Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2024 – 05:06 PM EST

PDB ID	:	3VS8
Title	:	Crystal structure of type III PKS ArsC
Authors	:	Satou, R.; Miyanaga, A.; Ozawa, H.; Funa, N.; Miyazono, K.; Tanokura, M.; Ohnishi, Y.; Horinouchi, S.
Deposited on	:	2012-04-23
Resolution	:	1.76 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

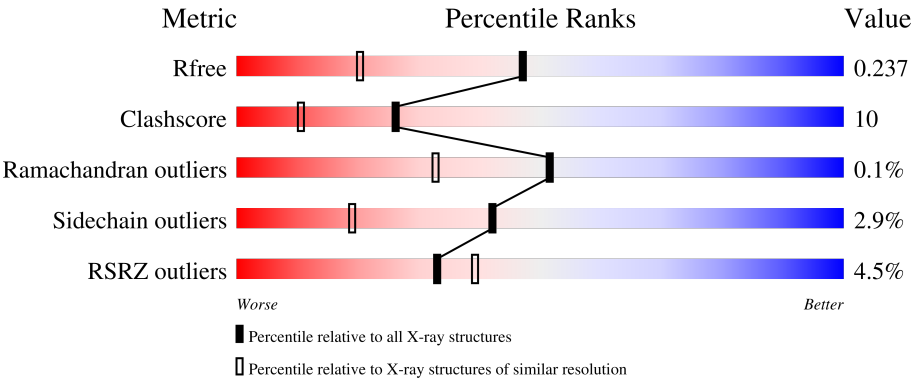
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 Å.

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



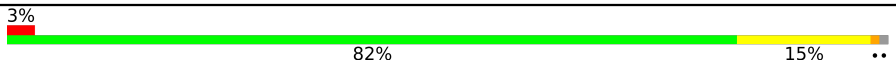
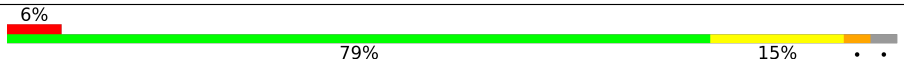
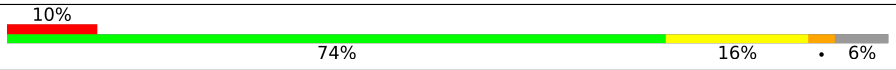
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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

Mol	Chain	Length	Quality of chain
1	A	410	85% 12%
1	B	410	5% 77% 19%
1	C	410	5% 81% 16%
1	D	410	4% 82% 14%
1	E	410	2% 83% 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	410	
1	G	410	
1	H	410	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 27375 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 Type III polyketide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3123	1984	542	582	15			
1	B	399	Total	C	N	O	S	0	0	0
			3084	1961	537	571	15			
1	C	402	Total	C	N	O	S	0	0	0
			3108	1973	540	580	15			
1	D	401	Total	C	N	O	S	0	0	0
			3100	1969	539	577	15			
1	E	401	Total	C	N	O	S	0	0	0
			3107	1976	539	577	15			
1	F	404	Total	C	N	O	S	0	0	0
			3123	1984	542	582	15			
1	G	398	Total	C	N	O	S	0	0	0
			3078	1958	536	569	15			
1	H	384	Total	C	N	O	S	0	0	0
			2968	1891	518	544	15			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		
2	E	1	Total	Na	0	0
			1	1		
2	F	1	Total	Na	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Na 1 1	0	0
2	H	1	Total Na 1 1	0	0

- Molecule 3 is water.

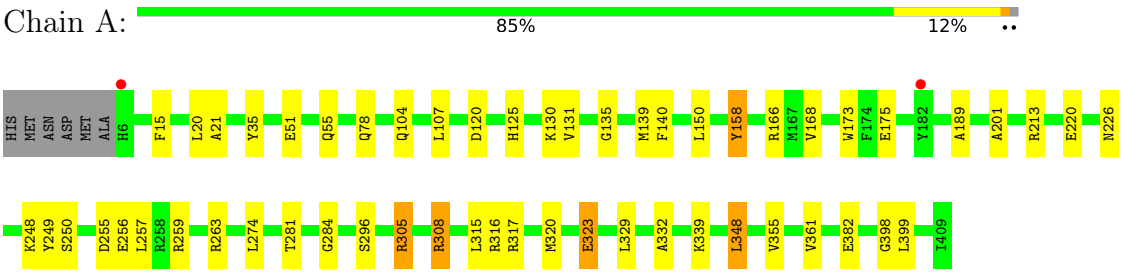
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	437	Total O 437 437	0	0
3	B	258	Total O 258 258	0	0
3	C	361	Total O 361 361	0	0
3	D	356	Total O 356 356	0	0
3	E	417	Total O 417 417	0	0
3	F	330	Total O 330 330	0	0
3	G	283	Total O 283 283	0	0
3	H	234	Total O 234 234	0	0

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.

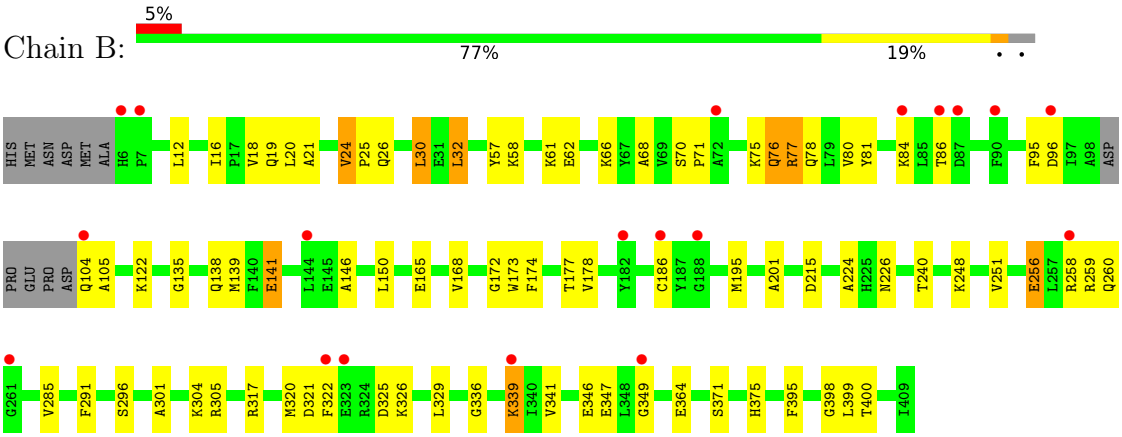
• Molecule 1: Type III polyketide synthase

Chain A:



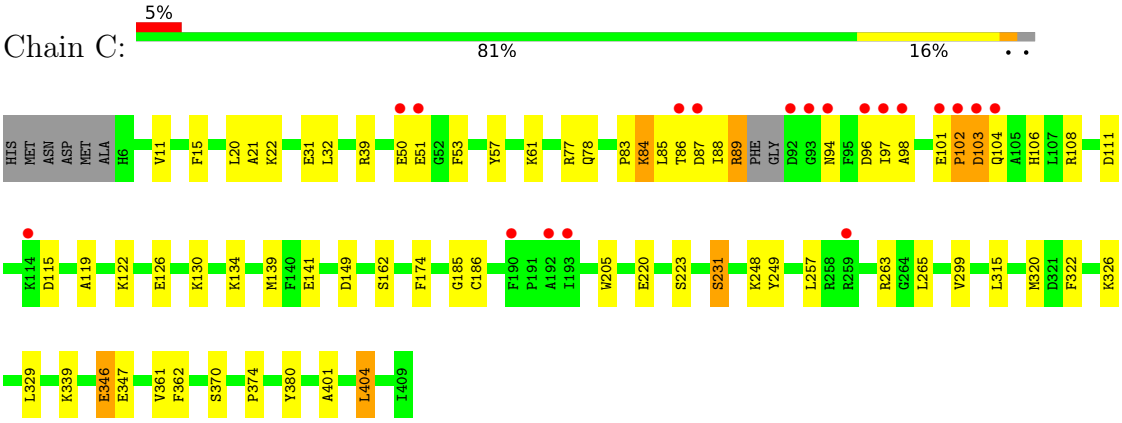
• Molecule 1: Type III polyketide synthase

Chain B:



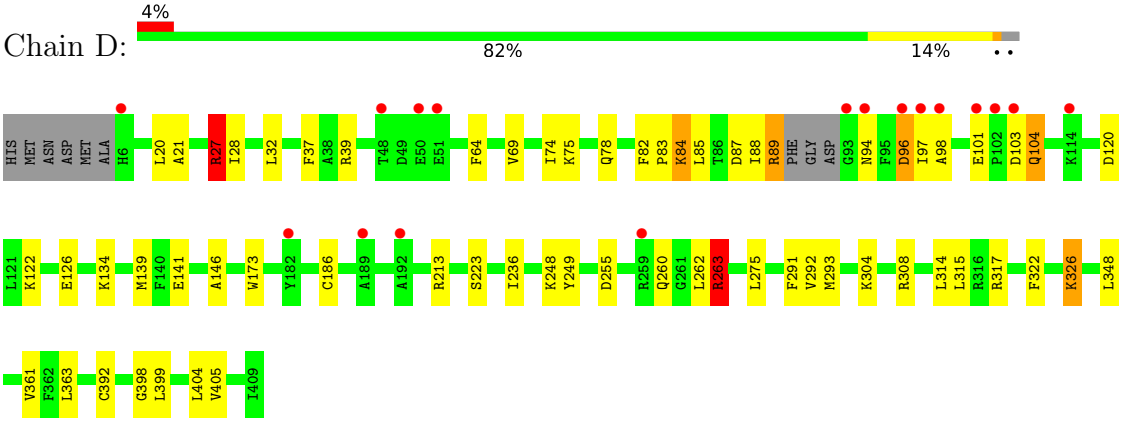
• Molecule 1: Type III polyketide synthase

Chain C:



