



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:32 AM UTC

PDB ID : 6DFW / pdb_00006dfw
Title : TCR 8F10 in complex with IAg7-p8G9E
Authors : Wang, Y.; Dai, S.
Deposited on : 2018-05-15
Resolution : 3.20 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:

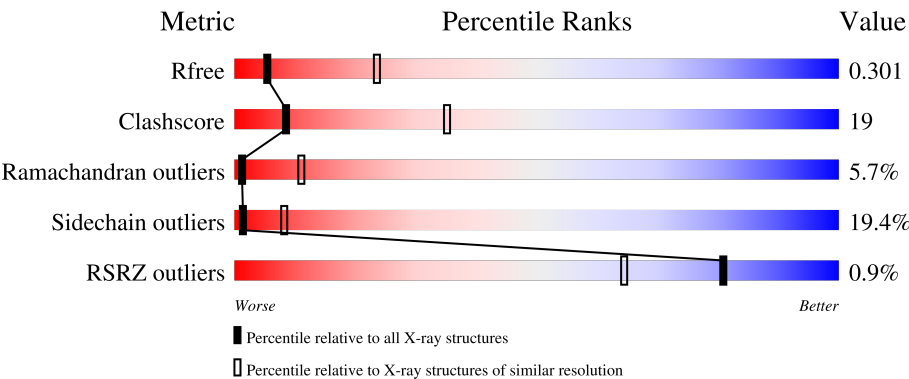
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	183	28%48%19% . .
1	C	183	28%47%19% 5% .
2	B	221	% 41%31%12% . 13%
2	D	221	41%31%12% . 13%
3	E	210	37%22%7%34%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	210	2%49%27%7%16%
4	F	241	%67%27%.
4	H	241	%68%25%...

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12219 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 H-2 class II histocompatibility antigen, A-D alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	2	0
			1489	962	241	284	2			
1	C	182	Total	C	N	O	S	0	1	0
			1477	954	239	282	2			

- Molecule 2 is a protein called H2-Ab1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	192	Total	C	N	O	S	0	0	0
			1595	1003	288	297	7			
2	D	192	Total	C	N	O	S	0	0	0
			1584	997	283	297	7			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-28	HIS	-	expression tag	UNP Q31135
B	-27	LEU	-	expression tag	UNP Q31135
B	-26	VAL	-	expression tag	UNP Q31135
B	-25	GLU	-	expression tag	UNP Q31135
B	-24	ARG	-	expression tag	UNP Q31135
B	-23	LEU	-	expression tag	UNP Q31135
B	-22	TYR	-	expression tag	UNP Q31135
B	-21	LEU	-	expression tag	UNP Q31135
B	-20	VAL	-	expression tag	UNP Q31135
B	-19	CYS	-	expression tag	UNP Q31135
B	-18	GLY	-	expression tag	UNP Q31135
B	-17	GLY	-	expression tag	UNP Q31135
B	-16	GLU	-	expression tag	UNP Q31135
B	-15	GLY	-	expression tag	UNP Q31135
B	-9	ALA	-	expression tag	UNP Q31135
B	-8	GLY	-	expression tag	UNP Q31135

