

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	1XF1
Title	:	Structure of C5a peptidase- a key virulence factor from Streptococcus
Authors	:	Brown, C.K.; Gu, Z.Y.; Cleary, P.P.; Matsuka, Y.; Olmstead, S.; Ohlendorf,
		D.H.; Earhart, C.A.
Deposited on	:	2004-09-13
Resolution	:	1.90 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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 1.90 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.



Matria	Whole archive	Similar resolution
wietric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of cha	Quality of chain												
1	А	926	68%	27% ••	•											
1	В	926	60%	35% 5%	•											



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15509 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 C5a peptidase.

Mol	Chain	Residues		Α	toms			ZeroOcc	AltConf	Trace
1	А	926	Total 7182	C 4510	N 1211	0 1445	Se 16	0	0	0
1	В	926	Total 7182	C 4510	N 1211	0 1445	${ m Se}$ 16	4	0	0

Chain	Residue	Modelled	Actual	Comment	Reference						
А	219	MSE	MET	modified residue	UNP P15926						
А	227	MSE	MET	modified residue	UNP P15926						
A	259	MSE	MET	modified residue	UNP P15926						
А	353	MSE	MET	modified residue	UNP P15926						
А	433	MSE	MET	modified residue	UNP P15926						
А	513	MSE	MET	modified residue	UNP P15926						
А	522	MSE	MET	modified residue	UNP P15926						
А	536	MSE	MET	modified residue	UNP P15926						
А	550	MSE	MET	modified residue	UNP P15926						
А	585	MSE	MET	modified residue	UNP P15926						
А	648	THR	ALA	SEE REMARK 999	UNP P15926						
А	680	MSE	MET	modified residue	UNP P15926						
А	697	THR	LYS	SEE REMARK 999	UNP P15926						
А	702	MSE	MET	modified residue	UNP P15926						
А	794	PHE	LEU	SEE REMARK 999	UNP P15926						
А	969	MSE	MET	modified residue	UNP P15926						
А	996	MSE	THR	engineered mutation	UNP P15926						
А	1005	MSE	MET	modified residue	UNP P15926						
А	1015	MSE	MET	modified residue	UNP P15926						
В	219	MSE	MET	modified residue	UNP P15926						
В	227	MSE	MET	modified residue	UNP P15926						
В	259	MSE	MET	modified residue	UNP P15926						
В	353	MSE	MET	modified residue	UNP P15926						
В	433	MSE	MET	modified residue	UNP P15926						
В	513	MSE	MET	modified residue	UNP P15926						

There are 38 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
В	522	MSE	MET	modified residue	UNP P15926
В	536	MSE	MET	modified residue	UNP P15926
В	550	MSE	MET	modified residue	UNP P15926
В	585	MSE	MET	modified residue	UNP P15926
В	648	THR	ALA	SEE REMARK 999	UNP P15926
В	680	MSE	MET	modified residue	UNP P15926
В	697	THR	LYS	SEE REMARK 999	UNP P15926
В	702	MSE	MET	modified residue	UNP P15926
В	794	PHE	LEU	SEE REMARK 999	UNP P15926
В	969	MSE	MET	modified residue	UNP P15926
В	996	MSE	THR	engineered mutation	UNP P15926
В	1005	MSE	MET	modified residue	UNP P15926
В	1015 MSE		MET	modified residue	UNP P15926

• Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf						
3	А	1	Total Ca 1 1	0	0						
3	В	1	Total Ca 1 1	0	0						

• Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total C O 13 6 7	0	0
4	А	1	Total C O 13 6 7	0	0
4	А	1	Total C O 13 6 7	0	0
4	В	1	Total C O 13 6 7	0	0
4	В	1	Total C O 13 6 7	0	0
4	В	1	Total C O 13 6 7	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	544	Total O 544 544	0	0
5	В	513	Total O 513 513	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. 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. 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.

Note EDS was not executed.

• Molecule 1: C5a peptidase



 \bullet Molecule 1: C5a peptidase





D180	1011	G185 K186		V189 D190	<mark>Q191</mark>	G194	T195	H196 V197	S198	G199 T000	1200 L201	8202	0000	8207 8207	E208	T209	K210 F211	P212	Y213	R214	L215 E216	G217	A218	M219	E221	A222	0223	L224 L225	L226	M227 B228	V229	E230	1231 V737	N233		A230	R240	N241	Y242	I246	R247 D248		L252
G253	A254 K255	V256	M259	N263	A264	L266	t t	L2/1 P272	D273	E274	1210	F279		COZA	V287		A308	A321		V328	Y331		L337	T338	V341	R342	V343 V343	N344 T345	A346	D347	0103	M353	P354 V355	L356	S357	1.358 N.359	R360	F361	E362	N364	K365 A366	Y367	D368
Y369	A370 Y371	A372 N373		K377	D380 F361	K382	D383	V384 K385	G386	K387	1300 A389	L390	1391 5200		D3 <mark>97</mark>	F398	K399 D400	0	K406	K407	A408 G409	A410	V411	G412	V413 L414	I415	Y416	0419	-	1425 E426	E420 L427		D431	M433	P434	A435 A436	F437	1438	5439 R440	K441	D442	L445	L446
	P450	Q451 K460	T453	I 454 T 455	F456 MAE7		P460	K461 V462		T465	G468	-	L471	S476	W477		1485	P492	G493	Q494	D495 I496	-	V500		K504		M513	A515	P516	MECO	G523	L524	KE07	0528 0528	Y529	E530	0532	Y533	MERG	T537	P538	E540	R541
L542	A545	К546 К547	V548	L549	T554	L556	Y557	K562		0570	4572 A572	G573	C L L	1504 M585	-	D589	K590 D591	N592	T593		969X	N601		F606	T609	V610	N611	N614	K615	S616 D617	K618	P619	ц620 т621	L622	Y623	4626	0704	F638	A639 1.640		V644	q651	K652
1653 201	1054 1655	P656 A657	N658	S659	0662 Vee3	T664	V665	P666 T667		R671	0679		F685	R691	-	0694 2001	D695	K698	E699	E700	1704	P705	¥706	1707	F713		1723 V72A	1/24	G7 <mark>29</mark>	<u>п73</u> Л	E735	A736	N737 5738	D739	A740	K/41 D742	Q743	L744	D745	L749	N757	F758	T759
A760	K772	K775	E776	G777 V778	E779	I781	E782	D/83	E785	S786	G796	T797	F798	0801		H806	TROO		Y818		678X	0833	F834	Q 835	F838		N844	V849		K852	W858	T859	5860 F861	V862		N809	L874		R /8	R882	F883 F884	K885	T886
R887		K8 <mark>9</mark> 3 D804	H 000	V898	Y903	T910	P911	1912 S913		P932	000	F940	S941	1942 E943	D944	R945	R946	K952	P953	K954	GG6.I.	P958	V959	Y960	E962	R963	1964 Agee	ABOO	M969	DQ7 A		<mark>¥97</mark> 8	DQ84	1	E991	E994	T995	M996	E997	A999	V1010		D1014
M1015	N1018	11019 T1020		K1026	E1029	H1031																																					



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	114.70Å 75.11Å 132.39Å	Depositor
a, b, c, α , β , γ	90.00° 104.95° 90.00°	Depositor
Resolution (Å)	50.00 - 1.90	Depositor
% Data completeness	(Not available) (50.00-1.90)	Depositor
(in resolution range)	(100 available) (50.00 1.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.269	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15509	wwPDB-VP
Average B, all atoms $(Å^2)$	51.0	wwPDB-VP



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: CIT, CA, ACT

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	Bond	angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.34	0/7312	0.63	0/9884
1	В	0.33	0/7312	0.61	0/9884
All	All	0.33	0/14624	0.62	0/19768

There are no bond length outliers.

There are no bond angle outliers.

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	7182	0	7004	319	0
1	В	7182	0	7005	384	0
2	А	4	0	3	0	0
2	В	4	0	3	0	0
3	А	1	0	0	0	0
3	В	1	0	0	0	0
4	А	39	0	15	0	0
4	В	39	0	15	2	0
5	А	544	0	0	34	0
5	В	513	0	0	23	0
All	All	15509	0	14045	688	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 24.