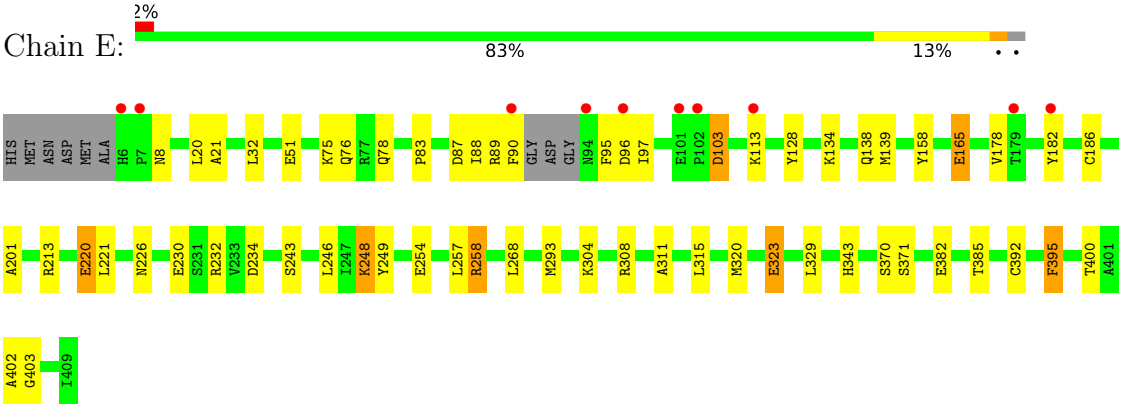
• Molecule 1: Type III polyketide synthase

Chain D:



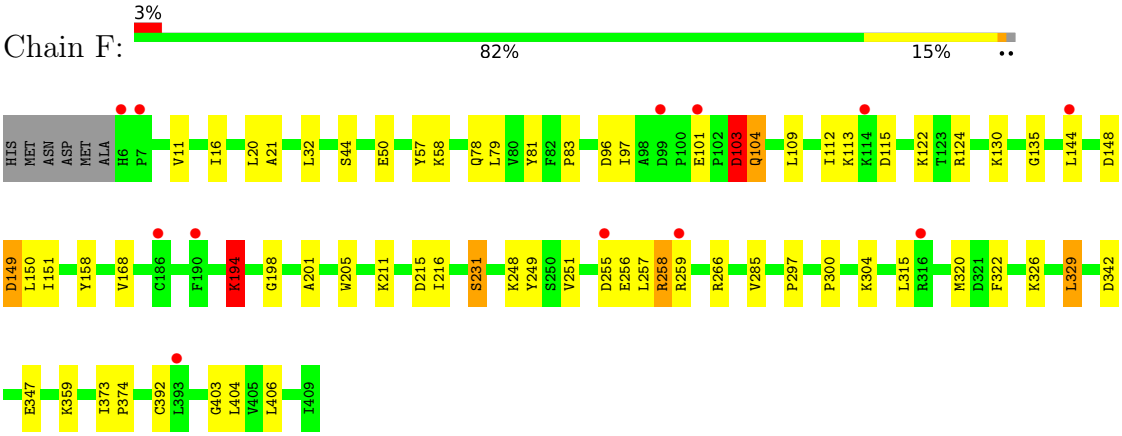
• Molecule 1: Type III polyketide synthase

Chain E:



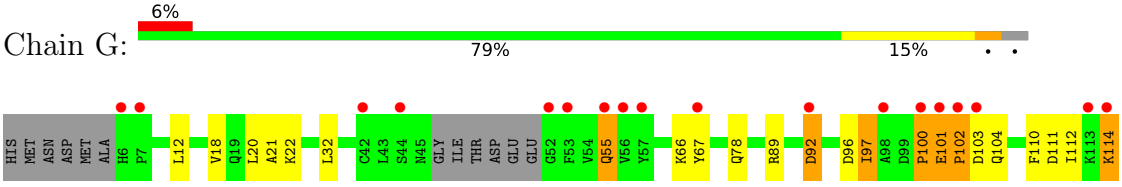
• Molecule 1: Type III polyketide synthase

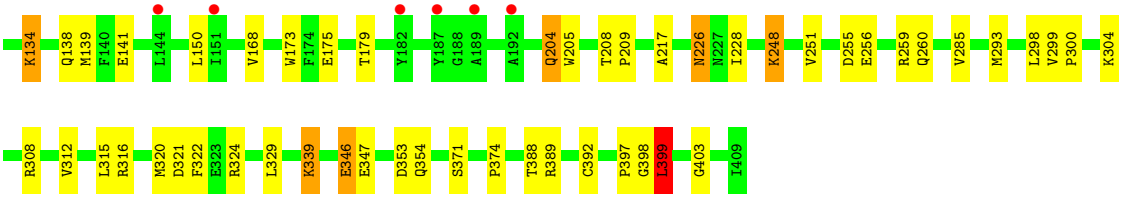
Chain F:



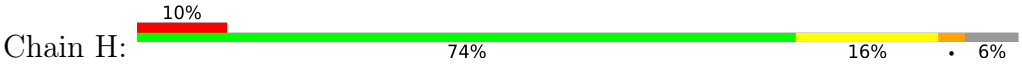
• Molecule 1: Type III polyketide synthase

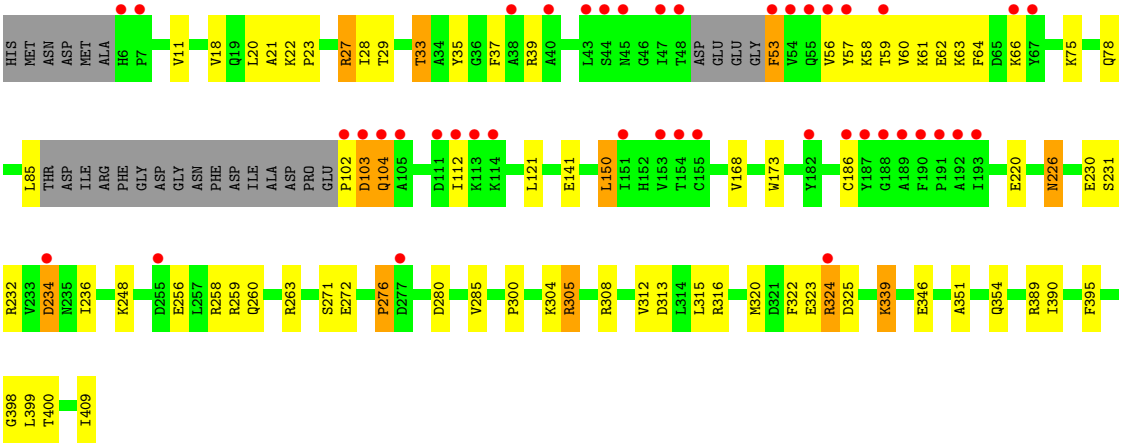
Chain G:





• Molecule 1: Type III polyketide synthase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	102.32Å 143.39Å 129.62Å 90.00° 110.33° 90.00°	Depositor
Resolution (Å)	37.57 – 1.76 35.27 – 1.76	Depositor EDS
% Data completeness (in resolution range)	97.4 (37.57-1.76) 97.4 (35.27-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.183 , 0.230 0.194 , 0.237	Depositor DCC
R_{free} test set	16976 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	22.9	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 49.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	27375	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 72.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2090e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.36	14/3194 (0.4%)	1.17	13/4331 (0.3%)
1	B	1.18	6/3152 (0.2%)	1.07	8/4270 (0.2%)
1	C	1.25	16/3177 (0.5%)	1.08	6/4307 (0.1%)
1	D	1.25	6/3169 (0.2%)	1.11	13/4296 (0.3%)
1	E	1.32	14/3177 (0.4%)	1.11	13/4307 (0.3%)
1	F	1.22	11/3194 (0.3%)	1.04	5/4331 (0.1%)
1	G	1.05	0/3148	0.98	2/4267 (0.0%)
1	H	1.08	3/3034 (0.1%)	0.99	5/4110 (0.1%)
All	All	1.22	70/25245 (0.3%)	1.07	65/34219 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
1	G	0	2
All	All	0	3

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	186	CYS	CB-SG	9.00	1.97	1.82
1	E	182	TYR	CD1-CE1	8.70	1.52	1.39
1	A	220	GLU	CB-CG	8.15	1.67	1.52
1	B	186	CYS	CB-SG	-8.04	1.68	1.82
1	E	186	CYS	CA-CB	7.44	1.70	1.53
1	H	220	GLU	CD-OE1	7.20	1.33	1.25
1	B	24	VAL	CB-CG1	7.02	1.67	1.52
1	B	195	MET	C-O	6.93	1.36	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	402	ALA	CA-CB	6.82	1.66	1.52
1	A	158	TYR	CD1-CE1	6.81	1.49	1.39
1	A	250	SER	CB-OG	6.69	1.50	1.42
1	C	361	VAL	CB-CG2	6.67	1.66	1.52
1	A	249	TYR	CE2-CZ	6.62	1.47	1.38
1	D	249	TYR	CD2-CE2	6.62	1.49	1.39
1	A	140	PHE	CE2-CZ	6.53	1.49	1.37
1	D	292	VAL	CB-CG1	6.50	1.66	1.52
1	E	165	GLU	CB-CG	6.46	1.64	1.52
1	F	57	TYR	CD1-CE1	6.34	1.48	1.39
1	F	251	VAL	CB-CG2	6.34	1.66	1.52
1	E	249	TYR	CG-CD1	6.24	1.47	1.39
1	A	189	ALA	CA-CB	6.04	1.65	1.52
1	E	323	GLU	CG-CD	6.03	1.60	1.51
1	C	174	PHE	CD2-CE2	6.00	1.51	1.39
1	A	332	ALA	CA-CB	6.00	1.65	1.52
1	D	223	SER	CB-OG	5.95	1.50	1.42
1	A	35	TYR	CD2-CE2	5.95	1.48	1.39
1	C	380	TYR	CD2-CE2	5.88	1.48	1.39
1	A	323	GLU	CG-CD	5.86	1.60	1.51
1	E	128	TYR	CD1-CE1	5.84	1.48	1.39
1	F	50	GLU	CB-CG	5.82	1.63	1.52
1	H	11	VAL	CB-CG2	5.81	1.65	1.52
1	A	131	VAL	CB-CG2	5.76	1.65	1.52
1	B	301	ALA	CA-CB	5.74	1.64	1.52
1	E	395	PHE	CB-CG	5.74	1.61	1.51
1	D	249	TYR	CG-CD1	5.73	1.46	1.39
1	F	158	TYR	CD1-CE1	5.72	1.48	1.39
1	D	361	VAL	CB-CG2	5.70	1.64	1.52
1	C	401	ALA	CA-CB	5.65	1.64	1.52
1	E	243	SER	CB-OG	5.65	1.49	1.42
1	C	15	PHE	CE2-CZ	5.59	1.48	1.37
1	B	256	GLU	CG-CD	5.54	1.60	1.51
1	C	249	TYR	CD1-CE1	5.52	1.47	1.39
1	E	370	SER	CB-OG	5.51	1.49	1.42
1	C	362	PHE	CE2-CZ	5.51	1.47	1.37
1	F	81	TYR	CD2-CE2	5.46	1.47	1.39
1	A	284	GLY	N-CA	5.43	1.54	1.46
1	F	168	VAL	C-O	5.40	1.33	1.23
1	A	361	VAL	CB-CG2	5.38	1.64	1.52
1	F	194	LYS	CD-CE	5.38	1.64	1.51
1	E	371	SER	CB-OG	5.36	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	249	TYR	CE1-CZ	-5.34	1.31	1.38
1	F	215	ASP	CB-CG	5.29	1.62	1.51
1	H	271	SER	CB-OG	-5.26	1.35	1.42
1	C	223	SER	CB-OG	5.25	1.49	1.42
1	E	158	TYR	CD2-CE2	5.21	1.47	1.39
1	C	370	SER	CB-OG	5.20	1.49	1.42
1	F	124	ARG	CB-CG	5.19	1.66	1.52
1	A	355	VAL	CB-CG1	5.16	1.63	1.52
1	E	201	ALA	CA-CB	5.14	1.63	1.52
1	D	291	PHE	CE1-CZ	5.13	1.47	1.37
1	F	198	GLY	C-O	5.13	1.31	1.23
1	B	201	ALA	CA-CB	5.12	1.63	1.52
1	C	149	ASP	N-CA	5.11	1.56	1.46
1	C	185	GLY	C-O	5.09	1.31	1.23
1	F	79	LEU	CG-CD1	5.09	1.70	1.51
1	C	299	VAL	CB-CG1	5.09	1.63	1.52
1	A	15	PHE	CD1-CE1	5.07	1.49	1.39
1	C	220	GLU	CG-CD	5.06	1.59	1.51
1	C	119	ALA	CA-CB	5.04	1.63	1.52
1	C	162	SER	CB-OG	5.02	1.48	1.42