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	GLY	-	expression tag	UNP Q31135
B	-6	GLY	-	expression tag	UNP Q31135
B	-5	SER	-	expression tag	UNP Q31135
B	-4	LEU	-	expression tag	UNP Q31135
B	-3	VAL	-	expression tag	UNP Q31135
B	-2	GLY	-	expression tag	UNP Q31135
B	-1	GLY	-	expression tag	UNP Q31135
B	0	SER	-	expression tag	UNP Q31135
B	1	GLY	-	expression tag	UNP Q31135
B	2	GLY	-	expression tag	UNP Q31135
B	3	GLY	-	expression tag	UNP Q31135
B	192	GLY	-	expression tag	UNP Q31135
B	193	GLY	-	expression tag	UNP Q31135
B	194	LEU	-	expression tag	UNP Q31135
B	195	VAL	-	expression tag	UNP Q31135
B	196	PRO	-	expression tag	UNP Q31135
B	197	ARG	-	expression tag	UNP Q31135
D	-28	HIS	-	expression tag	UNP Q31135
D	-27	LEU	-	expression tag	UNP Q31135
D	-26	VAL	-	expression tag	UNP Q31135
D	-25	GLU	-	expression tag	UNP Q31135
D	-24	ARG	-	expression tag	UNP Q31135
D	-23	LEU	-	expression tag	UNP Q31135
D	-22	TYR	-	expression tag	UNP Q31135
D	-21	LEU	-	expression tag	UNP Q31135
D	-20	VAL	-	expression tag	UNP Q31135
D	-19	CYS	-	expression tag	UNP Q31135
D	-18	GLY	-	expression tag	UNP Q31135
D	-17	GLY	-	expression tag	UNP Q31135
D	-16	GLU	-	expression tag	UNP Q31135
D	-15	GLY	-	expression tag	UNP Q31135
D	-9	ALA	-	expression tag	UNP Q31135
D	-8	GLY	-	expression tag	UNP Q31135
D	-7	GLY	-	expression tag	UNP Q31135
D	-6	GLY	-	expression tag	UNP Q31135
D	-5	SER	-	expression tag	UNP Q31135
D	-4	LEU	-	expression tag	UNP Q31135
D	-3	VAL	-	expression tag	UNP Q31135
D	-2	GLY	-	expression tag	UNP Q31135
D	-1	GLY	-	expression tag	UNP Q31135
D	0	SER	-	expression tag	UNP Q31135
D	1	GLY	-	expression tag	UNP Q31135

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	2	GLY	-	expression tag	UNP Q31135
D	3	GLY	-	expression tag	UNP Q31135
D	192	GLY	-	expression tag	UNP Q31135
D	193	GLY	-	expression tag	UNP Q31135
D	194	LEU	-	expression tag	UNP Q31135
D	195	VAL	-	expression tag	UNP Q31135
D	196	PRO	-	expression tag	UNP Q31135
D	197	ARG	-	expression tag	UNP Q31135

- Molecule 3 is a protein called 8F10 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	139	Total	C	N	O	S	0	0	0
			1075	671	183	216	5			
3	G	177	Total	C	N	O	S	0	1	0
			1381	868	230	276	7			

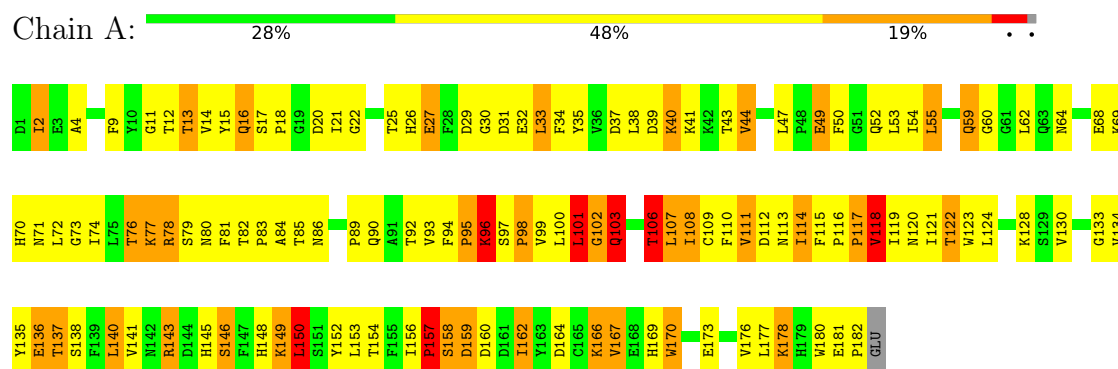
- Molecule 4 is a protein called 8F10 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	237	Total	C	N	O	S	0	0	0
			1811	1148	316	341	6			
4	H	235	Total	C	N	O	S	0	0	0
			1807	1145	318	338	6			

3 Residue-property plots

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.

