.41
3:D:607:LEU:HD23	3:D:614:PHE:HE1	1.85	0.41
2:C:265:ARG:NH1	2:C:267:TYR:HD1	2.18	0.41
3:D:184:GLU:HA	3:D:202:VAL:HA	2.03	0.41
3:D:416:ALA:HB3	3:D:419:ASP:OD1	2.20	0.41
3:D:703:ASN:HB3	3:D:746:ALA:HB3	2.02	0.41
3:D:1378:TYR:O	3:D:1420:LEU:HB3	2.21	0.41
3:D:1394:VAL:HB	3:D:1397:LYS:HG2	2.02	0.41
7:T:11:DT:H2"	7:T:12:DC:O5'	2.20	0.41
1:B:190:THR:HG21	3:D:720:LEU:O	2.20	0.41
2:C:18:LEU:HD21	2:C:542:VAL:HG11	2.02	0.41
2:C:710:ILE:HD11	2:C:758:ARG:NH2	2.28	0.41
3:D:1209:LEU:HD12	3:D:1213:ARG:HD3	2.01	0.41
3:D:1401:GLU:CD	3:D:1415:VAL:HG22	2.40	0.41
1:A:25:LEU:HD22	1:B:225:PHE:CE1	2.55	0.41
2:C:384:GLU:HA	2:C:388:ARG:NH2	2.33	0.41
2:C:555:ALA:HB2	3:D:1070:TYR:HE2	1.86	0.41
2:C:580:MET:HG3	2:C:902:ILE:HG12	2.02	0.41
2:C:1005:MET:HB2	3:D:724:GLN:NE2	2.31	0.41
3:D:655:PRO:HA	3:D:658:LEU:HD12	2.01	0.41
3:D:717:GLN:HA	3:D:718:PRO:HD3	1.87	0.41
1:A:34:VAL:HG21	2:C:939:ARG:NE	2.36	0.41
2:C:726:ILE:HA	2:C:727:PRO:HD3	1.81	0.41
3:D:62:LYS:HD2	3:D:75:ARG:HD2	2.03	0.41
3:D:646:LYS:HE3	3:D:722:GLU:HG2	2.02	0.41
3:D:1309:ALA:HB1	3:D:1326:THR:HG23	2.03	0.41
2:C:409:ARG:HA	2:C:454:SER:HA	2.03	0.41
2:C:1097:LEU:HD11	3:D:103:TRP:CZ3	2.56	0.41
3:D:131:LYS:HB2	3:D:568:ARG:HG2	2.03	0.41
3:D:165:LYS:CG	3:D:199:LEU:HB3	2.49	0.41
3:D:826:PRO:HB2	3:D:829:VAL:HG23	2.01	0.41
3:D:880:ILE:HD12	3:D:880:ILE:HA	1.93	0.41
3:D:1279:GLY:O	3:D:1319:VAL:HG12	2.21	0.41
3:D:1398:TRP:HA	3:D:1398:TRP:CE3	2.56	0.41
3:D:1472:ILE:HA	3:D:1473:PRO:HD3	1.82	0.41
3:D:756:GLN:O	3:D:760:ARG:HG2	2.21	0.41
3:D:1284:GLU:HG2	3:D:1291:SER:HB2	2.02	0.41
3:D:1364:HIS:ND1	3:D:1366:LYS:HG3	2.35	0.41
4:E:59:ASN:OD1	4:E:60:ALA:N	2.53	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:C:23:VAL:HG22	2:C:121:MET:HE1	2.03	0.41
2:C:196:LEU:HA	2:C:199:VAL:HG23	2.02	0.41
2:C:290:LEU:HD11	2:C:301:GLU:N	2.23	0.41
2:C:443:THR:HG22	2:C:453:THR:HG22	2.02	0.41
2:C:607:ASP:OD1	2:C:608:GLY:N	2.49	0.41
2:C:743:VAL:HG11	2:C:755:LEU:HD12	2.02	0.41
2:C:1081:VAL:HB	2:C:1086:ARG:NH1	2.36	0.41
3:D:111:LYS:HB2	3:D:111:LYS:HE2	1.88	0.41
3:D:832:ARG:HD2	3:D:832:ARG:HA	1.86	0.41
3:D:1295:GLU:HB3	3:D:1296:SER:H	1.53	0.41
4:E:51:LEU:HG	4:E:53:GLY:H	1.86	0.41
2:C:436:GLY:HA2	2:C:538:GLN:O	2.21	0.41
2:C:586:ARG:HH12	2:C:590:ASP:CG	2.25	0.41
3:D:704:ARG:NH2	3:D:743:ASP:OD2	2.53	0.41
3:D:861:GLN:N	3:D:861:GLN:OE1	2.54	0.41
3:D:1108:ARG:NH1	3:D:1460:ILE:HG13	2.36	0.41
1:B:25:LEU:HD23	1:B:28:LEU:HD21	2.04	0.40
2:C:34:VAL:HG11	2:C:38:LYS:HZ1	1.85	0.40
2:C:200:LEU:HD23	2:C:298:PHE:HB3	2.03	0.40
2:C:474:VAL:HG12	2:C:479:VAL:HG13	2.03	0.40
2:C:729:LEU:HD23	2:C:729:LEU:HA	1.93	0.40
2:C:1085:PHE:CD1	3:D:1468:LEU:HB3	2.55	0.40
3:D:1119:SER:HB2	3:D:1185:GLU:CB	2.51	0.40
3:D:1128:VAL:HG23	3:D:1133:ARG:HH22	1.85	0.40
7:T:2:DG:H2"	7:T:3:DG:C8	2.56	0.40
1:A:179:PHE:HB3	1:A:197:LEU:HD12	2.03	0.40
1:B:185:ARG:HB3	1:B:190:THR:HA	2.03	0.40
2:C:259:GLY:CA	2:C:291:ALA:HB2	2.51	0.40
2:C:559:LEU:HD12	2:C:559:LEU:O	2.21	0.40
2:C:589:ARG:HB3	2:C:596:TYR:CZ	2.56	0.40
3:D:367:ILE:HG13	3:D:368:VAL:H	1.85	0.40
4:E:22:VAL:CG1	4:E:68:LEU:HD21	2.51	0.40
2:C:205:GLU:OE1	2:C:206:THR:HG23	2.20	0.40
2:C:350:ARG:CB	2:C:377:PRO:HB3	2.51	0.40
2:C:503:LEU:HD21	2:C:508:ILE:HD13	2.03	0.40
2:C:690:ILE:HG12	2:C:691:SER:N	2.37	0.40
3:D:549:ASN:O	3:D:553:ARG:HB2	2.21	0.40
2:C:831:ARG:HH21	2:C:1000:MET:HG3	1.86	0.40
3:D:192:ALA:HB2	3:D:393:ILE:HD12	2.04	0.40
3:D:760:ARG:HD3	4:E:61:VAL:HG11	2.04	0.40
3:D:1004:THR:HG23	3:D:1036:ARG:HB2	2.02	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:GLU:HA	1:A:27:PRO:HA	1.88	0.40
2:C:69:LEU:O	2:C:97:ARG:HB2	2.22	0.40
2:C:222:MET:O	2:C:222:MET:HG2	2.19	0.40
3:D:57:GLU:HG2	3:D:58:CYS:N	2.37	0.40
3:D:116:LEU:HA	3:D:116:LEU:HD23	1.85	0.40
3:D:849:ALA:O	3:D:853:VAL:HG23	2.21	0.40
4:E:45:ARG:HA	4:E:46:PRO:HD3	1.95	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	P	\mathbf{erc}	entiles
1	А	221/315~(70%)	193 (87%)	19 (9%)	9 (4%)		3	23
1	В	221/315~(70%)	199 (90%)	21 (10%)	1 (0%)		29	68
2	С	1077/1119~(96%)	901 (84%)	149 (14%)	27~(2%)		5	34
3	D	1352/1534~(88%)	1112 (82%)	189 (14%)	51 (4%)		3	25
4	Е	91/99~(92%)	74 (81%)	14 (15%)	3(3%)		4	28
All	All	2962/3382 (88%)	2479 (84%)	392 (13%)	91 (3%)		4	30