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	27	ARG	NE-CZ-NH2	-15.83	112.38	120.30
1	B	77	ARG	NE-CZ-NH2	-12.60	114.00	120.30
1	D	27	ARG	NE-CZ-NH1	12.47	126.53	120.30
1	E	186	CYS	CA-CB-SG	-12.02	92.37	114.00
1	A	305	ARG	NE-CZ-NH1	11.49	126.05	120.30
1	B	77	ARG	NE-CZ-NH1	10.71	125.65	120.30
1	C	186	CYS	CA-CB-SG	-9.85	96.27	114.00
1	A	317	ARG	NE-CZ-NH2	-9.50	115.55	120.30
1	H	276	PRO	C-N-CA	-8.89	99.47	121.70
1	A	317	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	A	305	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	D	27	ARG	CB-CG-CD	8.09	132.63	111.60
1	D	263	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	E	221	LEU	CB-CG-CD1	-7.00	99.09	111.00
1	E	232	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	H	27	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	H	186	CYS	CA-CB-SG	-6.83	101.70	114.00
1	B	77	ARG	CD-NE-CZ	6.83	133.16	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	139	MET	CA-CB-CG	-6.82	101.71	113.30
1	D	317	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	A	213	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	F	255	ASP	CB-CG-OD1	6.41	124.07	118.30
1	A	348	LEU	CB-CG-CD1	6.37	121.83	111.00
1	D	404	LEU	CB-CG-CD2	-6.36	100.19	111.00
1	C	77	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A	255	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	308	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	D	186	CYS	CA-CB-SG	-6.22	102.80	114.00
1	G	399	LEU	CB-CG-CD1	6.12	121.41	111.00
1	E	308	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	77	ARG	CG-CD-NE	-6.03	99.14	111.80
1	D	249	TYR	CB-CG-CD2	-6.02	117.39	121.00
1	G	101	GLU	C-N-CD	-6.00	107.41	120.60
1	H	27	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	H	150	LEU	CB-CG-CD2	-5.87	101.01	111.00
1	A	15	PHE	CB-CG-CD2	-5.82	116.72	120.80
1	B	30	LEU	CA-CB-CG	5.82	128.68	115.30
1	C	265	LEU	CB-CG-CD1	-5.69	101.33	111.00
1	C	404	LEU	CA-CB-CG	5.62	128.23	115.30
1	D	275	LEU	CB-CG-CD2	-5.60	101.48	111.00
1	F	103	ASP	N-CA-C	5.56	126.01	111.00
1	D	120	ASP	CB-CG-OD2	5.56	123.30	118.30
1	F	115	ASP	CB-CG-OD1	5.53	123.28	118.30
1	E	234	ASP	CB-CG-OD1	5.52	123.27	118.30
1	E	304	LYS	CD-CE-NZ	-5.47	99.12	111.70
1	F	149	ASP	CB-CG-OD2	5.44	123.20	118.30
1	E	213	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	166	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	141	GLU	CB-CA-C	-5.40	99.61	110.40
1	D	392	CYS	CA-CB-SG	-5.39	104.30	114.00
1	E	320	MET	CG-SD-CE	-5.35	91.65	100.20
1	C	139	MET	CG-SD-CE	-5.30	91.72	100.20
1	E	232	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	320	MET	CG-SD-CE	-5.28	91.76	100.20
1	B	76	GLN	CB-CA-C	-5.21	99.99	110.40
1	D	213	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	C	263	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	B	317	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	F	404	LEU	CB-CG-CD2	-5.08	102.36	111.00
1	A	308	ARG	NE-CZ-NH2	-5.08	117.76	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	220	GLU	OE1-CD-OE2	-5.07	117.21	123.30
1	A	274	LEU	CB-CG-CD2	-5.02	102.46	111.00
1	E	308	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	E	182	TYR	CG-CD1-CE1	-5.00	117.30	121.30
1	E	258	ARG	NE-CZ-NH2	5.00	122.80	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	103	ASP	Peptide
1	G	100	PRO	Peptide
1	G	92	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3123	0	3112	30	0
1	B	3084	0	3083	86	0
1	C	3108	0	3099	72	0
1	D	3100	0	3095	55	0
1	E	3107	0	3101	42	0
1	F	3123	0	3112	66	0
1	G	3078	0	3074	77	0
1	H	2968	0	2986	97	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	437	0	0	8	1
3	B	258	0	0	13	0
3	C	361	0	0	8	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	356	0	0	13	2
3	E	417	0	0	9	0
3	F	330	0	0	13	0
3	G	283	0	0	11	0
3	H	234	0	0	7	0
All	All	27375	0	24662	514	2

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 10.