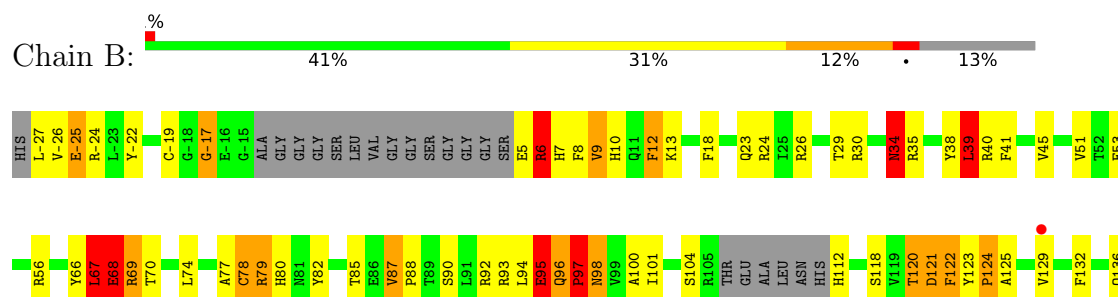
- Molecule 1: H-2 class II histocompatibility antigen, A-D alpha chain



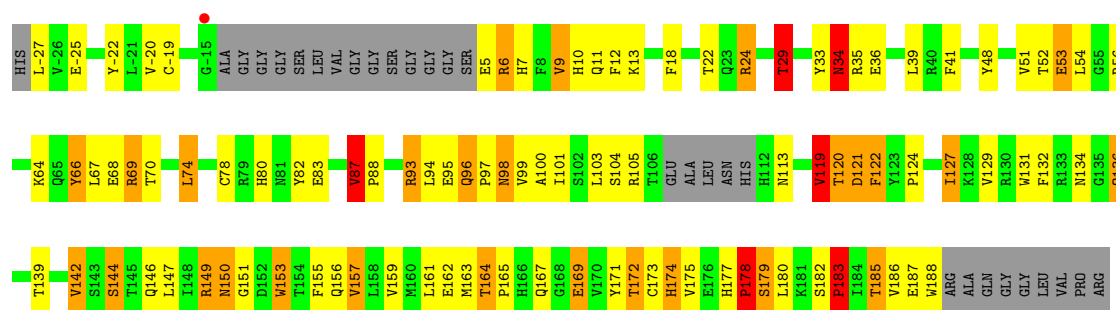
- Molecule 1: H-2 class II histocompatibility antigen, A-D alpha chain