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	184	THR
2	С	2	GLU
2	С	111	ASP
2	С	164	PRO
2	С	213	ALA
2	С	217	LEU
2	C	223	ASP



Mol	Chain	Res	Type
2	С	320	HIS
2	C	369	PRO
3	D	136	ASP
3	D	176	ASP
3	D	363	ALA
3	D	806	PHE
3	D	808	THR
3	D	830	ALA
3	D	1273	VAL
3	D	1294	VAL
3	D	1295	GLU
3	D	1327	ARG
3	D	1454	GLY
1	А	47	SER
1	А	161	ARG
2	С	248	PRO
2	С	262	ALA
2	С	274	ARG
2	С	476	GLY
2	С	517	ARG
2	С	795	GLY
3	D	50	PHE
3	D	200	ASP
3	D	522	PRO
3	D	594	PRO
3	D	616	GLN
3	D	823	LEU
3	D	1411	GLY
3	D	1459	LEU
4	Е	58	PRO
1	A	48	ILE
1	A	186	LEU
1	A	226	SER
2	C	96	ALA
2	C	188	LYS
2	C	$27\overline{2}$	ALA
2	C	815	LEU
2	С	984	GLU
3	D	166	GLN
3	D	345	TYR
3	D	417	PRO
3	D	735	ALA