All (514) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:ARG:CB	1:C:96:ASP:HB3	1.55	1.35
1:C:89:ARG:HB2	1:C:96:ASP:CB	1.62	1.29
1:D:122:LYS:HD3	3:D:872:HOH:O	1.32	1.26
1:C:39:ARG:NH2	1:C:94:ASN:ND2	1.86	1.22
1:H:104:GLN:HE21	1:H:104:GLN:CA	1.51	1.22
1:F:103:ASP:N	1:F:104:GLN:HB2	1.56	1.20
1:F:103:ASP:OD2	1:F:104:GLN:HG2	1.41	1.18
1:C:39:ARG:HH21	1:C:94:ASN:ND2	1.37	1.18
1:H:104:GLN:HA	1:H:104:GLN:NE2	1.46	1.14
1:F:101:GLU:O	1:F:104:GLN:HB3	1.48	1.13
1:B:304:LYS:HE2	1:B:346:GLU:OE1	1.47	1.12
1:G:111:ASP:OD2	1:G:114:LYS:HD3	1.52	1.09
1:H:320:MET:HE1	1:H:389:ARG:HH11	1.17	1.09
1:C:84:LYS:HB2	1:C:86:THR:O	1.53	1.08
1:F:258:ARG:HG2	1:F:258:ARG:HH11	1.16	1.07
1:H:324:ARG:HG2	1:H:324:ARG:HH11	1.18	1.07
1:B:18:VAL:HG21	1:B:139:MET:HG3	1.37	1.06
1:C:39:ARG:NH2	1:C:94:ASN:HD21	1.49	1.06
1:B:66:LYS:HD2	1:B:66:LYS:O	1.54	1.05
1:B:104:GLN:O	1:B:105:ALA:HB3	1.56	1.05
1:F:101:GLU:O	1:F:104:GLN:CB	2.07	1.03
1:D:122:LYS:HE3	3:D:910:HOH:O	1.59	1.03
1:B:339:LYS:HE2	3:B:753:HOH:O	1.57	1.02
1:B:18:VAL:HG21	1:B:139:MET:CG	1.91	1.00
1:B:26:GLN:OE1	1:B:77:ARG:HD2	1.61	0.99
1:G:134:LYS:HE3	1:G:138:GLN:HE22	1.25	0.98
1:E:382:GLU:OE2	3:E:993:HOH:O	1.82	0.97
1:F:20:LEU:H	1:F:78:GLN:NE2	1.62	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:305:ARG:HD3	3:H:834:HOH:O	1.65	0.95
1:D:39:ARG:NH2	1:D:94:ASN:OD1	1.99	0.95
1:C:346:GLU:C	1:C:346:GLU:OE1	2.07	0.93
1:B:20:LEU:H	1:B:78:GLN:HE22	1.12	0.93
1:D:37:PHE:CE2	1:D:236:ILE:HD13	2.05	0.91
1:A:382:GLU:OE2	3:A:824:HOH:O	1.87	0.91
1:H:320:MET:HE1	1:H:389:ARG:NH1	1.84	0.91
1:G:111:ASP:OD2	1:G:114:LYS:CD	2.19	0.89
1:E:89:ARG:O	1:E:96:ASP:N	2.04	0.89
1:D:104:GLN:OE1	1:D:104:GLN:HA	1.71	0.89
1:F:20:LEU:H	1:F:78:GLN:HE22	1.18	0.89
1:C:86:THR:HB	1:C:87:ASP:OD1	1.73	0.89
1:F:103:ASP:H	1:F:104:GLN:HB2	1.36	0.89
1:F:103:ASP:OD2	1:F:104:GLN:CG	2.22	0.87
1:D:263:ARG:HG2	1:D:263:ARG:HH11	1.39	0.87
1:C:84:LYS:NZ	1:C:108:ARG:HH21	1.73	0.86
1:B:104:GLN:O	1:B:105:ALA:CB	2.25	0.85
1:G:20:LEU:H	1:G:78:GLN:HE22	1.25	0.85
1:A:20:LEU:H	1:A:78:GLN:HE22	1.21	0.84
1:B:20:LEU:H	1:B:78:GLN:NE2	1.75	0.84
1:C:20:LEU:H	1:C:78:GLN:HE22	1.24	0.84
1:G:134:LYS:HE3	1:G:138:GLN:NE2	1.92	0.84
1:H:324:ARG:HG2	1:H:324:ARG:NH1	1.81	0.83
1:H:104:GLN:HE21	1:H:104:GLN:HA	0.70	0.83
1:H:35:TYR:CZ	1:H:39:ARG:HD2	2.13	0.82
1:H:320:MET:HE1	1:H:389:ARG:HD3	1.59	0.82
1:B:21:ALA:H	1:B:78:GLN:HE21	1.25	0.82
1:D:20:LEU:H	1:D:78:GLN:NE2	1.77	0.82
1:H:320:MET:CE	1:H:389:ARG:HH11	1.92	0.81
1:H:324:ARG:HH11	1:H:324:ARG:CG	1.92	0.81
1:D:20:LEU:H	1:D:78:GLN:HE22	1.26	0.81
1:C:57:TYR:CZ	1:C:61:LYS:HE3	2.15	0.81
1:H:39:ARG:NH1	1:H:53:PHE:HE1	1.79	0.80
1:C:20:LEU:H	1:C:78:GLN:NE2	1.79	0.80
1:G:293:MET:HE2	3:G:669:HOH:O	1.82	0.80
1:F:258:ARG:HG2	1:F:258:ARG:NH1	1.93	0.79
1:G:111:ASP:OD2	1:G:114:LYS:CE	2.30	0.79
1:H:20:LEU:H	1:H:78:GLN:HE22	1.29	0.79
1:A:305:ARG:HD2	3:A:758:HOH:O	1.80	0.79
1:H:141:GLU:OE1	3:H:829:HOH:O	2.01	0.79
1:H:351:ALA:H	1:H:354:GLN:HE21	1.29	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:111:ASP:OD2	1:G:114:LYS:HE2	1.84	0.77
1:C:126:GLU:OE2	3:C:903:HOH:O	2.03	0.77
1:E:20:LEU:H	1:E:78:GLN:HE22	1.31	0.77
1:A:305:ARG:CD	3:A:758:HOH:O	2.33	0.76
1:H:300:PRO:O	1:H:304:LYS:HG3	1.85	0.76
1:G:20:LEU:H	1:G:78:GLN:NE2	1.82	0.76
1:B:18:VAL:CG2	1:B:139:MET:CG	2.64	0.76
1:A:20:LEU:H	1:A:78:GLN:NE2	1.83	0.75
1:B:321:ASP:O	1:B:325:ASP:HB2	1.86	0.75
1:A:139:MET:HE3	1:A:248:LYS:HB3	1.67	0.75
1:E:139:MET:HG3	1:E:248:LYS:HG2	1.68	0.75
1:H:21:ALA:H	1:H:78:GLN:HE21	1.34	0.75
1:A:21:ALA:H	1:A:78:GLN:HE21	1.34	0.74
1:D:37:PHE:HE2	1:D:236:ILE:HD13	1.50	0.74
1:G:21:ALA:H	1:G:78:GLN:HE21	1.36	0.74
1:B:84:LYS:HE3	3:B:781:HOH:O	1.87	0.74
1:D:37:PHE:CE2	1:D:236:ILE:CD1	2.71	0.74
1:D:304:LYS:HE3	3:D:777:HOH:O	1.88	0.74
1:C:51:GLU:H	1:C:51:GLU:CD	1.91	0.74
1:A:175:GLU:O	3:A:873:HOH:O	2.05	0.73
1:H:57:TYR:CE1	1:H:61:LYS:HD2	2.23	0.73
1:D:126:GLU:OE2	3:D:910:HOH:O	2.06	0.73
1:E:21:ALA:H	1:E:78:GLN:HE21	1.36	0.73
1:C:57:TYR:CE1	1:C:61:LYS:HE3	2.22	0.73
1:E:75:LYS:HE2	3:E:695:HOH:O	1.88	0.73
1:F:103:ASP:CA	1:F:104:GLN:HB2	2.18	0.73
1:H:33:THR:HG21	3:H:804:HOH:O	1.90	0.72
1:B:304:LYS:HZ3	1:B:347:GLU:HB2	1.54	0.72
1:D:89:ARG:NH2	1:D:98:ALA:HB2	2.04	0.72
1:D:89:ARG:HG2	1:D:96:ASP:O	1.89	0.72
1:E:139:MET:CG	1:E:248:LYS:HG2	2.20	0.72
1:H:230:GLU:OE1	1:H:232:ARG:NH2	2.23	0.72
1:C:87:ASP:HB2	1:C:98:ALA:HB3	1.72	0.71
1:F:194:LYS:NZ	1:G:179:THR:OG1	2.23	0.71
1:C:103:ASP:C	1:C:103:ASP:OD1	2.28	0.71
1:F:101:GLU:O	1:F:104:GLN:HB2	1.90	0.71
1:G:97:ILE:HD12	1:G:97:ILE:N	2.05	0.71
1:A:323:GLU:OE2	3:A:1030:HOH:O	2.07	0.71
1:E:75:LYS:CE	3:E:695:HOH:O	2.39	0.70
1:C:21:ALA:H	1:C:78:GLN:HE21	1.36	0.70
1:E:89:ARG:HB3	1:E:90:PHE:CD2	2.26	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:VAL:CG2	1:B:139:MET:HG2	2.22	0.70
1:H:37:PHE:CE2	1:H:236:ILE:HD13	2.26	0.70
1:F:21:ALA:H	1:F:78:GLN:HE21	1.38	0.70
1:C:84:LYS:HZ3	1:C:108:ARG:HH21	1.36	0.70
1:C:86:THR:CB	1:C:87:ASP:OD1	2.40	0.70
1:F:113:LYS:NZ	3:F:895:HOH:O	2.22	0.70
1:D:89:ARG:CZ	1:D:98:ALA:HB2	2.22	0.69
1:E:89:ARG:HB2	1:E:96:ASP:HB3	1.74	0.69
1:G:66:LYS:HE3	1:G:67:TYR:OH	1.92	0.69
1:D:21:ALA:H	1:D:78:GLN:HE21	1.40	0.69
1:G:315:LEU:HG	1:G:320:MET:HE3	1.75	0.69
1:D:64:PHE:CE1	1:D:236:ILE:HD12	2.28	0.69
1:D:126:GLU:OE1	3:D:890:HOH:O	2.11	0.69
1:A:125:HIS:HE1	1:A:158:TYR:H	1.41	0.68
1:B:326:LYS:NZ	1:B:349:GLY:O	2.27	0.68
1:B:18:VAL:CG2	1:B:139:MET:HG3	2.20	0.68
1:C:101:GLU:O	1:C:103:ASP:N	2.26	0.68
1:F:258:ARG:HH11	1:F:258:ARG:CG	1.96	0.66
1:A:120:ASP:OD2	3:A:929:HOH:O	2.12	0.66
1:C:86:THR:CA	1:C:87:ASP:OD1	2.43	0.66
1:H:320:MET:CE	1:H:389:ARG:NH1	2.56	0.66
1:C:106:HIS:NE2	1:C:130:LYS:HE2	2.10	0.66
1:G:388:THR:OG1	3:G:844:HOH:O	2.14	0.66
1:C:89:ARG:HB2	1:C:96:ASP:HB3	0.72	0.65
1:F:101:GLU:HB2	1:F:104:GLN:HG3	1.77	0.65
1:C:31:GLU:OE2	3:C:769:HOH:O	2.14	0.65
1:C:86:THR:HA	1:C:87:ASP:OD1	1.96	0.65
1:B:304:LYS:CE	1:B:346:GLU:OE1	2.37	0.65
1:C:39:ARG:HH21	1:C:94:ASN:HD22	1.42	0.65
1:G:139:MET:HE3	1:G:248:LYS:HB3	1.78	0.65
1:G:293:MET:CE	3:G:669:HOH:O	2.41	0.65
1:D:101:GLU:HG3	1:D:104:GLN:HB2	1.79	0.65
1:H:27:ARG:HG3	1:H:28:ILE:N	2.11	0.65
1:C:89:ARG:CZ	1:C:98:ALA:HB2	2.27	0.64
1:H:64:PHE:CE1	1:H:236:ILE:HD12	2.33	0.64
1:H:324:ARG:HG3	1:H:325:ASP:OD1	1.97	0.64
1:F:231:SER:HB2	3:F:679:HOH:O	1.95	0.64
1:H:39:ARG:HD3	1:H:112:ILE:HD12	1.80	0.63
1:G:321:ASP:HB3	1:G:324:ARG:HD3	1.81	0.63
1:H:320:MET:HB2	1:H:325:ASP:OD2	1.98	0.63
1:C:103:ASP:OD1	1:C:104:GLN:HG3	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:102:PRO:CD	1:H:104:GLN:HB2	2.27	0.63
1:H:308:ARG:NH2	1:H:323:GLU:OE2	2.31	0.63
1:D:104:GLN:OE1	1:D:104:GLN:CA	2.45	0.62
1:A:308:ARG:NH2	1:A:323:GLU:OE2	2.31	0.62
1:E:89:ARG:N	1:E:89:ARG:HD3	2.13	0.62
1:F:150:LEU:C	1:F:150:LEU:HD23	2.19	0.62
1:H:39:ARG:NH1	1:H:53:PHE:CE1	2.66	0.62
1:E:134:LYS:HE3	1:E:138:GLN:NE2	2.14	0.62
1:F:150:LEU:HD23	1:F:151:ILE:N	2.14	0.62
1:C:103:ASP:OD1	1:C:103:ASP:O	2.18	0.61
1:A:125:HIS:CE1	1:A:158:TYR:H	2.18	0.61
1:B:20:LEU:N	1:B:78:GLN:NE2	2.48	0.61
1:H:112:ILE:HG13	1:H:112:ILE:O	2.00	0.61
1:B:76:GLN:HG3	3:B:757:HOH:O	2.00	0.61
1:C:57:TYR:CZ	1:C:61:LYS:CE	2.83	0.61
1:H:102:PRO:HG2	1:H:103:ASP:OD2	2.01	0.61
1:E:20:LEU:H	1:E:78:GLN:NE2	1.99	0.60
1:H:37:PHE:CE2	1:H:236:ILE:CD1	2.83	0.60
1:D:32:LEU:HD21	1:D:83:PRO:HG2	1.83	0.60
1:G:101:GLU:HG2	1:G:104:GLN:HG3	1.83	0.60
1:G:111:ASP:CG	1:G:114:LYS:HD3	2.21	0.60