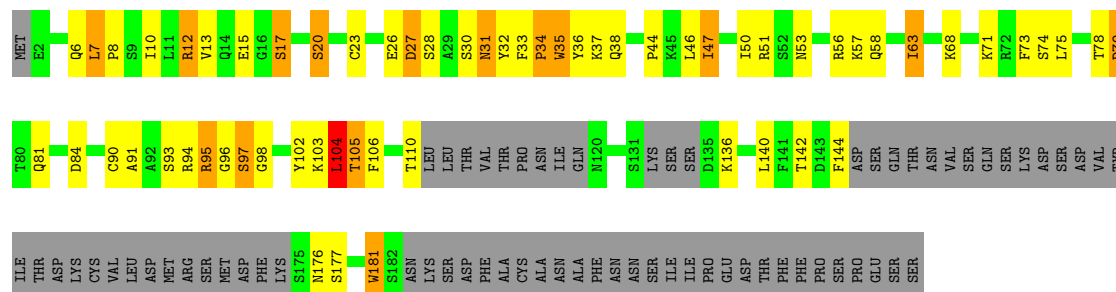
- Molecule 2: H2-Ab1 protein



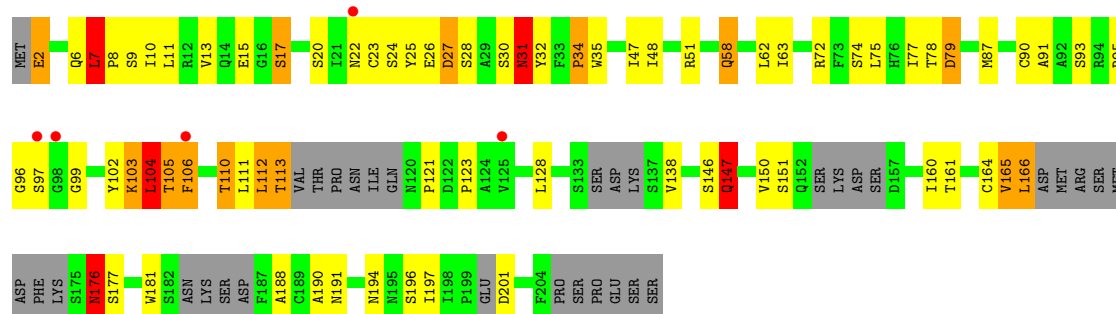
- Molecule 2: H2-Ab1 protein



- Molecule 3: 8F10 alpha chain



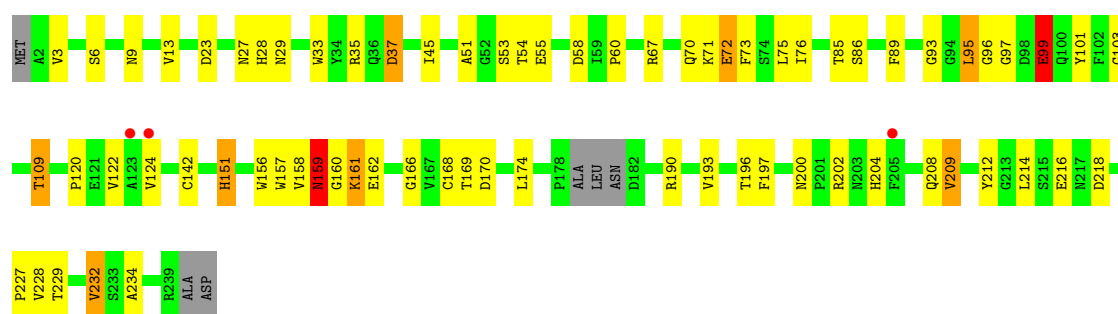
- Molecule 3: 8F10 alpha chain



- Molecule 4: 8F10 beta chain



- Molecule 4: 8F10 beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.09Å 102.04Å 136.00Å 90.00° 107.83° 90.00°	Depositor
Resolution (Å)	50.01 – 3.20 50.01 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.7 (50.01-3.20) 96.7 (50.01-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.233 , 0.297 0.239 , 0.301	Depositor DCC
R_{free} test set	1981 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	94.4	Xtriage
Anisotropy	0.767	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 99.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.089 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12219	wwPDB-VP
Average B, all atoms (Å ²)	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	1.85	26/1535 (1.7%)	1.61	15/2096 (0.7%)
1	C	1.78	30/1523 (2.0%)	1.55	22/2080 (1.1%)
2	B	1.82	30/1631 (1.8%)	1.51	16/2207 (0.7%)
2	D	1.65	23/1620 (1.4%)	1.42	17/2194 (0.8%)
3	E	1.07	0/1095	1.27	6/1478 (0.4%)
3	G	0.99	0/1407	1.22	8/1897 (0.4%)
4	F	0.87	2/1862 (0.1%)	1.09	3/2543 (0.1%)
4	H	0.92	2/1857 (0.1%)	1.10	5/2531 (0.2%)
All	All	1.43	113/12530 (0.9%)	1.35	92/17026 (0.5%)

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	A	0	2
1	C	0	3
2	B	0	1
2	D	0	3
All	All	0	9