All (688) 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:A:778:VAL:HG21	1:A:784:ILE:HD11	1.40	1.03
1:A:210:LYS:HA	1:A:337:LEU:HD12	1.40	1.03
1:B:343:VAL:HG12	1:B:454:ILE:HG22	1.41	1.02
1:A:465:THR:HG23	1:A:468:GLY:H	1.23	1.01
1:B:465:THR:HG23	1:B:468:GLY:H	1.25	1.00
1:A:271:LEU:HD23	1:A:271:LEU:H	1.26	1.00
1:B:271:LEU:HD23	1:B:271:LEU:H	1.27	1.00
1:A:952:LYS:HB3	1:A:953:PRO:HA	1.43	1.00
1:A:343:VAL:HG12	1:A:454:ILE:HG22	1.41	0.99
1:B:536:MSE:HE2	1:B:540:GLU:HB3	1.41	0.99
1:B:958:PRO:HG2	1:B:1015:MSE:HG3	1.43	0.99
1:A:440:ARG:NH1	1:A:444:LEU:HD11	1.78	0.99
1:A:219:MSE:HE2	1:A:520:GLY:HA2	1.44	0.98
1:A:246:ILE:HD11	1:A:278:ALA:HB1	1.48	0.96
1:B:995:THR:HG23	1:B:997:GLU:H	1.31	0.95
1:B:360:ARG:HH11	1:B:360:ARG:HB3	1.31	0.95
1:B:556:LEU:H	1:B:570:GLN:HE22	1.05	0.93
1:A:556:LEU:H	1:A:570:GLN:HE22	1.04	0.93
1:A:216:GLU:HG2	1:A:224:LEU:HD21	1.51	0.92
1:A:141:ARG:HE	1:A:141:ARG:HA	1.37	0.90
1:B:835:GLN:HE21	1:B:882:ARG:HE	1.20	0.89
1:B:522:MSE:HG3	1:B:549:LEU:HD22	1.54	0.89
1:B:749:LEU:HD23	1:B:749:LEU:H	1.37	0.89
1:A:160:LYS:HB2	1:A:165:ILE:HB	1.54	0.88
1:B:528:GLN:HE21	1:B:532:GLN:HE22	1.23	0.87
1:A:960:TYR:HA	1:A:1015:MSE:HE3	1.56	0.87
1:B:139:ALA:HB1	1:B:206:PRO:HA	1.56	0.87
1:B:838:PHE:H	1:B:869:ASN:HD22	1.19	0.87
1:B:944:ASP:OD2	1:B:946:ARG:HD3	1.76	0.86
1:B:611:ASN:ND2	1:B:662:GLN:HG2	1.91	0.85
1:A:522:MSE:HG3	1:A:549:LEU:HD22	1.57	0.85
1:A:622:LEU:HD21	1:A:655:ILE:HD13	1.60	0.84
1:B:749:LEU:H	1:B:749:LEU:CD2	1.90	0.84
1:A:835:GLN:NE2	1:A:882:ARG:HE	1.76	0.82
1:A:991:GLU:OE2	1:B:263:ASN:HB3	1.80	0.82
1:A:536:MSE:O	1:A:537:THR:HB	1.79	0.81
1:A:150:TYR:H	1:A:223:GLN:HE22	1.29	0.81



• • • •	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:522:MSE:HE1	1:B:542:LEU:HD12	1.63	0.81
1:B:200:ILE:HG22	1:B:201:LEU:HG	1.63	0.81
1:B:585:MSE:HG2	1:B:614:ASN:HA	1.64	0.80
1:A:835:GLN:HE21	1:A:882:ARG:HE	1.26	0.79
1:A:421:LYS:HG3	1:A:560:ASP:OD2	1.82	0.79
1:B:160:LYS:HE3	1:B:168:GLY:H	1.47	0.79
1:A:644:VAL:HG12	5:A:1124:HOH:O	1.83	0.79
1:B:835:GLN:NE2	1:B:882:ARG:HE	1.80	0.79
1:B:145:LYS:N	1:B:145:LYS:HD2	2.00	0.77
1:B:139:ALA:HB2	1:B:208:GLU:HG3	1.66	0.77
1:B:209:THR:HG22	1:B:210:LYS:HG3	1.67	0.77
1:B:219:MSE:HE3	1:B:527:LYS:HZ1	1.48	0.77
1:B:780:ASN:ND2	1:B:783:ASP:H	1.83	0.77
1:B:621:GLU:HG2	1:B:654:THR:HG22	1.65	0.77
1:A:644:VAL:HG23	5:A:1332:HOH:O	1.83	0.77
1:B:353:MSE:HE1	1:B:446:LEU:HD11	1.66	0.76
1:A:823:PRO:HG2	1:A:929:ASN:HD21	1.50	0.76
1:B:271:LEU:HD21	1:B:321:ALA:HB3	1.67	0.76
1:B:656:PRO:HG2	1:B:659:SER:OG	1.86	0.75
1:B:137:HIS:HD1	1:B:513:MSE:HE3	1.52	0.75
1:A:698:LYS:HG2	1:A:699:GLU:H	1.50	0.75
1:B:995:THR:HG22	1:B:999:ALA:H	1.51	0.75
1:A:838:PHE:H	1:A:869:ASN:HD22	1.31	0.75
1:B:124:THR:HG21	1:B:219:MSE:HE1	1.69	0.75
1:A:226:LEU:C	1:A:227:MSE:HE3	2.06	0.75
1:A:952:LYS:CB	1:A:953:PRO:HA	2.16	0.75
1:A:952:LYS:HB3	1:A:953:PRO:CA	2.17	0.75
1:B:337:LEU:HD21	1:B:460:PRO:HB2	1.65	0.75
1:B:503:ASN:HD22	1:B:504:LYS:HD2	1.52	0.74
1:A:898:VAL:HG12	1:A:903:TYR:OH	1.86	0.74
1:A:343:VAL:CG1	1:A:454:ILE:HG22	2.15	0.74
1:A:271:LEU:H	1:A:271:LEU:CD2	1.99	0.74
1:B:781:ILE:HA	1:B:784:ILE:HG23	1.69	0.74
1:B:147:LYS:HB2	1:B:147:LYS:NZ	2.03	0.74
1:B:271:LEU:HB2	1:B:272:PRO:HD2	1.69	0.74
1:B:838:PHE:H	1:B:869:ASN:ND2	1.85	0.74
1:B:691:ARG:HD2	1:B:700:GLU:OE2	1.88	0.73
1:A:246:ILE:HD11	1:A:278:ALA:CB	2.19	0.73
1:A:378:GLU:O	1:A:379:ASP:HB2	1.88	0.72
1:A:780:ASN:HD21	1:A:782:GLU:HG3	1.54	0.72
1:A:379:ASP:HA	1:A:382:LYS:HG3	1.70	0.71



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:355:VAL:HG12	1:B:438:ILE:HG22	1.71	0.71
1:B:171:VAL:O	1:B:172:ASN:HB3	1.90	0.71
1:A:303:THR:HB	5:A:1144:HOH:O	1.90	0.71
1:A:536:MSE:O	1:A:540:GLU:HB2	1.89	0.71
1:A:967:THR:HG23	5:A:1535:HOH:O	1.91	0.71
1:B:742:ASP:HB3	1:B:809:ILE:HB	1.73	0.71
1:B:167:TYR:HB2	1:B:179:HIS:CD2	2.26	0.70
1:A:388:ILE:HD12	1:A:454:ILE:HD11	1.73	0.70
1:A:254:ALA:O	1:A:255:LYS:HB2	1.91	0.70
1:B:671:ARG:HG2	5:B:1162:HOH:O	1.90	0.70
5:A:1173:HOH:O	1:B:996:MSE:HE3	1.91	0.70
1:A:168:GLY:HA3	1:A:177:TYR:CE1	2.27	0.69
1:B:342:ARG:HG3	1:B:457:ASN:HD21	1.58	0.69
1:A:440:ARG:HH12	1:A:444:LEU:HD11	1.54	0.69
1:A:465:THR:HG23	1:A:468:GLY:N	2.03	0.69
1:B:337:LEU:CD2	1:B:460:PRO:HB2	2.22	0.69
1:A:384:VAL:HG13	1:A:410:ALA:HB2	1.75	0.68
1:B:123:GLY:HA2	1:B:148:ALA:HB3	1.75	0.68
1:B:528:GLN:HE21	1:B:532:GLN:NE2	1.91	0.68
1:B:932:PRO:HD2	1:B:1020:THR:HG23	1.76	0.68
1:A:622:LEU:HD23	1:A:622:LEU:N	2.09	0.68
1:B:242:TYR:O	1:B:246:ILE:HG23	1.93	0.68
1:A:150:TYR:H	1:A:223:GLN:NE2	1.90	0.68
1:A:205:ALA:N	1:A:206:PRO:HD3	2.09	0.68
1:A:838:PHE:H	1:A:869:ASN:ND2	1.91	0.68
1:B:522:MSE:CE	1:B:542:LEU:HD12	2.23	0.68
1:B:264:ALA:HB1	5:B:1395:HOH:O	1.93	0.67
1:B:271:LEU:H	1:B:271:LEU:CD2	2.04	0.67
1:B:610:VAL:C	1:B:611:ASN:HD22	1.97	0.67
1:A:440:ARG:HH11	1:A:444:LEU:HD11	1.55	0.67
1:B:644:VAL:HG12	5:B:1128:HOH:O	1.95	0.67
1:B:1020:THR:HG22	5:B:1251:HOH:O	1.95	0.66
1:A:172:ASN:HB2	1:A:174:LYS:O	1.96	0.66
1:B:173:ASP:O	1:B:175:VAL:N	2.28	0.66
1:B:522:MSE:HG3	1:B:549:LEU:CD2	2.25	0.66
1:B:556:LEU:H	1:B:570:GLN:NE2	1.88	0.66
1:B:745:ASP:OD2	1:B:806:HIS:HD2	1.78	0.66
1:A:140:TRP:O	1:A:141:ARG:HB2	1.95	0.66
1:B:433:MSE:HA	1:B:433:MSE:HE2	1.77	0.66
1:A:960:TYR:CA	1:A:1015:MSE:HE3	2.24	0.66
1:B:232:VAL:O	1:B:233:ASN:HB2	1.96	0.65