1:G:97:ILE:N	1:G:97:ILE:CD1	2.63	0.60
1:G:353:ASP:OD1	1:G:354:GLN:N	2.34	0.60
1:H:102:PRO:C	1:H:104:GLN:H	2.05	0.60
1:C:32:LEU:HD11	1:C:88:ILE:HG12	1.84	0.60
1:D:84:LYS:HB2	1:D:87:ASP:HB2	1.84	0.60
1:E:89:ARG:HB3	1:E:90:PHE:CE2	2.36	0.60
1:H:263:ARG:HH11	1:H:263:ARG:HG2	1.67	0.60
1:G:55:GLN:HE21	1:G:55:GLN:HA	1.66	0.60
1:B:371:SER:O	1:B:375:HIS:HD2	1.84	0.59
1:F:258:ARG:NH1	1:F:258:ARG:CG	2.57	0.59
1:B:122:LYS:HZ1	1:H:285:VAL:HG21	1.68	0.59
1:F:256:GLU:CD	1:F:259:ARG:HH21	2.06	0.59
1:F:11:VAL:HG11	1:F:257:LEU:HD22	1.85	0.59
1:H:20:LEU:H	1:H:78:GLN:NE2	2.00	0.58
1:C:39:ARG:HD3	1:C:53:PHE:CE1	2.38	0.58
1:F:101:GLU:CB	1:F:104:GLN:HG3	2.33	0.58
1:F:285:VAL:HG13	3:F:734:HOH:O	2.03	0.58
1:H:102:PRO:CG	1:H:103:ASP:H	2.15	0.58
1:H:320:MET:HE1	1:H:389:ARG:CD	2.32	0.58
1:H:29:THR:O	1:H:33:THR:CG2	2.51	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:102:PRO:HD2	1:G:103:ASP:H	1.68	0.58
1:G:134:LYS:CE	1:G:138:GLN:NE2	2.64	0.58
1:H:102:PRO:HD2	1:H:104:GLN:HG2	1.86	0.58
1:B:305:ARG:NH2	1:F:103:ASP:O	2.37	0.58
1:D:101:GLU:HB2	1:D:103:ASP:OD1	2.04	0.58
1:F:103:ASP:CG	1:F:104:GLN:HG2	2.22	0.58
1:B:75:LYS:HE3	3:B:741:HOH:O	2.01	0.58
1:B:75:LYS:HE3	1:B:76:GLN:HE22	1.69	0.58
1:E:20:LEU:HD11	1:E:246:LEU:HD22	1.84	0.58
1:F:326:LYS:HA	1:F:329:LEU:HD22	1.86	0.57
1:H:104:GLN:CA	1:H:104:GLN:NE2	2.27	0.57
1:H:29:THR:O	1:H:33:THR:HG23	2.04	0.57
1:B:122:LYS:NZ	3:B:775:HOH:O	2.38	0.57
1:E:134:LYS:HE3	1:E:138:GLN:HE22	1.70	0.57
1:B:395:PHE:HD2	3:B:653:HOH:O	1.88	0.56
1:D:32:LEU:CD2	1:D:83:PRO:HG2	2.35	0.56
1:G:134:LYS:HD3	1:G:138:GLN:NE2	2.20	0.56
1:C:101:GLU:C	1:C:103:ASP:N	2.57	0.56
1:C:315:LEU:HD12	1:C:322:PHE:HA	1.86	0.56
1:C:89:ARG:CB	1:C:96:ASP:CB	2.47	0.56
1:H:75:LYS:NZ	3:H:796:HOH:O	2.37	0.56
1:A:315:LEU:HD21	1:A:329:LEU:HD11	1.88	0.56
1:D:263:ARG:NH2	1:F:44:SER:O	2.38	0.56
1:E:103:ASP:OD2	1:E:103:ASP:N	2.39	0.56
1:F:320:MET:CE	1:F:329:LEU:HD11	2.35	0.56
1:C:346:GLU:OE1	1:C:346:GLU:O	2.23	0.56
1:H:226:ASN:ND2	3:H:707:HOH:O	2.39	0.56
1:B:285:VAL:HG13	3:B:695:HOH:O	2.05	0.55
1:H:60:VAL:HA	1:H:63:LYS:HE2	1.88	0.55
1:A:315:LEU:HD21	1:A:329:LEU:CD1	2.36	0.55
1:B:320:MET:CE	1:B:329:LEU:HD11	2.36	0.55
1:C:141:GLU:HG3	3:C:603:HOH:O	2.07	0.55
1:G:141:GLU:OE1	3:G:803:HOH:O	2.18	0.55
1:H:53:PHE:C	1:H:53:PHE:CD2	2.80	0.55
1:E:293:MET:HE1	3:E:985:HOH:O	2.05	0.55
1:G:100:PRO:HA	1:G:101:GLU:OE1	2.07	0.55
1:H:58:LYS:O	1:H:62:GLU:HG3	2.06	0.55
1:H:320:MET:CE	1:H:389:ARG:HD3	2.34	0.55
1:A:139:MET:CE	1:A:248:LYS:HB3	2.35	0.55
1:E:113:LYS:HD3	3:E:770:HOH:O	2.07	0.55
1:C:101:GLU:O	1:C:102:PRO:C	2.46	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:371:SER:C	1:G:374:PRO:HD2	2.28	0.54
1:G:89:ARG:HG3	1:G:96:ASP:HB3	1.89	0.54
1:A:305:ARG:HD3	3:A:758:HOH:O	2.05	0.54
1:B:150:LEU:HD12	1:B:215:ASP:O	2.07	0.54
1:H:258:ARG:O	1:H:259:ARG:C	2.46	0.54
1:D:87:ASP:OD1	1:D:98:ALA:HB3	2.08	0.54
3:F:921:HOH:O	1:G:175:GLU:HG2	2.06	0.54
1:E:323:GLU:CD	1:E:323:GLU:H	2.11	0.53
1:F:256:GLU:OE2	1:F:259:ARG:NH2	2.38	0.53
1:H:315:LEU:HD22	1:H:322:PHE:HA	1.90	0.53
1:C:106:HIS:CD2	1:C:130:LYS:HE2	2.43	0.53
1:D:263:ARG:HH11	1:D:263:ARG:CG	2.17	0.53
1:C:89:ARG:CA	1:C:96:ASP:HB3	2.34	0.53
1:A:51:GLU:OE2	1:A:55:GLN:HG2	2.08	0.53
1:C:84:LYS:HZ1	1:C:108:ARG:HH21	1.55	0.53
1:H:85:LEU:N	1:H:85:LEU:HD23	2.23	0.53
1:B:18:VAL:HG23	1:B:139:MET:HG2	1.89	0.53
1:B:66:LYS:HD2	1:B:66:LYS:C	2.23	0.53
1:F:16:ILE:HD12	1:F:248:LYS:HE3	1.90	0.53
1:F:320:MET:HE3	1:F:329:LEU:HD11	1.90	0.53
1:G:285:VAL:HG22	3:G:789:HOH:O	2.09	0.53
1:H:315:LEU:CD2	1:H:322:PHE:HA	2.38	0.53
1:B:21:ALA:H	1:B:78:GLN:NE2	2.01	0.52
1:H:58:LYS:HE3	1:H:62:GLU:OE2	2.08	0.52
1:B:320:MET:HE1	1:B:329:LEU:HD11	1.91	0.52
1:B:258:ARG:HH11	1:B:258:ARG:HG2	1.74	0.52
1:B:84:LYS:HD3	3:B:807:HOH:O	2.10	0.52
1:G:66:LYS:HE3	1:G:67:TYR:CZ	2.44	0.52
1:G:110:PHE:HB3	1:G:226:ASN:OD1	2.10	0.52
1:G:22:LYS:HE3	3:G:771:HOH:O	2.10	0.52
1:D:27:ARG:HG2	3:D:641:HOH:O	2.09	0.51
1:G:226:ASN:ND2	1:G:228:ILE:HG23	2.25	0.51
1:H:102:PRO:HG2	1:H:103:ASP:H	1.74	0.51
1:H:35:TYR:OH	1:H:39:ARG:HD2	2.10	0.51
1:H:232:ARG:HH11	1:H:234:ASP:HB3	1.74	0.51
1:C:89:ARG:N	1:C:96:ASP:O	2.39	0.51
1:H:102:PRO:HD2	1:H:103:ASP:OD2	2.11	0.51
1:E:88:ILE:C	1:E:89:ARG:HD3	2.31	0.51
1:F:342:ASP:OD1	1:F:359:LYS:HE2	2.11	0.51
1:G:12:LEU:HD23	1:G:251:VAL:HG22	1.93	0.51
1:C:39:ARG:HH22	1:C:94:ASN:HD21	1.48	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:GLU:OE1	3:B:662:HOH:O	2.20	0.50
1:F:194:LYS:CE	3:F:666:HOH:O	2.59	0.50
1:B:122:LYS:NZ	1:H:285:VAL:HG21	2.26	0.50
1:B:341:VAL:HG23	3:B:828:HOH:O	2.11	0.50
1:F:315:LEU:HD12	1:F:322:PHE:HD1	1.77	0.50
1:G:102:PRO:CD	1:G:103:ASP:H	2.23	0.50
1:G:102:PRO:C	1:G:104:GLN:H	2.13	0.50
1:H:35:TYR:CE2	1:H:39:ARG:HD2	2.47	0.50
1:C:106:HIS:CE1	1:C:130:LYS:CE	2.95	0.50
1:E:89:ARG:N	1:E:89:ARG:CD	2.73	0.50
1:C:86:THR:O	1:C:86:THR:OG1	2.29	0.50
1:B:81:TYR:CE1	1:B:224:ALA:HB2	2.47	0.50
1:B:138:GLN:O	1:B:141:GLU:HG3	2.12	0.50
1:H:27:ARG:HG3	1:H:28:ILE:H	1.74	0.50
1:D:89:ARG:HD3	1:D:89:ARG:N	2.27	0.50
1:F:148:ASP:HB3	1:F:211:LYS:NZ	2.26	0.50
1:D:27:ARG:HG3	1:D:28:ILE:N	2.26	0.49
1:G:134:LYS:CE	1:G:138:GLN:HE22	2.11	0.49
1:F:20:LEU:N	1:F:78:GLN:NE2	2.45	0.49
1:H:263:ARG:HD2	1:H:409:ILE:O	2.13	0.49
1:D:255:ASP:OD1	3:D:785:HOH:O	2.19	0.49
1:E:89:ARG:O	1:E:95:PHE:HA	2.13	0.49
1:F:113:LYS:CD	3:F:895:HOH:O	2.60	0.49
1:G:101:GLU:HG2	1:G:101:GLU:O	2.13	0.49
1:B:165:GLU:HG3	1:B:178:VAL:HG11	1.94	0.49
1:D:20:LEU:N	1:D:78:GLN:NE2	2.54	0.49
1:B:24:VAL:HG12	1:B:25:PRO:O	2.12	0.49
1:H:313:ASP:OD1	1:H:316:ARG:NH2	2.46	0.49
1:B:139:MET:HE3	1:B:248:LYS:HB2	1.95	0.48
1:F:373:ILE:N	1:F:374:PRO:CD	2.76	0.48
1:F:149:ASP:OD2	1:F:211:LYS:NZ	2.45	0.48
1:H:75:LYS:CE	3:H:796:HOH:O	2.60	0.48
1:G:101:GLU:CG	1:G:104:GLN:HG3	2.43	0.48
1:D:82:PHE:CG	1:D:83:PRO:HD2	2.48	0.48
1:C:89:ARG:N	1:C:89:ARG:HD3	2.28	0.48
1:D:134:LYS:HD3	3:D:870:HOH:O	2.14	0.48
1:H:150:LEU:C	1:H:150:LEU:HD23	2.34	0.48
1:B:21:ALA:N	1:B:78:GLN:HE21	2.01	0.48
1:G:101:GLU:OE1	1:G:101:GLU:N	2.47	0.48
1:G:103:ASP:OD1	1:G:103:ASP:N	2.46	0.48
1:B:122:LYS:NZ	1:H:285:VAL:CG2	2.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:LEU:HD23	1:F:144:LEU:HA	1.68	0.48
1:G:134:LYS:CD	1:G:138:GLN:NE2	2.77	0.48
1:A:130:LYS:NZ	1:A:130:LYS:HB3	2.28	0.48
1:B:75:LYS:HE2	1:B:364:GLU:OE1	2.14	0.48
1:C:106:HIS:CE1	1:C:130:LYS:HE2	2.48	0.48
1:B:68:ALA:HB1	1:B:240:THR:HG21	1.96	0.48
1:F:130:LYS:HB3	1:F:130:LYS:HE3	1.63	0.48
1:G:315:LEU:CD2	1:G:322:PHE:HA	2.43	0.47
1:C:320:MET:CE	1:C:329:LEU:HD21	2.44	0.47
1:C:101:GLU:C	1:C:103:ASP:H	2.16	0.47
1:H:103:ASP:O	1:H:104:GLN:NE2	2.47	0.47
1:D:314:LEU:HG	1:D:405:VAL:CG2	2.44	0.47
1:E:20:LEU:CD1	1:E:246:LEU:HD22	2.44	0.47
1:G:150:LEU:C	1:G:150:LEU:HD23	2.35	0.47
1:B:32:LEU:CD2	1:B:95:PHE:CD2	2.97	0.47
1:C:32:LEU:HD11	1:C:88:ILE:CD1	2.44	0.47
1:C:89:ARG:HB2	1:C:96:ASP:CG	2.32	0.47
1:F:201:ALA:HA	1:G:205:TRP:CZ2	2.50	0.47
1:F:304:LYS:HZ2	1:F:347:GLU:HB2	1.78	0.47
1:F:103:ASP:CA	1:F:104:GLN:CB	2.92	0.47
1:H:398:GLY:N	1:H:399:LEU:HA	2.28	0.47
1:B:395:PHE:HA	1:B:400:THR:O	2.15	0.47
1:C:20:LEU:N	1:C:78:GLN:NE2	2.56	0.47
1:B:32:LEU:HA	1:B:32:LEU:HD22	1.56	0.46
1:C:346:GLU:OE1	1:C:347:GLU:N	2.47	0.46
1:E:20:LEU:HD11	1:E:246:LEU:CD2	2.45	0.46
1:F:216:ILE:HD12	1:F:249:TYR:CE1	2.50	0.46
1:H:39:ARG:HH11	1:H:53:PHE:HE1	1.56	0.46
1:B:322:PHE:O	1:B:326:LYS:HB3	2.15	0.46
1:F:266:ARG:O	1:F:406:LEU:HA	2.15	0.46
1:E:83:PRO:HG3	1:E:97:ILE:HD13	1.97	0.46