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6	ARG	NE-CZ	22.09	1.57	1.33
1	A	102	GLY	C-O	18.53	1.49	1.24
2	B	9	VAL	C-O	16.93	1.41	1.24
1	A	98	PRO	C-O	15.22	1.43	1.24
2	D	9	VAL	C-O	10.94	1.35	1.24
2	D	149	ARG	CZ-NH1	10.90	1.48	1.32
2	D	179	SER	CB-OG	10.73	1.63	1.42
2	D	121	ASP	C-N	10.03	1.47	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	LYS	CA-C	9.98	1.65	1.52
2	B	179	SER	CB-OG	9.94	1.62	1.42
2	D	5	GLU	N-CA	9.93	1.65	1.46
2	B	5	GLU	N-CA	9.70	1.64	1.46
1	C	102	GLY	C-O	8.65	1.35	1.23
1	A	31	ASP	CA-C	-8.52	1.42	1.52
1	A	102	GLY	N-CA	8.52	1.56	1.45
2	B	169	GLU	C-O	8.40	1.34	1.23
1	C	150	LEU	C-O	7.91	1.32	1.24
1	C	154	THR	C-O	7.90	1.33	1.24
2	B	5	GLU	C-N	-7.79	1.21	1.33
1	C	98	PRO	C-O	7.79	1.34	1.24
2	D	119	VAL	CA-CB	7.69	1.62	1.53
1	C	27	GLU	CA-C	7.63	1.61	1.52
2	B	96	GLN	CA-C	7.53	1.62	1.52
2	B	95	GLU	CG-CD	7.40	1.70	1.52
2	D	175	VAL	CA-CB	7.36	1.64	1.54
2	B	121	ASP	CG-OD1	7.32	1.39	1.25
2	D	169	GLU	C-O	7.28	1.32	1.23
1	C	157	PRO	CA-CB	-7.23	1.43	1.53
1	A	101	LEU	C-O	7.21	1.33	1.24
1	A	107	LEU	N-CA	7.20	1.54	1.46
1	C	96	LYS	CA-C	7.14	1.61	1.52
1	C	94	PHE	C-N	7.12	1.42	1.33
2	B	150	ASN	CA-C	7.05	1.62	1.52
1	C	132	ASP	C-O	6.97	1.32	1.23
2	B	5	GLU	CA-CB	-6.92	1.39	1.53
1	C	96	LYS	CB-CG	-6.91	1.31	1.52
1	C	150	LEU	N-CA	6.89	1.54	1.46
2	B	149	ARG	C-O	-6.87	1.16	1.24
2	D	178	PRO	C-O	6.81	1.32	1.24
1	C	17	SER	CA-C	6.81	1.61	1.52
4	F	99	GLU	N-CA	6.77	1.54	1.46
1	A	38	LEU	CB-CG	6.74	1.67	1.53
1	C	50	PHE	C-O	6.70	1.32	1.24
2	B	100	ALA	CA-CB	6.69	1.64	1.53
2	D	132	PHE	C-O	6.68	1.32	1.24
2	D	97	PRO	CA-C	-6.61	1.46	1.52
1	A	27	GLU	CD-OE2	6.55	1.37	1.25
1	C	106	THR	C-O	6.54	1.31	1.23
2	B	180	LEU	CB-CG	6.42	1.66	1.53
2	B	172	THR	CA-C	6.38	1.59	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	74	ILE	CG1-CD1	6.31	1.76	1.51
1	A	102	GLY	C-N	6.28	1.56	1.33
4	H	99	GLU	N-CA	6.27	1.54	1.46
2	B	100	ALA	N-CA	6.25	1.53	1.46
1	C	156	ILE	CA-C	6.23	1.59	1.52