	A O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:958:PRO:HG2	1:B:1015:MSE:CG	2.21	0.65
1:A:749:LEU:HD12	1:B:749:LEU:HG	1.77	0.65
1:A:931:THR:HG22	5:A:1249:HOH:O	1.95	0.65
1:B:515:ALA:HB3	1:B:516:PRO:HD3	1.77	0.65
1:B:844:ASN:HB3	5:B:1610:HOH:O	1.96	0.65
1:A:200:ILE:HG22	1:A:201:LEU:HG	1.77	0.65
1:A:503:ASN:HD22	1:A:503:ASN:H	1.45	0.65
1:B:590:LYS:HD3	1:B:609:THR:HG21	1.77	0.65
1:B:644:VAL:HG23	5:B:1347:HOH:O	1.97	0.65
1:A:209:THR:HG22	1:A:210:LYS:HG3	1.78	0.64
1:B:384:VAL:C	1:B:409:GLY:HA3	2.17	0.64
1:B:213:TYR:HA	5:B:1416:HOH:O	1.96	0.64
1:B:360:ARG:HB3	1:B:360:ARG:NH1	2.09	0.64
1:A:556:LEU:H	1:A:570:GLN:NE2	1.87	0.64
1:B:153:LYS:O	1:B:157:GLU:HG2	1.97	0.64
1:B:671:ARG:HG2	1:B:671:ARG:HH11	1.63	0.64
1:B:137:HIS:ND1	1:B:513:MSE:HE3	2.13	0.64
1:B:601:ASN:HD21	1:B:713:PHE:H	1.45	0.64
1:A:140:TRP:HA	1:A:174:LYS:HD2	1.79	0.64
1:A:528:GLN:HE21	1:A:532:GLN:NE2	1.95	0.63
1:B:562:LYS:HE2	1:B:562:LYS:HA	1.80	0.63
1:A:135:LYS:HB2	1:B:943:GLU:OE1	1.99	0.63
1:B:384:VAL:O	1:B:409:GLY:HA3	1.98	0.63
1:B:124:THR:HG22	1:B:125:VAL:N	2.14	0.63
1:B:359:ASN:HB2	1:B:434:PRO:HA	1.80	0.63
1:A:174:LYS:O	1:A:175:VAL:HB	1.99	0.63
1:B:389:ALA:HB3	1:B:413:VAL:HG12	1.81	0.63
1:A:149:ARG:HH12	1:A:253:GLY:HA3	1.63	0.63
1:B:427:LEU:CD2	1:B:437:PHE:HB2	2.29	0.62
1:B:995:THR:HG21	5:B:1345:HOH:O	1.99	0.62
1:A:485:ILE:HD12	1:A:571:GLY:HA2	1.82	0.62
1:B:219:MSE:HE3	1:B:527:LYS:NZ	2.13	0.62
1:B:898:VAL:HG22	1:B:903:TYR:OH	2.00	0.62
1:B:144:ASP:C	1:B:145:LYS:HD2	2.19	0.62
1:B:112:LYS:O	1:B:116:GLU:HG3	1.99	0.62
1:B:749:LEU:HD23	1:B:749:LEU:N	2.12	0.62
1:B:829:ARG:NH1	5:B:1173:HOH:O	2.31	0.62
1:A:530:GLU:HA	1:A:541:ARG:HE	1.65	0.62
1:B:433:MSE:HE2	1:B:434:PRO:HD2	1.82	0.62
1:A:193:HIS:HB2	1:A:197:VAL:HA	1.82	0.61
1:A:522:MSE:HE3	1:A:545:ALA:HB3	1.82	0.61



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:462:VAL:HG23	1:B:462:VAL:O	2.00	0.61
1:A:515:ALA:HB3	1:A:516:PRO:HD3	1.83	0.61
1:B:485:ILE:CG1	1:B:596:LYS:HD2	2.30	0.61
1:A:738:SER:O	1:A:739:ASP:HB2	1.99	0.61
1:A:964:ILE:HD13	1:A:1010:TYR:HA	1.81	0.61
1:B:365:LYS:H	1:B:455:THR:HG23	1.65	0.61
1:B:737:ASN:HD22	1:B:743:GLN:NE2	1.99	0.61
1:A:343:VAL:HG11	1:A:446:LEU:CD2	2.30	0.61
1:A:548:VAL:O	1:A:552:SER:HB2	2.00	0.61
1:A:271:LEU:CD2	1:A:321:ALA:HB3	2.31	0.61
1:A:216:GLU:CG	1:A:224:LEU:HD21	2.28	0.60
1:A:507:LYS:HD3	5:A:1436:HOH:O	2.01	0.60
1:B:215:LEU:O	1:B:216:GLU:HG3	2.01	0.60
1:A:882:ARG:NH1	1:B:996:MSE:HE1	2.17	0.60
1:B:343:VAL:CG1	1:B:454:ILE:HG22	2.26	0.60
1:A:331:TYR:HB2	1:A:471:LEU:HD22	1.83	0.60
1:A:867:VAL:HG13	5:A:1115:HOH:O	2.02	0.60
1:B:522:MSE:HE3	1:B:545:ALA:HB3	1.82	0.60
1:B:780:ASN:HD21	1:B:783:ASP:H	1.50	0.60
1:B:958:PRO:O	1:B:1015:MSE:HG2	2.02	0.60
1:A:144:ASP:O	1:A:145:LYS:HB2	2.02	0.60
1:B:136:ASN:O	1:B:137:HIS:HB3	2.02	0.59
1:B:780:ASN:C	1:B:782:GLU:H	2.04	0.59
1:B:893:LYS:O	1:B:894:ASP:C	2.40	0.59
1:A:384:VAL:CG1	1:A:410:ALA:HB2	2.31	0.59
1:A:379:ASP:OD2	1:A:382:LYS:HE3	2.01	0.59
1:B:852:LYS:HE3	5:B:1324:HOH:O	2.00	0.59
1:B:126:VAL:HG22	1:B:256:VAL:HG11	1.84	0.59
1:A:180:ASP:O	1:A:183:LYS:HD2	2.03	0.59
1:B:124:THR:HG21	1:B:219:MSE:CE	2.32	0.59
1:B:465:THR:HG23	1:B:468:GLY:N	2.08	0.59
1:A:214:ARG:HG2	5:A:1578:HOH:O	2.03	0.59
1:A:536:MSE:HE2	1:A:540:GLU:HB3	1.85	0.59
1:B:414:LEU:HD23	1:B:436:ALA:HB3	1.86	0.58
1:B:952:LYS:HD2	1:B:952:LYS:C	2.22	0.58
1:A:723:ILE:HD11	1:A:760:ALA:HB2	1.86	0.58
1:B:107:ASP:OD2	1:B:110:GLN:HA	2.02	0.58
1:B:338:THR:HG21	1:B:354:PRO:HB3	1.85	0.58
1:B:454:ILE:O	1:B:454:ILE:HD12	2.02	0.58
1:B:838:PHE:N	1:B:869:ASN:HD22	1.96	0.58
1:A:960:TYR:CB	1:A:1015:MSE:HE3	2.33	0.58



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:533:TYR:N	1:A:534:PRO:HD3	2.18	0.58
1:B:655:ILE:N	1:B:655:ILE:HD12	2.18	0.58
1:A:585:MSE:HG3	5:A:1620:HOH:O	2.04	0.58
1:A:602:VAL:HG13	1:A:603:SER:O	2.03	0.58
1:B:590:LYS:HD3	1:B:609:THR:CG2	2.34	0.58
1:B:557:TYR:OH	1:B:562:LYS:HE2	2.03	0.58
1:B:995:THR:HG23	1:B:997:GLU:N	2.11	0.58
1:A:273:ASP:HA	1:A:276:LYS:NZ	2.19	0.57
1:A:379:ASP:CG	1:A:382:LYS:HE3	2.25	0.57
1:B:171:VAL:O	1:B:172:ASN:CB	2.51	0.57
1:A:183:LYS:HD3	1:A:183:LYS:H	1.69	0.57
1:B:367:TYR:HB2	1:B:454:ILE:CD1	2.34	0.57
1:A:355:VAL:CG2	1:A:436:ALA:HB1	2.33	0.57
1:B:932:PRO:HB3	1:B:955:THR:HG22	1.86	0.57
1:B:228:ARG:HG3	1:B:228:ARG:HH11	1.69	0.57
1:B:148:ALA:O	1:B:149:ARG:O	2.22	0.57
1:B:440:ARG:HG3	1:B:440:ARG:HH11	1.69	0.57
1:A:536:MSE:O	1:A:537:THR:CB	2.52	0.57
1:A:729:GLY:C	1:A:736:ALA:HB2	2.24	0.57
1:B:723:ILE:HD11	1:B:760:ALA:HB2	1.85	0.57
1:A:775:LYS:HE3	1:A:775:LYS:N	2.19	0.57
1:A:833:GLN:HE22	1:A:887:ARG:HH21	1.52	0.57
1:B:427:LEU:HD21	1:B:437:PHE:HB2	1.87	0.57
1:A:376:THR:HG22	5:A:1342:HOH:O	2.04	0.57
1:A:302:LYS:NZ	1:A:302:LYS:HB3	2.20	0.57
1:B:945:ARG:CZ	1:B:991:GLU:HG2	2.35	0.57
1:A:691:ARG:HD2	1:A:700:GLU:OE2	2.05	0.56
1:A:850:LEU:CD2	1:A:856:VAL:HG22	2.36	0.56
1:B:150:TYR:HB2	1:B:223:GLN:HE22	1.70	0.56
1:B:153:LYS:HB2	5:B:1253:HOH:O	2.03	0.56
1:B:272:PRO:HB2	1:B:274:GLU:OE1	2.05	0.56
1:B:160:LYS:CE	1:B:168:GLY:H	2.18	0.56
1:B:388:ILE:HD12	1:B:454:ILE:HD11	1.88	0.56
1:B:738:SER:O	1:B:739:ASP:HB2	2.06	0.56
1:B:933:GLU:OE2	1:B:954:LYS:HE3	2.06	0.56
1:A:146:THR:O	1:A:146:THR:HG22	2.06	0.56
1:B:137:HIS:HD1	1:B:513:MSE:CE	2.18	0.56
1:B:168:GLY:HA2	1:B:177:TYR:CE1	2.40	0.56
1:A:254:ALA:O	1:A:255:LYS:CB	2.54	0.56
1:B:410:ALA:O	1:B:411:VAL:HB	2.06	0.56
1:B:621:GLU:HG2	1:B:654:THR:CG2	2.35	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:271:LEU:HD21	1:A:321:ALA:HB3	1.87	0.56
1:A:634:ASP:HB2	5:A:1583:HOH:O	2.05	0.56
1:A:734:HIS:HD2	5:A:1116:HOH:O	1.88	0.56
1:A:912:ILE:HD12	1:A:913:SER:N	2.21	0.56
1:A:177:TYR:CD2	1:A:227:MSE:HE2	2.41	0.56
1:B:893:LYS:HD2	5:B:1550:HOH:O	2.06	0.56
1:A:637:HIS:HD2	5:A:1250:HOH:O	1.88	0.55
1:B:137:HIS:NE2	1:B:211:GLU:HG2	2.21	0.55
1:A:264:ALA:O	1:A:265:ALA:HB3	2.07	0.55
1:A:171:VAL:O	1:A:172:ASN:O	2.23	0.55
1:B:611:ASN:HD22	1:B:611:ASN:N	2.03	0.55
1:A:738:SER:O	1:A:739:ASP:CB	2.54	0.55
1:A:343:VAL:HG11	1:A:446:LEU:HD21	1.88	0.55
1:B:206:PRO:O	1:B:207:SER:HB3	2.07	0.55
1:A:210:LYS:HA	1:A:337:LEU:CD1	2.26	0.55
1:A:263:ASN:HB2	1:B:991:GLU:OE1	2.06	0.55
1:A:503:ASN:H	1:A:503:ASN:ND2	2.04	0.55
1:B:353:MSE:SE	1:B:442:ASP:HB3	2.57	0.55
1:A:132:GLY:HA3	1:B:942:THR:HG23	1.88	0.54
1:A:944:ASP:OD1	1:A:946:ARG:HD2	2.08	0.54
1:B:454:ILE:HD13	1:B:456:PHE:HE1	1.72	0.54
1:A:113:THR:HG21	1:A:578:LYS:HG3	1.89	0.54
1:A:141:ARG:HE	1:A:141:ARG:CA	2.14	0.54
1:A:181:TYR:O	1:A:241:ASN:ND2	2.41	0.54
1:A:602:VAL:HG22	5:A:1453:HOH:O	2.06	0.54
1:A:912:ILE:HD12	1:A:912:ILE:C	2.27	0.54
1:A:587:VAL:HG22	1:A:612:VAL:HG22	1.90	0.54
1:A:171:VAL:HG12	1:A:172:ASN:OD1	2.08	0.54
1:A:737:ASN:ND2	1:A:740:ALA:HB3	2.23	0.54
1:A:772:LYS:O	1:A:776:GLU:HG3	2.07	0.54
1:A:838:PHE:N	1:A:869:ASN:HD22	2.03	0.54
1:A:926:ILE:HD12	1:A:927:VAL:N	2.22	0.54
1:A:537:THR:HG22	1:A:539:SER:H	1.71	0.54
1:B:216:GLU:O	1:B:218:ALA:N	2.39	0.54
1:B:537:THR:HG23	1:B:540:GLU:H	1.72	0.54
1:A:833:GLN:NE2	1:A:887:ARG:HH21	2.06	0.54
1:A:932:PRO:HD3	1:A:1018:ASN:HB3	1.88	0.54
1:A:655:ILE:HD12	1:A:655:ILE:N	2.23	0.53
1:A:296:ASP:OD2	1:A:302:LYS:HG3	2.07	0.53
1:B:213:TYR:CD1	1:B:513:MSE:HB3	2.43	0.53
1:A:823:PRO:HG2	1:A:929:ASN:ND2	2.22	0.53