1:E:89:ARG:CB	1:E:96:ASP:HB3	2.44	0.46
1:H:53:PHE:C	1:H:53:PHE:HD2	2.18	0.46
1:C:111:ASP:HB3	1:C:115:ASP:O	2.16	0.46
1:H:168:VAL:HG13	1:H:173:TRP:HB2	1.96	0.46
1:A:339:LYS:HA	1:A:339:LYS:HD3	1.58	0.46
1:B:305:ARG:HD3	3:F:620:HOH:O	2.15	0.46
1:F:194:LYS:HE2	3:F:666:HOH:O	2.15	0.46
1:G:299:VAL:HB	1:G:300:PRO:HD3	1.98	0.46
1:C:89:ARG:NH2	1:C:98:ALA:HB2	2.31	0.46
1:F:194:LYS:HE3	3:F:666:HOH:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:LYS:NZ	1:B:347:GLU:OE1	2.49	0.46
1:E:8:ASN:ND2	3:E:970:HOH:O	2.43	0.46
1:D:37:PHE:CD2	1:D:236:ILE:CD1	2.99	0.46
1:B:174:PHE:CE1	1:H:276:PRO:HA	2.51	0.45
1:D:263:ARG:CG	1:D:263:ARG:NH1	2.77	0.45
1:H:21:ALA:H	1:H:78:GLN:NE2	2.09	0.45
1:H:280:ASP:HB3	3:H:751:HOH:O	2.15	0.45
1:A:201:ALA:HA	1:C:205:TRP:CZ2	2.51	0.45
1:B:20:LEU:N	1:B:78:GLN:HE22	1.95	0.45
1:B:177:THR:HG23	1:H:272:GLU:HB3	1.98	0.45
1:H:20:LEU:N	1:H:78:GLN:HE22	2.06	0.45
1:C:11:VAL:HG11	1:C:257:LEU:HD22	1.97	0.45
1:C:83:PRO:HA	1:C:84:LYS:HZ2	1.80	0.45
1:E:51:GLU:O	1:E:51:GLU:HG3	2.16	0.45
1:F:20:LEU:HD21	1:F:135:GLY:HA2	1.98	0.45
1:H:312:VAL:HA	1:H:322:PHE:HB2	1.98	0.45
1:B:146:ALA:HB2	1:B:173:TRP:CD1	2.51	0.45
1:B:256:GLU:OE2	1:B:259:ARG:NH1	2.50	0.45
1:B:259:ARG:NH1	1:B:260:GLN:HE21	2.14	0.45
1:C:87:ASP:HB3	1:C:89:ARG:NH1	2.31	0.45
1:G:100:PRO:CA	1:G:101:GLU:OE1	2.65	0.45
1:E:139:MET:HG2	1:E:248:LYS:HG2	1.98	0.45
1:A:135:GLY:O	1:A:139:MET:HG3	2.16	0.45
1:G:139:MET:HE1	1:G:217:ALA:HB1	1.99	0.45
1:G:285:VAL:CG2	3:G:789:HOH:O	2.64	0.45
1:H:304:LYS:HE3	1:H:304:LYS:HB3	1.71	0.45
1:B:32:LEU:HD21	1:B:95:PHE:CG	2.51	0.45
1:B:285:VAL:HG13	1:B:285:VAL:O	2.17	0.45
1:F:392:CYS:O	1:F:403:GLY:HA2	2.17	0.45
1:A:20:LEU:HD23	1:A:20:LEU:HA	1.82	0.44
1:B:16:ILE:HD12	1:B:248:LYS:HE3	1.99	0.44
1:D:101:GLU:H	1:D:101:GLU:HG2	1.34	0.44
1:B:12:LEU:HD23	1:B:251:VAL:HG22	2.00	0.44
1:D:315:LEU:HD12	1:D:322:PHE:HA	1.99	0.44
1:E:230:GLU:OE2	3:E:951:HOH:O	2.20	0.44
1:D:304:LYS:CE	3:D:777:HOH:O	2.57	0.44
1:E:87:ASP:OD2	3:E:978:HOH:O	2.21	0.44
1:F:285:VAL:HG11	3:F:794:HOH:O	2.16	0.44
1:H:102:PRO:CD	1:H:103:ASP:N	2.80	0.44
1:C:85:LEU:HD12	1:C:88:ILE:HD12	2.00	0.44
1:G:89:ARG:HE	1:G:89:ARG:HB2	1.64	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:102:PRO:CG	1:H:103:ASP:N	2.80	0.44
1:C:51:GLU:CD	1:C:51:GLU:N	2.63	0.44
1:D:146:ALA:HB2	1:D:173:TRP:CD1	2.52	0.44
1:E:89:ARG:HG2	1:E:96:ASP:HB3	2.00	0.44
1:G:226:ASN:HD21	1:G:228:ILE:HG23	1.82	0.44
1:B:18:VAL:HG21	1:B:139:MET:HG2	1.78	0.44
1:C:134:LYS:CE	3:C:690:HOH:O	2.65	0.44
1:F:83:PRO:HG3	1:F:97:ILE:HD12	2.00	0.44
1:G:32:LEU:HD11	1:G:97:ILE:HD11	2.00	0.44
1:B:76:GLN:NE2	3:B:741:HOH:O	2.50	0.44
1:D:398:GLY:N	1:D:399:LEU:HA	2.33	0.44
1:H:29:THR:O	1:H:33:THR:HG22	2.18	0.43
1:B:75:LYS:HB3	1:B:76:GLN:NE2	2.33	0.43
1:C:32:LEU:HD11	1:C:88:ILE:CG1	2.47	0.43
1:C:339:LYS:HE3	3:C:801:HOH:O	2.17	0.43
1:D:141:GLU:HG3	3:D:642:HOH:O	2.18	0.43
1:E:254:GLU:O	1:E:258:ARG:HG2	2.18	0.43
1:G:20:LEU:N	1:G:78:GLN:NE2	2.59	0.43
1:B:26:GLN:OE1	1:B:77:ARG:CD	2.49	0.43
1:F:58:LYS:HB2	1:F:58:LYS:HE2	1.68	0.43
1:F:122:LYS:HE2	3:G:765:HOH:O	2.18	0.43
1:G:304:LYS:HZ3	1:G:347:GLU:HB2	1.83	0.43
1:A:168:VAL:HG13	1:A:173:TRP:HB2	2.00	0.43
3:A:938:HOH:O	1:C:122:LYS:HD3	2.18	0.43
1:B:291:PHE:N	1:B:291:PHE:CD1	2.86	0.43
1:D:326:LYS:HD2	3:D:737:HOH:O	2.18	0.43
1:G:134:LYS:HD3	1:G:138:GLN:HE21	1.84	0.43
1:G:134:LYS:HE2	3:G:818:HOH:O	2.18	0.43
1:B:58:LYS:O	1:B:62:GLU:HG3	2.19	0.43
1:B:75:LYS:CB	1:B:76:GLN:NE2	2.82	0.43
1:D:260:GLN:O	1:D:262:LEU:HD13	2.19	0.43
1:F:32:LEU:HD21	1:F:97:ILE:HD11	2.00	0.43
1:A:104:GLN:HE21	1:A:107:LEU:HD11	1.84	0.43
1:B:172:GLY:HA2	1:B:174:PHE:CE2	2.54	0.43
1:D:314:LEU:HG	1:D:405:VAL:HG23	2.00	0.43
1:F:300:PRO:HD2	3:F:809:HOH:O	2.17	0.43
1:G:398:GLY:N	1:G:399:LEU:HA	2.33	0.43
1:H:395:PHE:HA	1:H:400:THR:O	2.18	0.43
1:C:106:HIS:HE1	3:C:690:HOH:O	2.00	0.43
1:G:256:GLU:OE2	1:G:259:ARG:NH2	2.52	0.43
1:G:316:ARG:HG3	3:G:881:HOH:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:103:ASP:OD2	1:H:103:ASP:N	2.50	0.43
1:C:87:ASP:HB2	1:C:98:ALA:CB	2.45	0.42
1:D:89:ARG:N	1:D:89:ARG:CD	2.82	0.42
1:G:256:GLU:O	1:G:260:GLN:CG	2.67	0.42
1:D:263:ARG:HG2	1:D:263:ARG:NH1	2.15	0.42
1:F:150:LEU:C	1:F:150:LEU:CD2	2.87	0.42
1:F:205:TRP:HE1	1:G:204:GLN:HE21	1.67	0.42
1:G:321:ASP:OD2	1:G:324:ARG:CD	2.67	0.42
1:C:134:LYS:HE3	3:C:690:HOH:O	2.17	0.42
1:D:308:ARG:HA	1:D:348:LEU:HD21	2.01	0.42
1:F:148:ASP:HB3	1:F:211:LYS:HZ3	1.84	0.42
1:G:339:LYS:HB2	1:G:339:LYS:HE2	1.58	0.42
1:B:248:LYS:NZ	3:B:621:HOH:O	2.27	0.42
1:C:84:LYS:HZ3	1:C:108:ARG:NH2	2.09	0.42
1:D:75:LYS:HE3	1:D:363:LEU:HD21	2.01	0.42
1:D:85:LEU:HA	1:D:88:ILE:HD12	2.02	0.42
1:E:165:GLU:HG3	1:E:178:VAL:HG11	2.01	0.42
1:G:308:ARG:O	1:G:312:VAL:HG23	2.19	0.42
1:F:297:PRO:HD2	3:F:804:HOH:O	2.19	0.42
1:H:59:THR:O	1:H:63:LYS:HG3	2.20	0.42
1:H:263:ARG:HA	1:H:263:ARG:HD3	1.74	0.42
1:D:32:LEU:HD21	1:D:83:PRO:CG	2.49	0.42
1:A:150:LEU:C	1:A:150:LEU:HD23	2.40	0.42
1:H:308:ARG:O	1:H:312:VAL:HG23	2.19	0.42
1:B:66:LYS:O	1:B:66:LYS:CD	2.45	0.42
1:H:232:ARG:NH1	1:H:234:ASP:HB3	2.35	0.42
1:B:20:LEU:HD21	1:B:135:GLY:HA2	2.01	0.42
1:G:102:PRO:CD	1:G:103:ASP:N	2.81	0.42
1:G:256:GLU:O	1:G:260:GLN:HG3	2.20	0.42
1:G:304:LYS:NZ	1:G:347:GLU:HB2	2.35	0.42
1:A:104:GLN:NE2	1:A:107:LEU:HD11	2.35	0.41
1:C:231:SER:HB2	3:C:898:HOH:O	2.19	0.41
1:D:122:LYS:HD2	3:D:718:HOH:O	2.20	0.41
1:E:311:ALA:O	1:E:315:LEU:HD13	2.20	0.41
1:A:398:GLY:HA3	1:A:399:LEU:C	2.40	0.41
1:B:398:GLY:N	1:B:399:LEU:HA	2.36	0.41
1:B:57:TYR:CZ	1:B:61:LYS:HE3	2.55	0.41
1:G:97:ILE:HD13	1:G:112:ILE:HD11	2.01	0.41
1:G:329:LEU:HD22	1:G:389:ARG:HB2	2.02	0.41
1:A:256:GLU:OE1	1:A:259:ARG:NH2	2.45	0.41
1:H:102:PRO:N	1:H:104:GLN:HB2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:315:LEU:HD21	1:E:329:LEU:CD1	2.51	0.41
1:E:392:CYS:O	1:E:403:GLY:HA2	2.20	0.41
1:H:256:GLU:O	1:H:260:GLN:HG3	2.20	0.41
1:B:320:MET:HE2	1:B:329:LEU:HD11	2.03	0.41
1:H:263:ARG:HG2	1:H:263:ARG:NH1	2.34	0.41
1:A:281:THR:HB	1:A:296:SER:HB3	2.03	0.41
1:B:336:GLY:HA3	3:B:795:HOH:O	2.20	0.41
1:B:104:GLN:HB3	1:B:105:ALA:H	1.64	0.41
1:E:395:PHE:HA	1:E:400:THR:O	2.20	0.41
1:G:208:THR:HB	1:G:209:PRO:HD2	2.03	0.41
1:H:18:VAL:O	1:H:18:VAL:HG13	2.20	0.41
1:E:75:LYS:NZ	3:E:695:HOH:O	2.54	0.41
1:H:22:LYS:HA	1:H:23:PRO:HD3	1.97	0.41
1:B:80:VAL:O	1:B:80:VAL:CG1	2.68	0.41
1:C:101:GLU:HG3	1:C:103:ASP:CG	2.41	0.41
1:F:101:GLU:HB3	3:F:894:HOH:O	2.20	0.41
1:F:109:LEU:HD23	1:F:109:LEU:HA	1.89	0.41
1:G:168:VAL:HG13	1:G:173:TRP:HB2	2.02	0.41
1:H:339:LYS:HA	1:H:339:LYS:HD2	1.96	0.41
1:B:168:VAL:HG13	1:B:173:TRP:HB2	2.03	0.40
1:G:18:VAL:HG22	3:G:849:HOH:O	2.21	0.40
1:D:293:MET:HE2	3:D:685:HOH:O	2.20	0.40
1:F:112:ILE:HG13	1:F:113:LYS:HD2	2.03	0.40
1:F:149:ASP:OD2	1:F:211:LYS:CE	2.69	0.40
1:H:102:PRO:HD2	1:H:104:GLN:HB2	2.01	0.40
1:B:75:LYS:CB	1:B:76:GLN:HE22	2.34	0.40
1:D:69:VAL:HG11	1:D:74:ILE:HD12	2.04	0.40
1:G:392:CYS:O	1:G:403:GLY:HA2	2.21	0.40
1:H:121:LEU:HD12	1:H:121:LEU:HA	1.91	0.40
1:B:325:ASP:O	1:B:329:LEU:HD13	2.20	0.40
1:G:346:GLU:O	1:G:346:GLU:HG3	2.16	0.40
1:B:70:SER:HA	1:B:71:PRO:HD3	1.89	0.40
1:E:89:ARG:HB2	1:E:96:ASP:CB	2.46	0.40
1:E:220:GLU:HA	1:E:220:GLU:OE1	2.22	0.40
1:H:390:ILE:HG21	1:H:390:ILE:HD13	1.93	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:864:HOH:O	3:D:864:HOH:O[1_655]	2.04	0.16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:998:HOH:O	3:D:946:HOH:O[2_646]	2.16	0.04