2	B	9	VAL	C-N	6.18	1.42	1.33
1	C	58	PRO	CA-C	6.13	1.61	1.52
1	A	130	VAL	C-O	6.12	1.30	1.24
2	B	96	GLN	N-CA	6.11	1.54	1.46
2	B	176	GLU	CA-C	6.06	1.60	1.52
2	D	149	ARG	CZ-NH2	6.05	1.41	1.33
2	D	174	HIS	C-O	6.04	1.31	1.24
2	B	95	GLU	CD-OE1	6.01	1.36	1.25
4	H	93	GLY	CA-C	5.92	1.58	1.51
1	C	101	LEU	CA-CB	5.87	1.63	1.53
2	B	39	LEU	CA-C	5.79	1.59	1.52
2	B	7	HIS	C-O	5.74	1.30	1.23
1	A	170	TRP	NE1-CE2	5.73	1.43	1.37
2	D	34	ASN	CA-C	5.70	1.60	1.52
2	D	5	GLU	CD-OE2	5.67	1.36	1.25
1	A	12	THR	C-O	5.65	1.30	1.23
1	C	30	GLY	CA-C	5.64	1.60	1.51
1	A	122	THR	CA-C	5.60	1.59	1.52
2	D	180	LEU	CB-CG	5.59	1.64	1.53
2	B	121	ASP	C-N	5.59	1.41	1.33
2	B	148	ILE	CB-CG2	5.58	1.71	1.52
1	C	157	PRO	C-O	5.57	1.31	1.24
1	A	96	LYS	N-CA	-5.55	1.39	1.46
1	C	12	THR	CA-C	-5.54	1.47	1.53
1	C	115	PHE	N-CA	5.54	1.53	1.46
2	D	183	PRO	N-CD	5.54	1.55	1.47
1	C	74	ILE	CA-CB	5.50	1.62	1.54
1	C	118	VAL	CA-CB	5.50	1.61	1.54
2	B	176	GLU	CD-OE2	5.48	1.35	1.25
2	D	174	HIS	CA-C	5.45	1.59	1.52
2	D	188	TRP	C-O	5.42	1.34	1.23
2	B	121	ASP	C-O	5.41	1.30	1.24
4	F	119	PRO	CA-C	5.40	1.57	1.52
1	A	22	GLY	CA-C	5.40	1.56	1.52
2	D	96	GLN	N-CA	5.38	1.53	1.46
2	B	7	HIS	CA-C	-5.38	1.46	1.52
1	A	49	GLU	CD-OE1	5.37	1.35	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	121	ASP	C-O	5.33	1.30	1.24
2	B	175	VAL	CA-C	5.33	1.59	1.52
1	C	102	GLY	C-N	5.32	1.41	1.33
1	A	25	THR	CB-OG1	5.32	1.52	1.43
1	A	98	PRO	C-N	5.29	1.41	1.33
2	D	7	HIS	ND1-CE1	5.25	1.37	1.32
1	A	95	PRO	C-N	5.16	1.40	1.33
1	A	106	THR	C-N	5.13	1.40	1.33
1	A	137	THR	N-CA	5.12	1.52	1.46
1	A	133	GLY	C-O	5.12	1.29	1.24
1	C	110	PHE	C-O	5.10	1.30	1.24
2	B	34	ASN	C-O	5.09	1.30	1.24
1	C	157	PRO	CA-C	5.09	1.59	1.52
1	A	71	ASN	C-O	5.08	1.30	1.24
2	D	179	SER	CA-C	5.06	1.59	1.52
1	A	90	GLN	C-O	5.06	1.29	1.23
1	A	157	PRO	CA-C	5.04	1.59	1.52
2	B	150	ASN	CA-CB	5.04	1.62	1.53
1	C	27	GLU	CD-OE2	5.04	1.34	1.25
1	C	91	ALA	N-CA	5.03	1.52	1.45
1	C	117	PRO	N-CA	-5.01	1.41	1.47