	A t area D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:926:ILE:HD12	1:A:926:ILE:C	2.29	0.53
1:A:952:LYS:CB	1:A:953:PRO:CA	2.81	0.53
1:B:213:TYR:C	1:B:214:ARG:HD2	2.28	0.53
1:B:785:GLU:HG3	1:B:969:MSE:CE	2.39	0.53
1:B:158:LYS:O	1:B:162:GLU:HG3	2.09	0.53
1:B:362:GLU:OE1	1:B:365:LYS:HE3	2.08	0.53
1:B:178:TYR:HA	1:B:226:LEU:O	2.08	0.53
1:B:749:LEU:CD2	1:B:749:LEU:N	2.67	0.53
1:A:271:LEU:CD2	1:A:319:PRO:HB2	2.39	0.53
1:A:150:TYR:N	1:A:223:GLN:HE22	2.03	0.53
1:A:798:PHE:HB3	1:A:960:TYR:CE1	2.44	0.53
1:A:882:ARG:CZ	1:B:996:MSE:HE1	2.38	0.53
1:A:585:MSE:HG2	1:A:614:ASN:HA	1.91	0.53
1:B:360:ARG:HH11	1:B:360:ARG:CB	2.15	0.53
1:A:503:ASN:HD22	1:A:503:ASN:N	2.05	0.53
1:A:698:LYS:HG2	1:A:699:GLU:N	2.22	0.53
1:A:779:GLU:O	1:A:780:ASN:HB3	2.07	0.53
1:A:801:GLN:NE2	1:A:963:ARG:HG2	2.23	0.53
1:B:231:ILE:HD11	1:B:266:LEU:HD21	1.89	0.53
1:B:775:LYS:HE3	5:B:1431:HOH:O	2.07	0.53
1:B:652:LYS:NZ	1:B:654:THR:HG23	2.23	0.53
1:B:801:GLN:NE2	1:B:963:ARG:HG2	2.24	0.53
1:A:273:ASP:HA	1:A:276:LYS:HZ3	1.73	0.52
1:B:912:ILE:HD12	1:B:913:SER:N	2.23	0.52
1:A:738:SER:HA	1:A:741:LYS:HE3	1.90	0.52
1:A:440:ARG:CZ	5:A:1614:HOH:O	2.57	0.52
1:B:358:THR:O	1:B:359:ASN:HB2	2.10	0.52
1:A:145:LYS:CD	1:A:147:LYS:HB2	2.40	0.52
1:A:168:GLY:HA3	1:A:177:TYR:HE1	1.74	0.52
1:A:867:VAL:HG12	5:A:1229:HOH:O	2.08	0.52
1:B:530:GLU:HA	1:B:541:ARG:NE	2.25	0.52
1:B:801:GLN:HE22	1:B:963:ARG:HG2	1.74	0.52
1:A:129:ILE:HG21	1:A:242:TYR:CE2	2.45	0.52
1:A:597:VAL:O	1:A:706:TYR:HA	2.08	0.52
1:B:995:THR:CG2	1:B:999:ALA:H	2.21	0.52
1:A:858:TRP:CH2	1:A:860:SER:HB3	2.45	0.52
1:B:123:GLY:CA	1:B:148:ALA:HB3	2.38	0.52
1:A:140:TRP:HZ2	1:A:205:ALA:HB3	1.75	0.52
1:B:223:GLN:HG3	5:B:1314:HOH:O	2.09	0.52
1:A:414:LEU:HD11	1:A:454:ILE:HD13	1.92	0.51
1:A:271:LEU:HB2	1:A:272:PRO:HD2	1.92	0.51