Mol Chain Res Type 3 D 822 ALA 3 D 832 ARG 3 D 1208 ASP 4 E 4 PRO 1 A 29 GLU 1 A 191 ASP 2 C 114 PHE 3 D 82 LYS 3 D 109 PRO 3 D 132 TYR 3 D 146 PRO 3 D 32 GLY 3 D 425 GLY 3 D 595 GLY 3 D 711 LEU 3 D 1205 TYR 3 D 1205 TYR 3 D 1205 TYR 3 D 1205 TYR 3 D <t< th=""><th>Contr</th><th>naca jion</th><th>i previe</th><th>as paye</th></t<>	Contr	naca jion	i previe	as paye
3 D 822 ALA 3 D 1208 ASP 4 E 4 PRO 1 A 29 GLU 1 A 191 ASP 2 C 114 PHE 3 D 82 LYS 3 D 109 PRO 3 D 132 TYR 3 D 146 PRO 3 D 406 ASP 3 D 406 ASP 3 D 595 GLY 3 D 595 GLY 3 D 750 PRO 3 D 1205 TYR 3 D 1205 TYR 3 D 1269 LYS 3 D 1284 GLU 3 D 560 GLN 3 D 560<	Mol	Chain	Res	Type
3 D 832 ARG 3 D 1208 ASP 4 E 4 PRO 1 A 29 GLU 1 A 191 ASP 2 C 114 PHE 3 D 82 LYS 3 D 109 PRO 3 D 132 TYR 3 D 146 PRO 3 D 374 GLU 3 D 406 ASP 3 D 406 ASP 3 D 595 GLY 3 D 595 GLY 3 D 750 PRO 3 D 750 PRO 3 D 1205 TYR 3 D 1269 LYS 3 D 1284 GLU 2 C 905 </td <td>3</td> <td>D</td> <td>822</td> <td>ALA</td>	3	D	822	ALA
3 D 1208 ASP 4 E 4 PRO 1 A 29 GLU 1 A 191 ASP 2 C 114 PHE 3 D 82 LYS 3 D 109 PRO 3 D 132 TYR 3 D 146 PRO 3 D 406 ASP 3 D 406 ASP 3 D 406 ASP 3 D 595 GLY 3 D 595 GLY 3 D 711 LEU 3 D 750 PRO 3 D 1269 LYS 3 D 1269 LYS 3 D 1317 ASP 4 E 42 PRO 1 A 134 </td <td>3</td> <td>D</td> <td>832</td> <td>ARG</td>	3	D	832	ARG
4 E 4 PRO 1 A 29 GLU 1 A 191 ASP 2 C 114 PHE 3 D 82 LYS 3 D 109 PRO 3 D 132 TYR 3 D 146 PRO 3 D 406 ASP 3 D 425 GLY 3 D 595 GLY 3 D 595 GLY 3 D 750 PRO 3 D 750 PRO 3 D 1205 TYR 3 D 1269 LYS 3 D 1269 LYS 3 D 1317 ASP 4 E 42 PRO 1 A 134 GLU 2 C 751 PRO 2 C 125 PRO 3	3	D	1208	ASP
1 A 29 GLU 1 A 191 ASP 2 C 114 PHE 3 D 82 LYS 3 D 109 PRO 3 D 132 TYR 3 D 146 PRO 3 D 374 GLU 3 D 406 ASP 3 D 425 GLY 3 D 595 GLY 3 D 595 GLY 3 D 750 PRO 3 D 750 PRO 3 D 1269 LYS 3 D 1269 LYS 3 D 1269 LYS 3 D 1269 LYS 3 D 1317 ASP 4 E 42 PRO 1 A 134 GLU 2 C 751 PRO 2	4	Е	4	PRO
1 A 191 ASP 2 C 114 PHE 3 D 82 LYS 3 D 109 PRO 3 D 132 TYR 3 D 146 PRO 3 D 374 GLU 3 D 406 ASP 3 D 425 GLY 3 D 595 GLY 3 D 696 HIS 3 D 750 PRO 3 D 1205 TYR 3 D 1269 LYS 3 D 1284 GLU 3 D 1317 ASP 4 E 42 PRO 1 A 134 GLU 2 C 751 PRO 2 C 905 ILE 3 D 560 GLN 3 D 1314 LYS 1	1	А	29	GLU
2 C 114 PHE 3 D 82 LYS 3 D 109 PRO 3 D 132 TYR 3 D 146 PRO 3 D 374 GLU 3 D 406 ASP 3 D 425 GLY 3 D 595 GLY 3 D 696 HIS 3 D 750 PRO 3 D 1205 TYR 3 D 1269 LYS 3 D 1269 LYS 3 D 1284 GLU 3 D 1317 ASP 4 E 42 PRO 1 A 134 GLU 2 C 905 ILE 3 D 621 LYS 3 D 13	1	А	191	ASP
3 D 82 LYS 3 D 109 PRO 3 D 132 TYR 3 D 146 PRO 3 D 374 GLU 3 D 406 ASP 3 D 425 GLY 3 D 595 GLY 3 D 696 HIS 3 D 750 PRO 3 D 1205 TYR 3 D 1317 ASP 4 E 42 PRO 1 A 134 GLU 2 C <t< td=""><td>2</td><td>С</td><td>114</td><td>PHE</td></t<>	2	С	114	PHE
3D109PRO3D132TYR3D146PRO3D374GLU3D406ASP3D425GLY3D595GLY3D696HIS3D750PRO3D1205TYR3D1269LYS3D1269LYS3D1317ASP4E42PRO1A134GLU2C751PRO2C905ILE3D560GLN3D1314LYS3D1314LYS1B125PRO2C231PRO2C463GLU3D55ASP3D104HRO3D683ILE3D705ALA2C811PRO3D1032PRO3D1032PRO3D1057VAL2C244PRO	3	D	82	LYS