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	A	402/410 (98%)	391 (97%)	11 (3%)	0	100	100
1	B	395/410 (96%)	381 (96%)	14 (4%)	0	100	100
1	C	398/410 (97%)	386 (97%)	11 (3%)	1 (0%)	41	22
1	D	397/410 (97%)	385 (97%)	12 (3%)	0	100	100
1	E	397/410 (97%)	386 (97%)	11 (3%)	0	100	100
1	F	402/410 (98%)	389 (97%)	12 (3%)	1 (0%)	47	29
1	G	394/410 (96%)	376 (95%)	16 (4%)	2 (0%)	29	12
1	H	378/410 (92%)	360 (95%)	18 (5%)	0	100	100
All	All	3163/3280 (96%)	3054 (97%)	105 (3%)	4 (0%)	51	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	104	GLN
1	G	92	ASP
1	C	102	PRO
1	G	102	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	333/338 (98%)	328 (98%)	5 (2%)	65 49
1	B	328/338 (97%)	320 (98%)	8 (2%)	49 26
1	C	332/338 (98%)	320 (96%)	12 (4%)	35 13
1	D	331/338 (98%)	322 (97%)	9 (3%)	44 22
1	E	332/338 (98%)	323 (97%)	9 (3%)	44 22
1	F	333/338 (98%)	327 (98%)	6 (2%)	59 40
1	G	328/338 (97%)	315 (96%)	13 (4%)	31 10
1	H	317/338 (94%)	303 (96%)	14 (4%)	28 8
All	All	2634/2704 (97%)	2558 (97%)	76 (3%)	42 19