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:271:LEU:HG	1:A:321:ALA:HB3	1.92	0.51
1:B:123:GLY:HA2	1:B:148:ALA:CB	2.40	0.51
1:B:383:ASP:C	1:B:385:LYS:H	2.11	0.51
1:B:414:LEU:CD2	1:B:436:ALA:HB3	2.40	0.51
1:A:943:GLU:OE2	1:B:135:LYS:HB2	2.10	0.51
1:B:781:ILE:HA	1:B:784:ILE:CG2	2.38	0.51
1:B:419:GLN:HE22	4:B:1104:CIT:H41	1.75	0.51
1:B:964:ILE:HD13	1:B:1010:TYR:HA	1.93	0.51
1:A:246:ILE:CD1	1:A:278:ALA:HB1	2.31	0.51
1:A:666:PRO:HG2	5:A:1324:HOH:O	2.11	0.51
1:B:242:TYR:OH	1:B:259:MSE:HB3	2.10	0.51
1:B:618:LYS:NZ	1:B:620:GLN:HE22	2.09	0.51
1:B:125:VAL:HB	1:B:253:GLY:O	2.11	0.51
1:B:368:ASP:CB	1:B:387:LYS:HD3	2.41	0.51
1:A:503:ASN:ND2	1:A:504:LYS:HD3	2.26	0.51
1:A:145:LYS:C	1:A:147:LYS:H	2.15	0.50
1:B:371:TYR:HD1	1:B:390:LEU:HD22	1.76	0.50
1:B:1026:LYS:O	1:B:1029:GLU:HG2	2.12	0.50
1:B:653:ILE:HD13	1:B:663:VAL:HG22	1.93	0.50
5:A:1173:HOH:O	1:B:996:MSE:HG2	2.10	0.50
1:B:361:PHE:CE1	1:B:434:PRO:HB2	2.46	0.50
1:B:112:LYS:HG2	1:B:116:GLU:OE2	2.10	0.50
1:B:138:GLU:C	1:B:140:TRP:H	2.13	0.50
1:B:181:TYR:HE2	1:B:227:MSE:HG2	1.76	0.50
1:B:271:LEU:HD11	1:B:275:THR:HG21	1.94	0.50
1:B:345:THR:HG22	1:B:346:ALA:N	2.26	0.50
1:B:860:SER:HB2	1:B:885:LYS:O	2.12	0.50
1:A:528:GLN:HE21	1:A:532:GLN:HE22	1.56	0.50
1:B:213:TYR:H	1:B:213:TYR:HD2	1.58	0.50
1:B:367:TYR:HB2	1:B:454:ILE:HD11	1.93	0.50
1:B:371:TYR:CZ	1:B:373:ASN:HA	2.46	0.50
1:B:147:LYS:HB2	1:B:147:LYS:HZ2	1.74	0.50
1:A:271:LEU:HD22	1:A:319:PRO:HB2	1.94	0.50
1:A:358:THR:O	1:A:359:ASN:HB2	2.12	0.50
1:A:590:LYS:HA	1:A:611:ASN:OD1	2.12	0.50
1:B:584:THR:OG1	1:B:616:SER:HB3	2.11	0.50
1:B:213:TYR:N	1:B:213:TYR:CD2	2.79	0.49
1:B:849:VAL:HG23	1:B:858:TRP:HE3	1.77	0.49
1:B:178:TYR:CG	1:B:178:TYR:O	2.65	0.49
1:B:440:ARG:HG3	1:B:440:ARG:NH1	2.27	0.49
1:A:532:GLN:O	1:A:533:TYR:HB2	2.13	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:893:LYS:HE2	5:A:1334:HOH:O	2.12	0.49
1:A:945:ARG:HG3	1:A:989:LEU:O	2.12	0.49
1:B:210:LYS:O	1:B:212:PRO:HD3	2.12	0.49
1:B:331:TYR:HB2	1:B:471:LEU:HD22	1.94	0.49
1:B:496:ILE:HD11	5:B:1350:HOH:O	2.13	0.49
1:B:639:ALA:O	1:B:640:LEU:HB2	2.12	0.49
1:A:770:ILE:O	1:A:774:VAL:HG23	2.13	0.49
1:B:147:LYS:HB2	1:B:147:LYS:HZ3	1.76	0.49
1:A:250:ILE:HD11	1:A:282:ALA:HB2	1.95	0.49
1:A:671:ARG:HB2	5:A:1514:HOH:O	2.13	0.49
1:B:141:ARG:HH12	1:B:216:GLU:CD	2.16	0.49
1:B:606:PHE:CE1	1:B:667:ILE:HD12	2.48	0.49
1:B:149:ARG:O	1:B:223:GLN:NE2	2.46	0.49
1:B:283:LYS:NZ	1:B:283:LYS:HB2	2.28	0.49
1:A:542:LEU:HD23	1:A:542:LEU:C	2.34	0.49
1:A:924:ASP:HB3	5:A:1407:HOH:O	2.12	0.49
1:B:833:GLN:HE21	1:B:887:ARG:HB2	1.78	0.49
1:A:125:VAL:O	1:A:254:ALA:O	2.30	0.49
1:A:141:ARG:HA	1:A:172:ASN:HD22	1.77	0.49
1:A:203:GLY:O	1:A:204:ASN:HB2	2.13	0.49
1:A:898:VAL:HG11	1:A:903:TYR:CE2	2.48	0.49
1:B:128:VAL:HB	1:B:226:LEU:HD23	1.94	0.49
1:A:414:LEU:HD11	1:A:454:ILE:CD1	2.43	0.48
1:A:414:LEU:HD23	1:A:436:ALA:HB3	1.95	0.48
1:B:345:THR:HB	1:B:347:ASP:OD1	2.12	0.48
1:B:887:ARG:HG2	1:B:887:ARG:HH11	1.77	0.48
1:A:213:TYR:CE1	1:A:493:GLY:HA2	2.48	0.48
1:B:391:ILE:O	1:B:415:ILE:HA	2.13	0.48
1:A:215:LEU:O	1:A:216:GLU:CB	2.62	0.48
1:A:623:TYR:CD2	1:A:696:PRO:HD3	2.49	0.48
1:A:745:ASP:OD2	1:A:806:HIS:HD2	1.97	0.48
1:A:129:ILE:CD1	1:A:246:ILE:HG22	2.44	0.48
1:B:124:THR:CG2	1:B:125:VAL:N	2.76	0.48
1:B:503:ASN:ND2	1:B:504:LYS:HD2	2.24	0.48
1:A:1029:GLU:O	1:A:1030:GLY:C	2.52	0.48
1:B:782:GLU:HG3	1:B:783:ASP:OD1	2.13	0.48
1:A:174:LYS:O	1:A:175:VAL:CB	2.61	0.48
1:A:757:ASN:ND2	5:A:1129:HOH:O	2.47	0.48
1:A:845:LEU:HB3	1:A:863:THR:HB	1.96	0.48
1:B:346:ALA:C	1:B:348:GLN:H	2.16	0.48
1:A:898:VAL:CG1	1:A:903:TYR:OH	2.61	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:1004:LYS:NZ	1:A:1004:LYS:HB3	2.29	0.48
1:B:695:ASP:HB3	1:B:698:LYS:HD2	1.96	0.48
1:A:171:VAL:O	1:A:175:VAL:O	2.31	0.48
1:A:1015:MSE:HA	1:A:1015:MSE:HE2	1.94	0.48
1:B:171:VAL:O	1:B:171:VAL:HG12	2.13	0.48
1:A:533:TYR:H	1:A:534:PRO:HD3	1.79	0.48
5:A:1129:HOH:O	1:B:996:MSE:HE3	2.14	0.48
1:A:485:ILE:HG12	1:A:596:LYS:HE3	1.96	0.47
1:B:397:ASP:HB2	4:B:1106:CIT:O3	2.14	0.47
1:B:528:GLN:NE2	1:B:532:GLN:HE22	2.03	0.47
1:B:729:GLY:C	1:B:736:ALA:HB2	2.35	0.47
1:A:115:GLN:C	1:A:117:LYS:H	2.18	0.47
1:A:213:TYR:HE1	1:A:493:GLY:HA2	1.79	0.47
1:B:198:SER:HB2	1:B:202:SER:OG	2.14	0.47
1:B:849:VAL:HG23	1:B:858:TRP:CE3	2.49	0.47
1:B:946:ARG:NH2	1:B:984:ASP:OD2	2.47	0.47
1:A:391:ILE:O	1:A:415:ILE:HA	2.14	0.47
1:B:197:VAL:HG12	1:B:197:VAL:O	2.13	0.47
1:B:213:TYR:CE1	1:B:513:MSE:HB3	2.49	0.47
1:A:882:ARG:CZ	1:B:996:MSE:CE	2.92	0.47
1:B:591:ASP:OD1	1:B:593:THR:N	2.33	0.47
1:B:142:LEU:HD13	1:B:143:THR:H	1.79	0.47
1:B:912:ILE:HD12	1:B:912:ILE:C	2.35	0.47
1:A:180:ASP:OD2	1:A:228:ARG:HD3	2.14	0.47
1:A:445:LEU:C	1:A:445:LEU:HD23	2.35	0.47
1:B:141:ARG:O	1:B:142:LEU:O	2.32	0.47
1:A:226:LEU:O	1:A:227:MSE:HE3	2.14	0.47
1:A:750:GLN:HA	5:A:1616:HOH:O	2.14	0.47
1:B:213:TYR:CE1	1:B:493:GLY:HA2	2.50	0.47
1:B:833:GLN:NE2	1:B:884:GLU:HA	2.30	0.47
1:A:255:LYS:HZ2	1:A:255:LYS:HB3	1.80	0.47
1:B:874:LEU:HD23	1:B:878:LEU:HD21	1.97	0.47
1:A:265:ALA:HB3	5:A:1533:HOH:O	2.14	0.47
1:A:833:GLN:HE21	1:A:887:ARG:HE	1.62	0.47
1:B:398:PHE:CE1	1:B:425:ILE:HG21	2.50	0.47
1:A:198:SER:HB3	1:A:202:SER:OG	2.15	0.47
1:A:778:VAL:O	1:A:778:VAL:CG2	2.62	0.47
1:A:177:TYR:HB3	1:A:225:LEU:HD22	1.97	0.46
1:A:200:ILE:O	1:A:201:LEU:HB2	2.15	0.46
1:A:342:ARG:CD	1:A:457:ASN:HD21	2.28	0.46
1:A:820:ALA:CB	1:A:926:ILE:HG13	2.45	0.46



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:B:611:ASN:HD21	1:B:662:GLN:HG2	1.72	0.46	
1:A:149:ARG:HG2	1:A:149:ARG:HH11	1.80	0.46	
1:B:200:ILE:O	1:B:201:LEU:HB2	2.16	0.46	
1:B:111:VAL:HG11	1:B:218:ALA:HB1	1.98	0.46	
1:A:145:LYS:O	1:A:147:LYS:N	2.49	0.46	
1:A:392:GLU:HB2	1:A:416:TYR:CZ	2.50	0.46	
1:B:337:LEU:HA	1:B:462:VAL:HA	1.97	0.46	
1:B:341:VAL:HA	1:B:455:THR:O	2.16	0.46	
1:B:228:ARG:HG3	1:B:228:ARG:NH1	2.31	0.46	
1:A:183:LYS:HB2	1:A:183:LYS:NZ	2.31	0.46	
1:B:141:ARG:HG2	1:B:141:ARG:HH11	1.80	0.46	
1:A:137:HIS:O	1:A:138:GLU:O	2.34	0.46	
1:A:263:ASN:ND2	1:B:945:ARG:HG2	2.30	0.46	
1:A:723:ILE:HG12	1:A:758:PHE:CD2	2.51	0.46	
1:B:367:TYR:HB2	1:B:454:ILE:HD12	1.98	0.46	
1:A:215:LEU:O	1:A:216:GLU:HB2	2.16	0.45	
1:A:529:TYR:O	1:A:532:GLN:O	2.33	0.45	
1:A:960:TYR:CD1	1:A:961:ARG:HG3	2.52	0.45	
1:A:1026:LYS:HA	1:A:1029:GLU:HG2	1.97	0.45	
1:B:139:ALA:C	1:B:141:ARG:N	2.70	0.45	
1:B:384:VAL:O	1:B:385:LYS:C	2.55	0.45	
1:B:780:ASN:HD21	1:B:783:ASP:N	2.12	0.45	
1:B:898:VAL:HG21	1:B:903:TYR:CE2	2.51	0.45	
1:A:153:LYS:HE3	5:A:1622:HOH:O	2.17	0.45	
1:B:777:GLY:O	1:B:778:VAL:C	2.54	0.45	
1:B:780:ASN:HD21	1:B:783:ASP:HB2	1.81	0.45	
1:A:213:TYR:CE1	1:A:513:MSE:HB2	2.52	0.45	
1:A:728:ASP:O	1:A:741:LYS:HG3	2.17	0.45	
1:A:729:GLY:O	1:A:736:ALA:HB2	2.17	0.45	
1:A:960:TYR:HB2	1:A:1015:MSE:HE3	1.98	0.45	
1:B:125:VAL:CG1	1:B:225:LEU:HG	2.46	0.45	
1:B:454:ILE:HD13	1:B:456:PHE:CE1	2.50	0.45	
1:B:734:HIS:HE1	5:B:1328:HOH:O	1.98	0.45	
1:A:528:GLN:HG2	1:A:532:GLN:NE2	2.32	0.45	
1:A:775:LYS:NZ	5:A:1322:HOH:O	2.49	0.45	
1:B:368:ASP:HB3	1:B:387:LYS:HD3	1.96	0.45	
1:B:601:ASN:ND2	1:B:713:PHE:H	2.13	0.45	
1:B:671:ARG:HG2	1:B:671:ARG:NH1	2.29	0.45	
1:B:1029:GLU:O	1:B:1030:GLY:C	2.55	0.45	
1:A:271:LEU:HD23	1:A:271:LEU:N	2.09	0.45	
1:A:302:LYS:HB3	1:A:302:LYS:HZ3	1.80	0.45	