3 D 132 TYR 3 D 146 PRO 3 D 374 GLU 3 D 406 ASP 3 D 425 GLY 3 D 595 GLY 3 D 696 HIS 3 D 750 PRO 3 D 1205 TYR 3 D 1269 LYS 3 D 1269 LYS 3 D 1317 ASP 4 E 42 PRO 1 A 134 GLU 2 C 751 PRO 2 C 905 ILE 3 D 560 GLN 3 D 560 GLN 3 D 621 LYS 3 D 1314 LYS 1 B 125 PRO 2 C 463 GLU 3	3	D	109	PRO
3 D 146 PRO 3 D 374 GLU 3 D 406 ASP 3 D 595 GLY 3 D 595 GLY 3 D 696 HIS 3 D 750 PRO 3 D 750 PRO 3 D 1265 TYR 3 D 1269 LYS 3 D 1284 GLU 3 D 1284 GLU 3 D 1317 ASP 4 E 42 PRO 1 A 134 GLU 2 C 751 PRO 2 C 905 ILE 3 D 560 GLN 3 D 621 LYS 3 D 1314 LYS 1 B 125 PRO 2 C 231 PRO 2	3	D	132	TYR
3 D 374 GLU 3 D 406 ASP 3 D 595 GLY 3 D 595 GLY 3 D 696 HIS 3 D 711 LEU 3 D 750 PRO 3 D 1205 TYR 3 D 1269 LYS 3 D 1269 LYS 3 D 1284 GLU 3 D 1317 ASP 4 E 42 PRO 1 A 134 GLU 2 C 751 PRO 2 C 905 ILE 3 D 560 GLN 3 D 621 LYS 3 D 1314 LYS 1 B 125 PRO 2 C 231 PRO 3 D 55 AS	3	D	146	PRO
3 D 406 ASP 3 D 425 GLY 3 D 595 GLY 3 D 696 HIS 3 D 711 LEU 3 D 750 PRO 3 D 1205 TYR 3 D 1269 LYS 3 D 1284 GLU 3 D 1317 ASP 4 E 42 PRO 1 A 134 GLU 2 C 751 PRO 1 A 134 GLN 3 D 621 LYS 3 D 621 LYS 3 D 1314 LYS 1 B 125 PRO 2 C 231 PRO 2 C 463 GLU 3 D 55	3	D	374	GLU
3 D 425 GLY 3 D 595 GLY 3 D 696 HIS 3 D 711 LEU 3 D 750 PRO 3 D 1205 TYR 3 D 1269 LYS 3 D 1284 GLU 3 D 1317 ASP 4 E 42 PRO 1 A 134 GLU 2 C 751 PRO 2 C 905 ILE 3 D 621 LYS 3 D 621 LYS 3 D 1314 LYS 1 B 125 PRO 2 C 152 PRO 2 C 463 GLU 3 D 55 ASP 3 D 70	3	D	406	ASP
3 D 595 GLY 3 D 696 HIS 3 D 711 LEU 3 D 750 PRO 3 D 1205 TYR 3 D 1269 LYS 3 D 1269 LYS 3 D 1284 GLU 3 D 1284 GLU 3 D 1317 ASP 4 E 42 PRO 1 A 134 GLU 2 C 751 PRO 2 C 905 ILE 3 D 621 LYS 3 D 621 LYS 3 D 1314 LYS 1 B 125 PRO 2 C 463 GLU 3 D 55 ASP 3 D	3	D	425	GLY
3 D 696 HIS 3 D 711 LEU 3 D 750 PRO 3 D 1205 TYR 3 D 1269 LYS 3 D 1284 GLU 3 D 1317 ASP 4 E 42 PRO 1 A 134 GLU 2 C 751 PRO 2 C 905 ILE 3 D 560 GLN 3 D 621 LYS 3 D 1314 LYS 3 D 1314 LYS 1 B 125 PRO 2 C 152 PRO 2 C 463 GLU 3 D 55 ASP 3 D 705 ALA 2 C 8	3	D	595	GLY
3 D 711 LEU 3 D 750 PRO 3 D 1205 TYR 3 D 1269 LYS 3 D 1269 LYS 3 D 1284 GLU 3 D 1317 ASP 4 E 42 PRO 1 A 134 GLU 2 C 751 PRO 2 C 905 ILE 3 D 621 LYS 3 D 621 LYS 3 D 1314 LYS 3 D 1314 LYS 1 B 125 PRO 2 C 231 PRO 2 C 463 GLU 3 D 55 ASP 3 D 705 ALA 2 C	3	D	696	HIS
3 D 750 PRO 3 D 1205 TYR 3 D 1269 LYS 3 D 1284 GLU 3 D 1317 ASP 4 E 42 PRO 1 A 134 GLU 2 C 751 PRO 2 C 905 ILE 3 D 621 LYS 3 D 621 LYS 3 D 621 LYS 3 D 1314 LYS 3 D 1314 LYS 1 B 125 PRO 2 C 152 PRO 2 C 463 GLU 3 D 55 ASP 3 D 705 ALA 2 C 811 PRO 3 D 6	3	D	711	LEU
3 D 1205 TYR 3 D 1269 LYS 3 D 1284 GLU 3 D 1317 ASP 4 E 42 PRO 1 A 134 GLU 2 C 751 PRO 2 C 905 ILE 3 D 560 GLN 3 D 621 LYS 3 D 621 LYS 3 D 1314 LYS 1 B 125 PRO 2 C 152 PRO 2 C 463 GLU 3 D 55 ASP 3 D 705 ALA 2 C 811 PRO 3 D 683 ILE 3 D 683 ILE 3 D 68	3	D	750	PRO
3 D 1269 LYS 3 D 1284 GLU 3 D 1317 ASP 4 E 42 PRO 1 A 134 GLU 2 C 751 PRO 2 C 905 ILE 3 D 560 GLN 3 D 621 LYS 3 D 621 LYS 3 D 1314 LYS 3 D 1314 LYS 1 B 125 PRO 2 C 152 PRO 2 C 463 GLU 3 D 55 ASP 3 D 124 GLU 3 D 705 ALA 2 C 811 PRO 3 D 683 ILE 3 D 10	3	D	1205	TYR