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	GLY	N-CA-C	-12.65	99.42	114.48
2	B	150	ASN	N-CA-C	-9.79	101.34	113.28
2	D	7	HIS	CA-CB-CG	-8.98	104.82	113.80
2	B	179	SER	N-CA-C	-7.93	102.67	113.30
2	B	121	ASP	N-CA-C	7.75	127.31	110.80
1	A	96	LYS	CB-CG-CD	-7.50	94.05	111.30
2	B	172	THR	N-CA-C	7.29	121.51	107.44
2	D	122	PHE	N-CA-C	7.26	119.90	110.53
2	D	121	ASP	N-CA-C	7.15	126.02	110.80
1	C	101	LEU	O-C-N	-7.05	113.21	122.59
4	H	159	ASN	N-CA-C	7.05	121.12	111.54
3	G	31	ASN	N-CA-C	7.01	121.59	113.38
1	A	101	LEU	CA-C-N	-6.97	115.27	123.08
1	A	101	LEU	C-N-CA	-6.97	115.27	123.08
2	D	172	THR	N-CA-C	6.80	118.53	107.32
2	D	29	THR	CB-CA-C	6.77	121.43	109.72
1	C	14	VAL	CB-CA-C	6.63	119.14	110.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	96	LYS	N-CA-C	6.61	118.18	110.97
1	A	120	ASN	N-CA-C	6.60	119.17	108.41
3	G	104	LEU	CA-C-N	6.58	133.54	121.70
3	G	104	LEU	C-N-CA	6.58	133.54	121.70
1	C	44	VAL	CB-CA-C	6.49	117.81	110.41
3	E	35	TRP	N-CA-C	6.44	119.22	109.23
1	C	23	GLN	N-CA-C	6.44	117.99	107.23
4	F	150	ASP	N-CA-C	6.38	120.79	113.19
3	E	104	LEU	CA-C-N	6.35	133.12	121.70
3	E	104	LEU	C-N-CA	6.35	133.12	121.70
3	G	181	TRP	N-CA-C	6.34	118.49	108.79
1	A	103	GLN	CA-C-N	-6.32	113.44	119.76
1	A	103	GLN	C-N-CA	-6.32	113.44	119.76
1	A	96	LYS	N-CA-C	6.31	117.85	110.97
2	B	144	SER	N-CA-C	6.31	119.40	110.50
1	C	116	PRO	CA-C-N	6.27	127.68	119.84
1	C	116	PRO	C-N-CA	6.27	127.68	119.84
2	B	97	PRO	N-CD-CG	6.25	112.58	103.20
2	B	188	TRP	N-CA-C	6.24	118.57	108.34
2	D	119	VAL	CB-CA-C	-6.21	104.59	111.35
2	D	113	ASN	N-CA-C	6.11	119.18	109.65
1	C	74	ILE	CA-CB-CG1	6.04	120.67	110.40
2	B	186	VAL	N-CA-C	6.04	118.05	108.87
1	C	103	GLN	CA-C-N	5.98	126.00	119.90
1	C	103	GLN	C-N-CA	5.98	126.00	119.90
1	A	30	GLY	CA-C-N	-5.96	112.13	122.37
1	A	30	GLY	C-N-CA	-5.96	112.13	122.37
3	G	176	ASN	N-CA-C	5.94	118.31	108.99
2	D	35	ARG	N-CA-C	-5.88	107.09	114.56
2	B	6	ARG	NE-CZ-NH1	5.87	127.37	121.50
4	F	95	LEU	N-CA-C	5.86	123.29	110.80
1	C	167	VAL	N-CA-C	5.83	116.26	107.75
1	C	117	PRO	CA-C-N	-5.81	114.33	122.75
1	C	117	PRO	C-N-CA	-5.81	114.33	122.75
1	C	30	GLY	CA-C-O	5.80	125.47	118.86
1	A	167	VAL	N-CA-C	5.79	116.27	108.17
2	B	12	PHE	CB-CA-C	-5.79	101.42	110.74
2	B	124	PRO	CA-N-CD	-5.79	103.40	111.50
2	D	144	SER	N-CA-C	5.76	118.13	110.53
1	C	118	VAL	O-C-N	5.74	129.26	123.07
2	B	9	VAL	O-C-N	5.66	129.18	123.07
2	B	122	PHE	N-CA-C	5.66	118.16	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	VAL	O-C-N	5.63	129.28	123.20
4	H	103	GLY	CA-C-N	5.59	124.94	118.85
4	H	103	GLY	C-N-CA	5.59	124.94	118.85
2	D	97	PRO	CB-CA-C	-5.58	106.33	111.40
2	B	7	HIS	CA-CB-CG	-5.57	108.23	113.80
3	E	142	THR	N-CA-C	5.55	117.84	109.23
4	H	151	HIS	N-CA-C	5.55	118.42	107.98
3	E	56	ARG	N-CA-C	5.54	117.43	108.41
3	G	164	CYS	N-CA-C	5.51	115.82	108.38
1	A	150	LEU	CA-C-N	-5.44	115.04	122.93
1	A	150	LEU	C-N-CA	-5.44	115.04	122.93
2	D	98	ASN	OD1-CG-ND2	-5.41	117.19	122.60
2	B	150	ASN	O-C-N	5.38	130.04	122.41
3	E	97	SER	N-CA-C	5.36	126.01	111.00
2	D	66	TYR	O-C-N	5.34	125.52	120.71
4	F	115	LYS	N-CA-C	5.30	116.75	110.97
1	C	120	ASN	N-CA-C	5.29	117.01	108.34
3	G	103	LYS	CA-C-N	5.28	131.62	121.54
3	G	103	LYS	C-N-CA	5.28	131.62	121.54
1	C	93	VAL	N-CA-C	5.27	115.68	107.99
1	C	102	GLY	N-CA-C	5.26	125.64	113.18
2	D	87	VAL	CA-C-N	-5.22	113.31	119.84
2	D	87	VAL	C-N-CA	-5.22	113.31	119.84
1	A	102	GLY	CA-C-O	-5.21	114.16	119.37
4	H	72	GLU	N-CA-C	5.21	117.73	109.24
2	D	175	VAL	CA-C-O	5.18	124.83	120.22
2	D	182	SER	CA-C-N	5.17	126.30	119.84
2	D	182	SER	C-N-CA	5.17	126.30	119.84
1	C	139	PHE	CA-C-N	-5.12	115.77	122.99
1	C	139	PHE	C-N-CA	-5.12	115.77	122.99
1	C	103	GLN	CB-CA-C	-5.08	105.14	110.33
1	C	154	THR	CA-CB-OG1	5.07	117.20	109.60
2	B	-25	GLU	N-CA-C	5.02	117.74	109.76