A 4 1			Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:337:LEU:CD1	1:A:460:PRO:HB2	2.46	0.45	
1:B:173:ASP:O	1:B:174:LYS:C	2.55	0.45	
1:B:254:ALA:C	1:B:256:VAL:H	2.20	0.45	
1:A:476:SER:O	1:A:477:TRP:C	2.55	0.45	
1:A:803:ASP:HB2	5:A:1141:HOH:O	2.17	0.45	
1:A:157:GLU:CD	1:A:160:LYS:HE3	2.37	0.45	
1:B:364:ASN:C	1:B:364:ASN:HD22	2.20	0.45	
1:A:242:TYR:OH	1:A:259:MSE:HB3	2.17	0.45	
1:A:850:LEU:HD21	1:A:856:VAL:HG22	1.99	0.45	
1:B:228:ARG:HH21	1:B:230:GLU:CD	2.20	0.45	
1:B:626:ALA:CB	1:B:665:VAL:HG11	2.47	0.45	
1:A:271:LEU:CG	1:A:321:ALA:HB3	2.46	0.44	
1:A:149:ARG:HG2	1:A:149:ARG:NH1	2.33	0.44	
1:B:263:ASN:O	1:B:264:ALA:O	2.35	0.44	
1:B:265:ALA:HB2	5:B:1597:HOH:O	2.17	0.44	
1:A:556:LEU:N	1:A:570:GLN:HE22	1.89	0.44	
1:B:108:PRO:HB2	1:B:492:PRO:HG2	1.99	0.44	
1:B:111:VAL:HG11	1:B:218:ALA:CB	2.47	0.44	
1:B:172:ASN:OD1	1:B:173:ASP:N	2.50	0.44	
1:B:965:ALA:HB2	1:B:978:TYR:CE1	2.52	0.44	
1:B:138:GLU:C	1:B:140:TRP:N	2.70	0.44	
1:B:308:ALA:HA	1:B:638:PHE:CE1	2.53	0.44	
1:B:969:MSE:HE1	1:B:974:PRO:HB3	2.00	0.44	
1:A:378:GLU:HG2	1:A:379:ASP:N	2.33	0.44	
1:A:471:LEU:HD21	1:A:556:LEU:HD13	1.99	0.44	
1:A:528:GLN:NE2	1:A:532:GLN:NE2	2.65	0.44	
1:B:786:SER:HB2	5:B:1581:HOH:O	2.18	0.44	
1:A:125:VAL:CG1	1:A:225:LEU:HG	2.48	0.44	
1:B:406:LYS:NZ	1:B:431:ASP:HB3	2.32	0.44	
1:B:532:GLN:HG2	1:B:533:TYR:CE1	2.52	0.44	
1:B:960:TYR:CD1	1:B:961:ARG:HG3	2.53	0.44	
1:A:536:MSE:O	1:A:540:GLU:OE2	2.36	0.44	
1:A:898:VAL:CG1	1:A:903:TYR:CZ	3.00	0.44	
1:B:136:ASN:C	1:B:138:GLU:H	2.21	0.44	
1:B:264:ALA:O	1:B:265:ALA:HB3	2.17	0.44	
1:B:377:LYS:HB2	1:B:380:ASP:OD2	2.18	0.44	
1:A:131:ALA:HA	1:A:229:VAL:O	2.18	0.44	
1:A:378:GLU:O	1:A:379:ASP:CB	2.61	0.44	
1:A:476:SER:HB2	1:A:569:GLN:HA	1.98	0.44	
1:A:850:LEU:HD22	1:A:856:VAL:HA	2.00	0.44	
1:A:982:ASN:ND2	5:A:1191:HOH:O	2.50	0.44	



	1.5	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:137:HIS:CE1	1:B:513:MSE:HE3	2.53	0.44
1:B:356:LEU:O	1:B:436:ALA:HA	2.17	0.44
1:B:849:VAL:HG21	1:B:888:TRP:CD2	2.53	0.44
1:A:264:ALA:HB3	5:A:1500:HOH:O	2.17	0.44
1:A:623:TYR:CE1	1:A:652:LYS:HG2	2.53	0.44
1:A:723:ILE:HG12	1:A:758:PHE:CE2	2.53	0.44
1:A:965:ALA:HB2	1:A:978:TYR:CE1	2.53	0.44
1:B:126:VAL:HA	1:B:256:VAL:HG13	2.00	0.44
1:B:734:HIS:HD2	5:B:1138:HOH:O	2.00	0.44
1:B:1014:ASP:OD1	1:B:1014:ASP:C	2.57	0.44
1:A:585:MSE:HE2	1:A:620:GLN:NE2	2.33	0.43
1:A:622:LEU:HD21	1:A:655:ILE:CD1	2.40	0.43
1:A:801:GLN:HE22	1:A:963:ARG:HG2	1.83	0.43
1:A:874:LEU:HD23	1:A:878:LEU:HD21	1.99	0.43
1:B:126:VAL:HG22	1:B:256:VAL:CG1	2.48	0.43
1:A:256:VAL:CG1	1:A:519:ALA:HB1	2.48	0.43
1:A:528:GLN:HG2	1:A:532:GLN:HE21	1.82	0.43
1:B:142:LEU:HD13	1:B:143:THR:O	2.18	0.43
1:B:409:GLY:O	1:B:410:ALA:HB3	2.18	0.43
1:B:570:GLN:HE21	1:B:573:GLY:HA2	1.83	0.43
1:B:618:LYS:CE	1:B:620:GLN:HE22	2.31	0.43
1:A:242:TYR:CE2	1:A:259:MSE:SE	3.21	0.43
1:A:337:LEU:HD11	1:A:460:PRO:HB2	2.00	0.43
1:A:946:ARG:NH2	1:A:984:ASP:OD2	2.51	0.43
1:B:344:LYS:HB2	1:B:451:GLN:CD	2.39	0.43
1:B:589:ASP:OD1	1:B:591:ASP:OD1	2.36	0.43
1:A:835:GLN:HE21	1:A:882:ARG:NE	2.04	0.43
1:A:898:VAL:HG11	1:A:903:TYR:CZ	2.54	0.43
1:B:145:LYS:HE3	1:B:221:GLU:OE1	2.17	0.43
1:A:206:PRO:O	1:A:207:SER:HB3	2.19	0.43
1:A:235:LEU:HD22	1:A:235:LEU:N	2.33	0.43
1:A:528:GLN:NE2	1:A:532:GLN:HE22	2.16	0.43
1:A:749:LEU:CD1	1:B:749:LEU:HG	2.46	0.43
1:B:111:VAL:HG12	1:B:111:VAL:O	2.18	0.43
1:B:410:ALA:O	1:B:411:VAL:CB	2.67	0.43
1:B:142:LEU:HD13	1:B:143:THR:N	2.33	0.43
1:B:214:ARG:HD2	1:B:214:ARG:N	2.34	0.43
1:A:485:ILE:CG1	1:A:596:LYS:HE3	2.48	0.43
1:A:728:ASP:HB2	5:A:1636:HOH:O	2.19	0.43
1:A:785:GLU:HG3	1:A:969:MSE:HE1	2.00	0.43
1:A:967:THR:HG22	1:A:976:THR:HA	2.00	0.43