3 D 1284 GLU 3 D 1317 ASP 4 E 42 PRO 1 A 134 GLU 2 C 751 PRO 2 C 905 ILE 3 D 560 GLN 3 D 621 LYS 3 D 621 LYS 3 D 1314 LYS 1 B 125 PRO 2 C 231 PRO 2 C 463 GLU 3 D 55 ASP 3 D 55 ASP 3 D 705 ALA 2 C 811 PRO 3 D 683 ILE 3 D 683 ILE 3 D 809 PRO 3 D 1032<	3	D	1269	LYS
3 D 1317 ASP 4 E 42 PRO 1 A 134 GLU 2 C 751 PRO 2 C 905 ILE 3 D 560 GLN 3 D 621 LYS 3 D 1314 LYS 3 D 1314 LYS 1 B 125 PRO 2 C 152 PRO 2 C 231 PRO 2 C 463 GLU 3 D 55 ASP 3 D 124 GLU 3 D 705 ALA 2 C 811 PRO 3 D 683 ILE 3 D 809 PRO 3 D 1032 PRO 3 D 105	3	D	1284	GLU
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	3	D	1317	ASP
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	Е	42	PRO
2 C 751 PRO 2 C 905 ILE 3 D 560 GLN 3 D 621 LYS 3 D 1314 LYS 3 D 1314 LYS 1 B 125 PRO 2 C 152 PRO 2 C 231 PRO 2 C 463 GLU 3 D 55 ASP 3 D 705 ALA 2 C 811 PRO 3 D 683 ILE 3 D 809 PRO 3 D 1032 PRO 3 D 1057 VAL 2 C 244 PRO	1	А	134	GLU
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	С	751	PRO
3 D 560 GLN 3 D 621 LYS 3 D 1314 LYS 1 B 125 PRO 2 C 152 PRO 2 C 231 PRO 2 C 463 GLU 3 D 55 ASP 3 D 124 GLU 3 D 705 ALA 2 C 811 PRO 3 D 683 ILE 3 D 809 PRO 3 D 1032 PRO 3 D 1057 VAL 2 C 244 PRO	2	С	905	ILE
3 D 621 LYS 3 D 1314 LYS 1 B 125 PRO 2 C 152 PRO 2 C 231 PRO 2 C 231 PRO 2 C 463 GLU 3 D 55 ASP 3 D 705 ALA 2 C 811 PRO 3 D 683 ILE 3 D 809 PRO 3 D 1032 PRO 3 D 1057 VAL 2 C 244 PRO	3	D	560	GLN
3 D 1314 LYS 1 B 125 PRO 2 C 152 PRO 2 C 231 PRO 2 C 463 GLU 3 D 55 ASP 3 D 124 GLU 3 D 705 ALA 2 C 811 PRO 3 D 683 ILE 3 D 809 PRO 3 D 1032 PRO 3 D 1057 VAL 2 C 244 PRO	3	D	621	LYS
1 B 125 PRO 2 C 152 PRO 2 C 231 PRO 2 C 463 GLU 3 D 55 ASP 3 D 124 GLU 3 D 705 ALA 2 C 811 PRO 3 D 683 ILE 3 D 809 PRO 3 D 1032 PRO 3 D 1057 VAL 2 C 244 PRO	3	D	1314	LYS
2 C 152 PRO 2 C 231 PRO 2 C 463 GLU 3 D 55 ASP 3 D 124 GLU 3 D 705 ALA 2 C 811 PRO 3 D 683 ILE 3 D 809 PRO 3 D 1032 PRO 3 D 1057 VAL 2 C 244 PRO	1	В	125	PRO
2 C 231 PRO 2 C 463 GLU 3 D 55 ASP 3 D 124 GLU 3 D 705 ALA 2 C 811 PRO 3 D 683 ILE 3 D 1032 PRO 3 D 1057 VAL 2 C 244 PRO	2	С	152	PRO
2 C 463 GLU 3 D 55 ASP 3 D 124 GLU 3 D 705 ALA 2 C 811 PRO 3 D 683 ILE 3 D 809 PRO 3 D 1032 PRO 3 D 1057 VAL 2 C 244 PRO	2	С	231	PRO
3 D 55 ASP 3 D 124 GLU 3 D 705 ALA 2 C 811 PRO 3 D 683 ILE 3 D 809 PRO 3 D 1032 PRO 3 D 1057 VAL 2 C 244 PRO	2	С	463	GLU
3 D 124 GLU 3 D 705 ALA 2 C 811 PRO 3 D 683 ILE 3 D 809 PRO 3 D 1032 PRO 3 D 1057 VAL 2 C 244 PRO	3	D	55	ASP
3 D 705 ALA 2 C 811 PRO 3 D 683 ILE 3 D 809 PRO 3 D 1032 PRO 3 D 1057 VAL 2 C 244 PRO	3	D	124	GLU
2 C 811 PRO 3 D 683 ILE 3 D 809 PRO 3 D 1032 PRO 3 D 1057 VAL 2 C 244 PRO	3	D	705	ALA
3 D 683 ILE 3 D 809 PRO 3 D 1032 PRO 3 D 1057 VAL 2 C 244 PRO	2	С	811	PRO
3 D 809 PRO 3 D 1032 PRO 3 D 1057 VAL 2 C 244 PRO	3	D	683	ILE
3 D 1032 PRO 3 D 1057 VAL 2 C 244 PRO	3	D	809	PRO
3 D 1057 VAL 2 C 244 PRO	3	D	1032	PRO
2 C 244 PRO	3	D	1057	VAL
	2	С	244	PRO