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	GLY	Mainchain
1	A	117	PRO	Peptide
2	B	67	LEU	Peptide
1	C	117	PRO	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C	150	LEU	Mainchain
1	C	155	PHE	Sidechain
2	D	93	ARG	Sidechain
2	D	96	GLN	Mainchain
2	D	98	ASN	Sidechain

5.2 Too-close contacts ⓘ

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	1489	0	1418	104	0
1	C	1477	0	1402	97	0
2	B	1595	0	1533	76	0
2	D	1584	0	1510	65	0
3	E	1075	0	1015	48	0
3	G	1381	0	1313	39	0
4	F	1811	0	1687	39	0
4	H	1807	0	1694	40	0
All	All	12219	0	11572	452	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 19.

All (452) 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:74:ILE:CG1	1:C:74:ILE:CD1	1.76	1.53
2:D:179:SER:CB	2:D:179:SER:OG	1.63	1.43
3:E:31:ASN:HD22	3:E:95:ARG:HB3	1.17	1.05
1:A:17:SER:OG	1:A:18:PRO:HA	1.61	1.00
3:E:31:ASN:HD22	3:E:95:ARG:CB	1.75	0.99
1:A:59[A]:GLN:HE21	1:A:59[A]:GLN:CA	1.72	0.97
3:E:31:ASN:ND2	3:E:95:ARG:HB3	1.80	0.97
3:E:103:LYS:HB3	3:E:104:LEU:HD22	1.52	0.91
1:A:59[A]:GLN:HE21	1:A:59[A]:GLN:HA	1.37	0.90
3:G:27:ASP:H	3:G:28:SER:HA	1.36	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59[A]:GLN:N	1:A:59[A]:GLN:NE2	2.22	0.88
3:E:27:ASP:N	3:E:28:SER:HA	1.90	0.87
1:C:86:ASN:HD22	1:C:170:TRP:HB2	1.38	0.86
4:H:120:PRO:HG2	4:H:209:VAL:HG11	1.58	0.85
3:G:27:ASP:N	3:G:28:SER:HA	1.91	0.84
2:B:129:VAL:HG11	2:B:159:VAL:HG21	1.60	0.83
3:E:27:ASP:H	3:E:28:SER:HA	1.40	0.83
2:B:129:VAL:CG1	2:B:159:VAL:HG21	2.08	0.82
1:C:86:ASN:ND2	1:C:170:TRP:HB2	1.94	0.82
4:F:182:ASP:CB	4:F:183:SER:HA	2.08	0.82
3:E:31:ASN:HD22	3:E:95:ARG:CG	1.93	0.82
2:B:181:LYS:HE2	2:B:181:LYS:H	1.46	0.79
4:H:85:THR:HG23	4:H:109:THR:HA	1.65	0.79
1:C:16:GLN:HB3	2:D:9:VAL:HG22	1.65	0.78
4:F:214:LEU:HD23	4:F:218:ASP:HB3	1.67	0.77
3:E:31:ASN:ND2	3:E:95:ARG:CB	2.44	0.77
1:C:89:PRO:HD3	1:C:169:HIS:HD2	1.49	0.76
1:C:140:LEU:HB2	1:C:148:HIS:CD2	2.20	0.76
3:E:140:LEU:HD11	3:E:177:SER:HB2	1.69	0.74
1:A:59[A]:GLN:HE21	1:A:59[A]:GLN:N	1.84	0.74
3:G:51:