		Interatomic	Clash
Atom-1	Atom-1 Atom-2		overlap (Å)
1:A:1031:HIS:O	1:B:191:GLN:HG2	2.19	0.43
1:B:172:ASN:C	1:B:173:ASP:O	2.57	0.43
1:B:353:MSE:CE	1:B:446:LEU:HD11	2.44	0.43
1:B:392:GLU:HB2	1:B:416:TYR:CZ	2.53	0.43
1:B:623:TYR:HA	1:B:651:GLN:O	2.18	0.43
1:B:796:GLY:HA2	1:B:818:TYR:O	2.18	0.43
1:B:723:ILE:HG12	1:B:758:PHE:CD2	2.53	0.43
1:B:1014:ASP:OD2	1:B:1018:ASN:HB2	2.18	0.43
1:A:197:VAL:O	1:A:197:VAL:HG12	2.18	0.43
1:A:232:VAL:O	1:A:233:ASN:HB3	2.19	0.43
1:B:275:THR:O	1:B:279:PHE:HD1	2.01	0.43
1:A:209:THR:HG22	1:A:210:LYS:N	2.33	0.42
1:A:968:TYR:O	1:A:975:THR:HG22	2.19	0.42
1:B:476:SER:O	1:B:477:TRP:C	2.57	0.42
1:A:621:GLU:C	1:A:622:LEU:HD23	2.40	0.42
1:B:194:GLY:O	1:B:198:SER:HA	2.19	0.42
1:B:383:ASP:CG	1:B:384:VAL:H	2.23	0.42
1:B:485:ILE:HD12	1:B:571:GLY:HA2	2.00	0.42
1:B:556:LEU:N	1:B:570:GLN:HE22	1.90	0.42
1:B:610:VAL:HG11	1:B:704:ILE:HG21	2.01	0.42
1:A:205:ALA:N	1:A:206:PRO:CD	2.79	0.42
1:A:934:VAL:C	1:A:952:LYS:HG3	2.39	0.42
1:A:944:ASP:OD2	1:B:135:LYS:HE3	2.19	0.42
1:B:341:VAL:CG1	1:B:454:ILE:HB	2.49	0.42
1:B:384:VAL:O	1:B:384:VAL:HG12	2.19	0.42
1:B:451:GLN:O	1:B:453:THR:N	2.52	0.42
1:A:138:GLU:HG3	1:A:215:LEU:HD12	2.01	0.42
1:A:741:LYS:HE2	1:A:741:LYS:N	2.33	0.42
1:B:494:GLN:O	1:B:496:ILE:HD12	2.18	0.42
1:B:585:MSE:HE1	1:B:622:LEU:HD21	2.00	0.42
1:A:210:LYS:HD2	5:A:1303:HOH:O	2.19	0.42
1:B:369:TYR:CE1	1:B:452:LYS:HD2	2.55	0.42
1:B:554:THR:HA	1:B:700:GLU:OE1	2.19	0.42
1:A:215:LEU:C	1:A:216:GLU:HG3	2.40	0.42
1:A:388:ILE:CD1	1:A:454:ILE:HD11	2.46	0.42
1:A:537:THR:HG22	1:A:539:SER:N	2.35	0.42
1:B:780:ASN:O	1:B:782:GLU:N	2.52	0.42
1:B:858:TRP:CH2	1:B:860:SER:HB3	2.55	0.42
1:B:364:ASN:C	1:B:364:ASN:ND2	2.73	0.42
1:B:369:TYR:O	1:B:452:LYS:HB3	2.18	0.42
1:B:503:ASN:ND2	1:B:503:ASN:H	2.17	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:572:ALA:HA	1:A:705:PRO:HD3	2.00	0.42
1:B:441:LYS:HE2	5:B:1498:HOH:O	2.19	0.42
1:B:932:PRO:HD3	1:B:1018:ASN:HB3	2.02	0.42
1:A:192:GLU:C	1:A:194:GLY:H	2.23	0.42
1:A:229:VAL:HG12	1:A:238:TYR:CE1	2.55	0.42
1:B:137:HIS:CD2	1:B:211:GLU:HG2	2.55	0.42
1:B:218:ALA:O	1:B:524:LEU:HD11	2.20	0.41
1:B:584:THR:HG22	5:B:1386:HOH:O	2.20	0.41
1:A:175:VAL:O	1:A:175:VAL:HG12	2.21	0.41
1:A:1028:LEU:O	1:A:1029:GLU:C	2.58	0.41
1:B:537:THR:HG22	1:B:540:GLU:CG	2.49	0.41
1:B:611:ASN:ND2	1:B:611:ASN:N	2.68	0.41
1:B:740:ALA:HB1	1:B:743:GLN:HE21	1.85	0.41
1:A:833:GLN:NE2	1:A:884:GLU:HA	2.36	0.41
1:B:218:ALA:HB1	1:B:524:LEU:HD12	2.02	0.41
1:B:345:THR:HA	1:B:449:ASN:OD1	2.20	0.41
1:B:738:SER:O	1:B:739:ASP:CB	2.69	0.41
1:B:757:ASN:ND2	5:B:1122:HOH:O	2.53	0.41
1:B:135:LYS:O	1:B:137:HIS:N	2.53	0.41
1:B:331:TYR:HB3	1:B:471:LEU:HD13	2.03	0.41
1:B:398:PHE:HE1	1:B:425:ILE:HG21	1.84	0.41
1:A:833:GLN:NE2	1:A:887:ARG:HE	2.18	0.41
1:A:951:SER:OG	1:A:952:LYS:HG2	2.21	0.41
1:B:390:LEU:C	1:B:390:LEU:HD23	2.41	0.41
1:B:940:PHE:CZ	1:B:945:ARG:HA	2.55	0.41
1:A:156:LEU:HD13	1:A:156:LEU:C	2.41	0.41
1:A:275:THR:O	1:A:279:PHE:HD1	2.02	0.41
1:A:440:ARG:HD3	5:A:1624:HOH:O	2.20	0.41
1:B:780:ASN:C	1:B:782:GLU:N	2.71	0.41
1:B:141:ARG:HA	1:B:141:ARG:HD2	1.83	0.41
1:B:178:TYR:O	1:B:178:TYR:CD2	2.73	0.41
1:B:614:ASN:ND2	1:B:657:ALA:HA	2.36	0.41
1:B:679:GLN:HE21	1:B:679:GLN:HB2	1.67	0.41
1:A:232:VAL:O	1:A:233:ASN:CB	2.69	0.41
1:B:139:ALA:HB1	1:B:206:PRO:CA	2.38	0.41
1:B:255:LYS:HA	1:B:287:VAL:HG22	2.03	0.41
1:B:537:THR:OG1	1:B:538:PRO:HD2	2.21	0.41
1:B:801:GLN:HE22	1:B:963:ARG:CG	2.33	0.41
1:A:174:LYS:NZ	1:A:216:GLU:OE1	2.53	0.41
1:A:221:GLU:OE2	1:A:221:GLU:HA	2.20	0.41
1:A:503:ASN:ND2	1:A:503:ASN:N	2.64	0.41



	A 4 0	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:B:248:ASP:O	1:B:252:LEU:HG	2.21	0.41	
1:B:685:PHE:CD2	1:B:707:ILE:HD11	2.54	0.41	
1:A:259:MSE:HG3	1:A:289:ILE:HG23	2.02	0.41	
1:A:640:LEU:HD12	1:A:640:LEU:HA	1.89	0.41	
1:A:1028:LEU:O	1:A:1030:GLY:N	2.54	0.41	
1:B:133:PHE:CD1	1:B:133:PHE:N	2.89	0.41	
1:B:383:ASP:C	1:B:385:LYS:N	2.74	0.41	
1:B:416:TYR:HA	1:B:438:ILE:O	2.21	0.41	
1:B:442:ASP:O	1:B:445:LEU:HB3	2.21	0.41	
1:B:547:LYS:NZ	1:B:593:THR:O	2.54	0.41	
1:A:243:ALA:O	1:A:246:ILE:HG12	2.20	0.40	
1:A:946:ARG:HH21	1:B:500:VAL:HB	1.86	0.40	
1:B:236:ALA:O	1:B:240:ARG:HG3	2.21	0.40	
1:B:355:VAL:HG12	1:B:438:ILE:CG2	2.47	0.40	
1:B:365:LYS:HB3	1:B:366:ALA:H	1.60	0.40	
1:B:1029:GLU:O	1:B:1031:HIS:N	2.53	0.40	
1:A:247:ARG:NH2	1:A:277:LYS:NZ	2.69	0.40	
1:B:171:VAL:O	1:B:172:ASN:ND2	2.53	0.40	
1:B:206:PRO:O	1:B:207:SER:CB	2.68	0.40	
1:B:369:TYR:CZ	1:B:452:LYS:HA	2.57	0.40	
1:B:527:LYS:HE3	1:B:527:LYS:HB2	1.94	0.40	
1:B:772:LYS:O	1:B:776:GLU:HG3	2.21	0.40	
1:B:910:THR:HA	1:B:911:PRO:HD3	1.98	0.40	
1:A:944:ASP:O	1:A:945:ARG:CB	2.68	0.40	
1:A:946:ARG:NH2	1:B:500:VAL:HB	2.36	0.40	
1:B:381:PHE:O	1:B:382:LYS:C	2.59	0.40	
1:B:572:ALA:HA	1:B:705:PRO:HD3	2.03	0.40	
1:B:626:ALA:HB3	1:B:665:VAL:HG11	2.03	0.40	
1:B:723:ILE:HD12	1:B:724:TYR:H	1.86	0.40	
1:B:737:ASN:ND2	1:B:743:GLN:HE22	2.20	0.40	
1:B:798:PHE:HB3	1:B:960:TYR:CE1	2.56	0.40	
1:A:156:LEU:HG	1:A:176:ALA:O	2.21	0.40	
1:A:850:LEU:HD22	1:A:856:VAL:HG22	2.03	0.40	
1:B:264:ALA:HB3	5:B:1406:HOH:O	2.20	0.40	
1:B:346:ALA:C	1:B:348:GLN:N	2.74	0.40	
1:B:368:ASP:HB2	1:B:387:LYS:HD3	2.03	0.40	

There are no symmetry-related clashes.