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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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	196/273~(72%)	187~(95%)	9~(5%)	27 61
1	В	196/273~(72%)	191~(97%)	5(3%)	46 74
2	С	912/941~(97%)	837~(92%)	75~(8%)	11 40
3	D	1147/1289~(89%)	1058~(92%)	89~(8%)	12 42
4	Ε	82/88~(93%)	70~(85%)	12 (15%)	3 18
All	All	2533/2864~(88%)	2343 (92%)	190 (8%)	13 43

All (190) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	7	LYS
1	А	12	THR
1	А	15	THR
1	А	32	PHE
1	А	46	SER
1	А	126	ASP
1	А	131	THR
1	А	165	ILE
1	А	182	GLU
1	В	63	HIS
1	В	112	ARG
1	В	148	VAL
1	В	201	THR
1	В	205	VAL
2	С	8	ARG
2	С	30	LEU
2	С	38	LYS
2	С	39	ARG
2	С	49	ARG
2	С	52	PHE
2	С	81	ASP
2	С	98	LEU
2	С	102	HIS



Mol	Chain	Res	Type
2	С	104	ASP
2	С	118	ILE
2	С	127	PHE
2	С	135	VAL
2	С	154	ARG
2	С	157	ARG
2	С	189	ARG
2	С	193	LEU
2	С	205	GLU
2	С	214	TYR
2	С	223	ASP
2	С	243	ARG
2	С	267	TYR
2	С	274	ARG
2	С	279	GLU
2	С	281	LEU
2	С	284	ARG
2	С	288	ARG
2	С	289	THR
2	С	295	ASP
2	С	300	ASP
2	С	307	LEU
2	С	321	GLU
2	С	350	ARG
2	С	351	LEU
2	С	367	LEU
2	С	375	SER
2	С	376	ARG
2	С	378	LEU
2	С	388	ARG
2	С	391	LEU
2	С	394	PHE
2	С	403	SER
2	С	405	ARG
2	С	473	ARG
2	C	481	ASP
2	С	506	ASN
2	С	533	ASP
2	С	565	GLN
2	С	589	ARG
2	С	605	LYS
2	С	610	ARG