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	226	ASN
1	A	257	LEU
1	A	263	ARG
1	A	316	ARG
1	A	348	LEU
1	B	19	GLN
1	B	30	LEU
1	B	32	LEU
1	B	86	THR
1	B	96	ASP
1	B	226	ASN
1	B	296	SER
1	B	339	LYS
1	C	22	LYS
1	C	50	GLU
1	C	84	LYS
1	C	89	ARG
1	C	97	ILE
1	C	103	ASP
1	C	231	SER
1	C	248	LYS
1	C	326	LYS
1	C	346	GLU
1	C	374	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	404	LEU
1	D	27	ARG
1	D	84	LYS
1	D	89	ARG
1	D	96	ASP
1	D	97	ILE
1	D	104	GLN
1	D	248	LYS
1	D	263	ARG
1	D	326	LYS
1	E	32	LEU
1	E	76	GLN
1	E	103	ASP
1	E	226	ASN
1	E	248	LYS
1	E	257	LEU
1	E	268	LEU
1	E	343	HIS
1	E	385	THR
1	F	96	ASP
1	F	103	ASP
1	F	194	LYS
1	F	231	SER
1	F	258	ARG
1	F	329	LEU
1	G	55	GLN
1	G	97	ILE
1	G	114	LYS
1	G	134	LYS
1	G	204	GLN
1	G	226	ASN
1	G	248	LYS
1	G	255	ASP
1	G	298	LEU
1	G	339	LYS
1	G	346	GLU
1	G	397	PRO
1	G	399	LEU
1	H	33	THR
1	H	53	PHE
1	H	56	VAL
1	H	66	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	103	ASP
1	H	104	GLN
1	H	226	ASN
1	H	231	SER
1	H	234	ASP
1	H	248	LYS
1	H	305	ARG
1	H	324	ARG
1	H	339	LYS
1	H	346	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	78	GLN
1	A	104	GLN
1	A	125	HIS
1	A	226	ASN
1	A	290	GLN
1	B	19	GLN
1	B	76	GLN
1	B	78	GLN
1	B	226	ASN
1	B	260	GLN
1	B	290	GLN
1	B	343	HIS
1	B	375	HIS
1	C	6	HIS
1	C	78	GLN
1	C	94	ASN
1	C	106	HIS
1	C	226	ASN
1	C	290	GLN
1	D	41	HIS
1	D	78	GLN
1	D	226	ASN
1	D	290	GLN
1	E	8	ASN
1	E	55	GLN
1	E	78	GLN
1	E	138	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	226	ASN
1	E	290	GLN
1	E	343	HIS
1	F	78	GLN
1	F	290	GLN
1	G	55	GLN
1	G	78	GLN
1	G	106	HIS
1	G	138	GLN
1	G	204	GLN
1	G	290	GLN
1	H	78	GLN
1	H	104	GLN
1	H	226	ASN
1	H	260	GLN
1	H	290	GLN
1	H	354	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	404/410 (98%)	-0.21	2 (0%) 91 93	13, 21, 37, 48	0
1	B	399/410 (97%)	0.19	19 (4%) 30 36	21, 32, 52, 67	0
1	C	402/410 (98%)	0.06	19 (4%) 31 37	14, 23, 51, 79	0
1	D	401/410 (97%)	0.03	17 (4%) 36 42	14, 24, 53, 68	0
1	E	401/410 (97%)	-0.10	10 (2%) 57 63	13, 22, 46, 63	0
1	F	404/410 (98%)	-0.06	12 (2%) 50 56	18, 28, 45, 58	0
1	G	398/410 (97%)	0.17	24 (6%) 21 27	19, 31, 54, 68	0
1	H	384/410 (93%)	0.50	42 (10%) 5 7	19, 33, 63, 85	0
All	All	3193/3280 (97%)	0.07	145 (4%) 33 39	13, 27, 52, 85	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	102	PRO	7.1
1	D	102	PRO	6.8
1	H	53	PHE	6.0
1	H	56	VAL	5.8
1	F	144	LEU	5.4
1	G	92	ASP	5.3
1	H	6	HIS	5.2
1	G	102	PRO	4.9
1	H	112	ILE	4.9
1	H	47	ILE	4.8
1	B	144	LEU	4.7
1	F	6	HIS	4.6
1	G	6	HIS	4.5
1	H	114	LYS	4.4
1	C	96	ASP	4.4
1	G	55	GLN	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	53	PHE	4.1
1	C	86	THR	4.1
1	G	114	LYS	4.1
1	H	104	GLN	4.1
1	H	102	PRO	4.1
1	H	48	THR	4.0
1	C	98	ALA	4.0
1	H	45	ASN	4.0
1	C	92	ASP	3.9
1	H	44	SER	3.8
1	H	67	TYR	3.8
1	H	103	ASP	3.8
1	H	113	LYS	3.7
1	H	55	GLN	3.7
1	G	56	VAL	3.7
1	D	94	ASN	3.5
1	C	101	GLU	3.5
1	G	101	GLU	3.5
1	E	101	GLU	3.4
1	H	54	VAL	3.4
1	H	57	TYR	3.3
1	D	101	GLU	3.3
1	H	153	VAL	3.2
1	H	66	LYS	3.2
1	C	103	ASP	3.2
1	E	90	PHE	3.2
1	D	103	ASP	3.2
1	G	7	PRO	3.1
1	B	261	GLY	3.1
1	C	87	ASP	3.1
1	H	190	PHE	3.1
1	D	50	GLU	3.1
1	C	93	GLY	3.1
1	G	67	TYR	3.0
1	B	72	ALA	3.0
1	D	259	ARG	3.0
1	C	114	LYS	3.0
1	E	6	HIS	3.0
1	B	323	GLU	3.0
1	E	96	ASP	2.9
1	H	182	TYR	2.9
1	D	93	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	94	ASN	2.9
1	H	40	ALA	2.9
1	B	6	HIS	2.9
1	H	38	ALA	2.8
1	H	255	ASP	2.8
1	B	349	GLY	2.8
1	H	188	GLY	2.7
1	G	192	ALA	2.7
1	B	84	LYS	2.7
1	H	192	ALA	2.6
1	G	100	PRO	2.6
1	H	277	ASP	2.6
1	D	98	ALA	2.6
1	D	114	LYS	2.6
1	B	186	CYS	2.6
1	B	7	PRO	2.6
1	H	189	ALA	2.5
1	E	7	PRO	2.5
1	D	6	HIS	2.5
1	B	104	GLN	2.5
1	G	151	ILE	2.5
1	G	144	LEU	2.5
1	H	59	THR	2.5
1	H	324	ARG	2.5
1	H	186	CYS	2.5
1	D	96	ASP	2.5
1	F	255	ASP	2.4
1	B	339	LYS	2.4
1	H	155	CYS	2.4
1	B	188	GLY	2.4
1	H	43	LEU	2.4
1	F	99	ASP	2.4
1	C	51	GLU	2.4
1	D	182	TYR	2.4
1	H	7	PRO	2.4
1	B	96	ASP	2.4
1	D	189	ALA	2.4
1	C	50	GLU	2.3
1	C	259	ARG	2.3
1	F	259	ARG	2.3
1	C	192	ALA	2.3
1	H	151	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	182	TYR	2.3
1	H	193	ILE	2.3
1	B	258	ARG	2.3
1	E	179	THR	2.3
1	F	114	LYS	2.3
1	A	6	HIS	2.3
1	H	187	TYR	2.3
1	H	234	ASP	2.2
1	B	90	PHE	2.2
1	E	102	PRO	2.2
1	D	48	THR	2.2
1	H	105	ALA	2.2
1	H	111	ASP	2.2
1	G	113	LYS	2.2
1	B	182	TYR	2.2
1	E	113	LYS	2.2
1	C	97	ILE	2.2
1	B	87	ASP	2.2
1	G	44	SER	2.1
1	D	97	ILE	2.1
1	F	316	ARG	2.1
1	F	393	LEU	2.1
1	H	154	THR	2.1
1	G	103	ASP	2.1
1	H	191	PRO	2.1
1	F	101	GLU	2.1
1	G	52	GLY	2.1
1	G	98	ALA	2.1
1	C	104	GLN	2.1
1	C	193	ILE	2.1
1	B	86	THR	2.1
1	E	182	TYR	2.1
1	B	322	PHE	2.1
1	G	189	ALA	2.1
1	D	51	GLU	2.0
1	F	7	PRO	2.0
1	A	182	TYR	2.0
1	E	94	ASN	2.0
1	F	186	CYS	2.0
1	G	42	CYS	2.0
1	D	192	ALA	2.0
1	G	57	TYR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	187	TYR	2.0
1	C	190	PHE	2.0
1	F	190	PHE	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
2	NA	B	501	1/1	0.97	0.13	25,25,25,25	0
2	NA	G	501	1/1	0.98	0.15	25,25,25,25	0
2	NA	H	501	1/1	0.98	0.14	28,28,28,28	0
2	NA	A	501	1/1	0.99	0.09	20,20,20,20	0
2	NA	F	501	1/1	0.99	0.15	27,27,27,27	0
2	NA	C	501	1/1	1.00	0.12	19,19,19,19	0
2	NA	D	501	1/1	1.00	0.11	20,20,20,20	0
2	NA	E	501	1/1	1.00	0.12	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.