5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	924/926~(100%)	830 (90%)	64 (7%)	30 (3%)	4 0
1	В	924/926~(100%)	818 (88%)	70 (8%)	36 (4%)	3 0
All	All	1848/1852~(100%)	1648 (89%)	134 (7%)	66 (4%)	3 0

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	138	GLU
1	А	140	TRP
1	А	145	LYS
1	А	172	ASN
1	А	184	ASP
1	А	207	SER
1	А	254	ALA
1	А	264	ALA
1	А	592	ASN
1	А	952	LYS
1	А	1029	GLU
1	А	1030	GLY
1	В	141	ARG
1	В	142	LEU
1	В	146	THR
1	В	149	ARG
1	В	172	ASN
1	В	174	LYS
1	В	189	VAL
1	В	217	GLY
1	В	264	ALA
1	В	384	VAL
1	В	741	LYS
1	В	778	VAL
1	В	781	ILE



Mol	Chain	Res	Type
1	B	1030	GLY
1	A	146	THR
1	A	183	LYS
1	A	233	ASN
1	A	255	LYS
1	A	323	ASP
1	B	136	ASN
1	B	173	ASP
1	B	200	ILE
1	B	364	ASN
1	B	366	ALA
1	B	408	ALA
1	В	894	ASP
1	A	141	ARG
1	A	204	ASN
1	В	144	ASP
1	В	170	TRP
1	В	185	GLY
1	В	186	LYS
1	В	233	ASN
1	В	382	LYS
1	В	385	LYS
1	В	777	GLY
1	А	200	ILE
1	А	531	THR
1	А	739	ASP
1	А	971	GLU
1	В	207	SER
1	В	367	TYR
1	В	476	SER
1	А	136	ASN
1	А	495	ASP
1	А	780	ASN
1	В	206	PRO
1	A	175	VAL
1	A	379	ASP
1	В	195	THR
1	В	495	ASP
1	Α	189	VAL
1	А	537	THR
1	В	411	VAL

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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 Percer		\mathbf{ntiles}	
1	А	771/760~(101%)	736~(96%)	35~(4%)	27	18
1	В	771/760~(101%)	739~(96%)	32~(4%)	30	20
All	All	1542/1520~(101%)	1475 (96%)	67 (4%)	29	19

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	106	ASN
1	А	140	TRP
1	А	141	ARG
1	А	142	LEU
1	А	183	LYS
1	А	184	ASP
1	А	213	TYR
1	А	227	MSE
1	А	242	TYR
1	А	255	LYS
1	А	271	LEU
1	А	303	THR
1	А	336	GLN
1	А	384	VAL
1	А	390	LEU
1	А	407	LYS
1	А	503	ASN
1	А	552	SER
1	А	560	ASP
1	А	602	VAL
1	А	622	LEU
1	А	640	LEU
1	А	651	GLN
1	А	723	ILE
1	А	741	LYS
1	А	758	PHE
1	А	775	LYS



Mol	Chain	Res	Type
1	А	778	VAL
1	A	780	ASN
1	А	818	TYR
1	A	926	ILE
1	A	960	TYR
1	А	994	GLU
1	А	1004	LYS
1	А	1026	LYS
1	В	106	ASN
1	В	142	LEU
1	В	145	LYS
1	В	155	ASP
1	В	167	TYR
1	В	213	TYR
1	В	227	MSE
1	В	228	ARG
1	В	242	TYR
1	В	246	ILE
1	В	271	LEU
1	В	328	VAL
1	В	337	LEU
1	В	360	ARG
1	В	364	ASN
1	В	400	ASP
1	В	503	ASN
1	В	504	LYS
1	B	522	MSE
1	B	554	THR
1	B	640	LEU
1	B	694	GLN
1	B	723	ILE
1	B	749	LEU
1	B	758	PHE
1	B	783	ASP
1	B	785	GLU
1	В	862	VAL
1	В	952	LYS
1	В	960	TYR
1	В	994	GLU
1	В	995	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:



Mol	Chain	Res	Type
1	А	115	GLN
1	А	223	GLN
1	А	233	ASN
1	А	244	GLN
1	А	263	ASN
1	А	336	GLN
1	А	451	GLN
1	А	457	ASN
1	А	484	ASN
1	А	503	ASN
1	А	526	GLN
1	А	532	GLN
1	А	569	GLN
1	A	570	GLN
1	А	651	GLN
1	А	694	GLN
1	А	734	HIS
1	А	756	ASN
1	А	757	ASN
1	А	780	ASN
1	А	806	HIS
1	А	833	GLN
1	А	835	GLN
1	А	844	ASN
1	А	855	ASN
1	А	869	ASN
1	А	929	ASN
1	А	982	ASN
1	А	1018	ASN
1	В	115	GLN
1	В	136	ASN
1	В	204	ASN
1	В	223	GLN
1	В	241	ASN
1	В	263	ASN
1	В	349	GLN
1	B	364	ASN
1	В	419	GLN
1	В	494	GLN
1	В	503	ASN
1	В	526	GLN
1	В	532	GLN
1	В	569	GLN



Mol	Chain	Res	Type
1	В	570	GLN
1	В	601	ASN
1	В	611	ASN
1	В	620	GLN
1	В	658	ASN
1	В	679	GLN
1	В	743	GLN
1	В	756	ASN
1	В	780	ASN
1	В	801	GLN
1	В	806	HIS
1	В	833	GLN
1	В	835	GLN
1	В	844	ASN
1	В	869	ASN
1	В	982	ASN
1	В	1018	ASN

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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 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mol	Tuno	Chain	Dog	Link	B	ond leng	$_{ m gths}$	I	Bond an	gles
1VIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
4	CIT	В	1102	-	3,12,12	1.61	1 (33%)	$3,\!17,\!17$	4.52	3 (100%)
4	CIT	В	1106	-	3,12,12	1.69	0	3,17,17	4.33	3 (100%)
2	ACT	А	1107	-	1,3,3	0.31	0	$0,\!3,\!3$	-	-
4	CIT	А	1103	-	3,12,12	1.88	1 (33%)	$3,\!17,\!17$	3.73	2 (66%)
2	ACT	В	1108	-	1,3,3	0.56	0	0,3,3	-	-
4	CIT	А	1105	-	3,12,12	1.73	1 (33%)	$3,\!17,\!17$	4.04	2 (66%)
4	CIT	В	1104	-	3,12,12	1.81	1 (33%)	3,17,17	3.80	2 (66%)
4	CIT	А	1101	-	3,12,12	1.85	1 (33%)	3,17,17	4.85	3 (100%)

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

Mol	Type	Chain	\mathbf{Res}	Link	Chirals	Torsions	Rings
4	CIT	В	1102	-	-	4/6/16/16	-
4	CIT	В	1106	-	-	4/6/16/16	-
4	CIT	А	1103	-	-	4/6/16/16	-
4	CIT	А	1105	-	-	3/6/16/16	-
4	CIT	В	1104	-	-	4/6/16/16	-
4	CIT	А	1101	-	-	4/6/16/16	_

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	А	1103	CIT	C4-C3	-2.55	1.51	1.54
4	В	1104	CIT	C4-C3	-2.40	1.51	1.54
4	А	1101	CIT	O7-C3	2.37	1.46	1.43
4	А	1105	CIT	C4-C3	-2.17	1.51	1.54
4	В	1102	CIT	O7-C3	2.08	1.46	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	В	1106	CIT	C4-C3-C2	6.13	125.72	109.33
4	А	1105	CIT	C4-C3-C2	6.05	125.52	109.33
4	В	1102	CIT	C4-C3-C2	5.62	124.37	109.33
4	А	1101	CIT	C4-C3-C2	5.59	124.29	109.33
4	В	1104	CIT	C4-C3-C2	5.53	124.11	109.33



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$	
4	А	1103	CIT	C4-C3-C2	5.09	122.93	109.33	
4	А	1101	CIT	C3-C4-C5	4.56	122.29	114.98	
4	А	1101	CIT	C3-C2-C1	4.31	121.89	114.98	
4	А	1103	CIT	C3-C2-C1	3.97	121.34	114.98	
4	В	1102	CIT	C3-C2-C1	3.96	121.33	114.98	
4	В	1102	CIT	C3-C4-C5	3.74	120.97	114.98	
4	В	1104	CIT	C3-C2-C1	3.33	120.31	114.98	
4	В	1106	CIT	C3-C2-C1	3.26	120.20	114.98	
4	А	1105	CIT	C3-C2-C1	3.14	120.02	114.98	
4	В	1106	CIT	C3-C4-C5	2.82	119.50	114.98	

There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
4	А	1101	CIT	C1-C2-C3-O7
4	А	1101	CIT	C1-C2-C3-C6
4	А	1101	CIT	O7-C3-C4-C5
4	А	1103	CIT	C1-C2-C3-O7
4	А	1103	CIT	C1-C2-C3-C6
4	А	1103	CIT	O7-C3-C4-C5
4	А	1105	CIT	C1-C2-C3-O7
4	А	1105	CIT	C1-C2-C3-C6
4	А	1105	CIT	C2-C3-C4-C5
4	В	1102	CIT	C1-C2-C3-O7
4	В	1102	CIT	C1-C2-C3-C6
4	В	1102	CIT	O7-C3-C4-C5
4	В	1104	CIT	C1-C2-C3-O7
4	В	1104	CIT	C1-C2-C3-C6
4	В	1104	CIT	C2-C3-C4-C5
4	В	1106	CIT	C1-C2-C3-O7
4	В	1106	CIT	C1-C2-C3-C6
4	В	1106	CIT	C2-C3-C4-C5
4	В	1104	CIT	O7-C3-C4-C5
4	A	1101	CIT	C6-C3-C4-C5
4	В	1102	CIT	C6-C3-C4-C5
4	В	1106	CIT	C6-C3-C4-C5
4	A	1103	CIT	C2-C3-C4-C5

All (23) torsion outliers are listed below:

There are no ring outliers.

2 monomers are involved in 2 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	1106	CIT	1	0
4	В	1104	CIT	1	0

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