Mol	Chain	Res	Type
2	С	620	LEU
2	С	626	ARG
2	С	627	ARG
2	С	676	ILE
2	C	690	ILE
2	С	699	PHE
2	С	703	ILE
2	С	717	LEU
2	С	728	HIS
2	С	807	ARG
2	С	835	VAL
2	С	842	ARG
2	С	858	MET
2	C	899	GLN
2	C	953	VAL
2	С	966	LEU
2	С	978	ARG
2	С	1000	MET
2	С	1001	VAL
2	С	1008	ARG
2	С	1021	LEU
2	С	1035	MET
2	С	1099	VAL
2	С	1105	LYS
3	D	17	LYS
3	D	41	ARG
3	D	57	GLU
3	D	60	CYS
3	D	68	PHE
3	D	74	GLU
3	D	75	ARG
3	D	79	GLU
3	D	80	VAL
3	D	82	LYS
3	D	87	ARG
3	D	124	GLU
3	D	137	PRO
3	D	142	LEU
3	D	149	LYS
3	D	166	GLN
3	D	176	ASP
3	D	178	LEU



Mol	Chain	Res	Type
3		3/0	тнь
<u></u>		240	VAT
<u></u>	D	047 200	VAL CLU
<u>ა</u>	D	382	GLU
3 	D	392	SER VAL
<u> </u>	D	400	VAL
<u> </u>	D	405	ASP
<u> </u>	D	408	GLU
3	D	414	ARG
3	D	430	ASP
3	D	431	VAL
3	D	435	VAL
3	D	450	TYR
3	D	494	LYS
3	D	520	LEU
3	D	686	GLU
3	D	724	GLN
3	D	734	GLU
3	D	754	PHE
3	D	804	LEU
3	D	808	THR
3	D	813	LEU
3	D	817	GLU
3	D	823	LEU
3	D	828	LYS
3	D	833	GLU
3	D	892	ASP
3	D	935	LYS
3	D	943	THR
3	D	971	LEU
3	D	983	LEU
3	D	985	ASP
3	D	1001	GLU
3	D	1008	PHE
3	D	1012	GLU
3	D	1013	GLU
3	D	1029	ARG
3	D	1041	LEU
3	D	1044	LEU
3	D	1058	ARG
3	D	1070	TYR
3	D	1083	ASP
3	D	1106	VAL
0		1100	



Mol	Chain	Res	Type
3	D	1108	ARG
3	D	1109	GLU
3	D	1115	THR
3	D	1131	SER
3	D	1135	ARG
3	D	1151	ARG
3	D	1162	GLU
3	D	1170	ASP
3	D	1197	ARG
3	D	1207	TYR
3	D	1209	LEU
3	D	1235	GLN
3	D	1262	LEU
3	D	1290	LEU
3	D	1296	SER
3	D	1299	PHE
3	D	1304	LYS
3	D	1305	LEU
3	D	1314	LYS
3	D	1318	TYR
3	D	1325	LEU
3	D	1327	ARG
3	D	1342	GLU
3	D	1373	ARG
3	D	1383	ASP
3	D	1441	GLN
3	D	1460	ILE
3	D	1478	SER
3	D	1493	LYS
4	Е	14	ASP
4	Е	32	ARG
4	Е	35	PHE
4	Е	38	THR
4	Е	39	VAL
4	Е	40	LEU
4	Е	41	GLU
4	Е	47	LYS
4	Е	49	GLN
4	Е	51	LEU
4	Е	56	ASP
4	Е	83	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10)



such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	124	ASN
2	С	141	HIS
2	С	431	HIS
2	С	609	ASN
2	С	670	GLN
2	С	829	GLN
2	С	884	GLN
3	D	101	HIS
3	D	388	HIS
3	D	552	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	R	8/29~(27%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	R	22	U

There are no RNA pucker outliers to report.

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 3 ligands modelled in this entry, 3 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, 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	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	223/315~(70%)	-0.31	0 100 100	45, 90, 147, 194	0
1	В	223/315~(70%)	-0.38	0 100 100	40, 86, 139, 173	0
2	С	1083/1119~(96%)	-0.11	19 (1%) 68 62	32, 101, 186, 255	0
3	D	1358/1534~(88%)	0.02	68 (5%) 28 25	34, 102, 194, 264	0
4	Ε	93/99~(93%)	0.10	5 (5%) 25 23	58, 107, 184, 204	0
5	Ν	11/13~(84%)	2.78	9 (81%) 0 0	369, 412, 462, 465	0
6	R	9/29~(31%)	1.02	1 (11%) 5 6	178, 188, 215, 227	0
7	Т	22/22~(100%)	1.70	$6\ (27\%)\ 0\ 0$	202, 334, 453, 466	0
All	All	3022/3446~(87%)	-0.05	108 (3%) 42 38	32, 100, 193, 466	0

All ((108)	RSRZ	outliers	are	listed	below:
(100100	0.0101010	~~ ~	110000	0010111

Mol	Chain	Res	Type	RSRZ
4	Е	56	ASP	10.4
3	D	802	ALA	10.0
3	D	810	GLU	9.9
2	С	417	GLY	6.8
7	Т	9	DC	6.2
4	Е	57	ASP	5.7
3	D	1090	ASP	5.3
3	D	1296	SER	5.3
7	Т	1	DG	5.2
3	D	1324	PRO	4.9
3	D	1309	ALA	4.8
2	С	416	GLY	4.8
3	D	70	GLY	4.7
3	D	1295	GLU	4.7
2	С	270	GLY	4.5
3	D	365	ASP	4.4



4GZY

Mol	Chain	Res	Type	RSRZ	
3	D	194	GLY	4.3	
5	N	13	DC	4.3	
3	D	1308	GLU	4.1	
3	D	366	LYS	4.0	
7	Т	14	DA	4.0	
3	D	1279	GLY	4.0	
3	D	1280	VAL	4.0	
3	D	369	ALA	4.0	
3	D	367	ILE	3.9	
5	Ν	12	DC	3.9	
3	D	66	GLN	3.9	
5	Ν	11	DC	3.9	
3	D	1289	LYS	3.8	
3	D	1408	ILE	3.8	
3	D	79	GLU	3.7	
3	D	341	GLU	3.7	
2	С	1022	GLY	3.7	
2	С	320	HIS	3.6	
2	С	105	THR	3.6	
2	С	365	ASP	3.6	
3	D	63	TYR	3.6	
2	С	726	ILE	3.5	
7	Т	2	DG	3.4	
3	D	1313	VAL	3.3	
7	Т	3	DG	3.3	
3	D	368	VAL	3.2	
2	С	366	SER	3.2	
3	D	1491	THR	3.2	
3	D	58	CYS	3.1	
3	D	801	GLY	3.1	
3	D	81	THR	3.1	
2	С	167	LYS	3.0	
3	D	1273	VAL	3.0	
2	С	361	MET	3.0	
3	D	1316	GLY	3.0	
3	D	165	LYS	2.9	
3	D	372	ASP	2.9	
2	С	103	LYS	2.9	
3	D	67	ARG	2.9	
3	D	378	ILE	2.9	
3	D	215	TYR	2.9	
4	Е	55	PHE	2.9	



Mol	Chain	Res	Type	RSRZ
5	N	5	DG	2.9
3	D	371	ILE	2.9
3	D	2	LYS	2.8
5	N	8	DA	2.8
3	D	343	LYS	2.8
3	D	1312	LEU	2.8
3	D	1305	LEU	2.8
3	D	351	MET	2.7
2	С	418	LEU	2.7
2	С	112	GLU	2.7
3	D	62	LYS	2.7
2	С	741	GLY	2.7
3	D	65	ARG	2.7
3	D	370	ALA	2.6
5	Ν	10	DT	2.6
3	D	798	GLU	2.6
3	D	342	PRO	2.6
2	С	222	MET	2.6
3	D	211	VAL	2.5
3	D	350	HIS	2.5
3	D	1278	ASP	2.5
3	D	193	PRO	2.5
3	D	393	ILE	2.5
3	D	1317	ASP	2.5
3	D	1130	ARG	2.5
3	D	803	GLY	2.4
5	N	7	DG	2.4
3	D	28	LYS	2.4
3	D	57	GLU	2.4
5	N	9	DT	2.4
7	Т	8	DT	2.4
3	D	384	VAL	2.4
3	D	385	VAL	2.4
4	Е	2	ALA	2.3
5	N	3	DA	2.3
2	С	786	LYS	2.3
2	С	106	GLY	2.2
3	D	78	VAL	2.2
3	D	481	MET	2.2
3	D	71	LYS	2.2
3	D	61	GLY	2.1
3	D	69	GLU	2.1



Mol	Chain	Res	Type	RSRZ
3	D	44	LEU	2.1
3	D	73	CYS	2.1
2	С	1023	GLY	2.1
3	D	55	ASP	2.1
6	R	24	U	2.1
4	Е	41	GLU	2.1
3	D	1087	ARG	2.0
3	D	1285	GLU	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 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	$B-factors(Å^2)$	Q<0.9
8	ZN	D	1601	1/1	0.82	0.27	188,188,188,188	0
9	MG	D	1603	1/1	0.96	0.28	46,46,46,46	0
8	ZN	D	1602	1/1	0.98	0.12	80,80,80,80	0

6.5 Other polymers (i)

There are no such residues in this entry.

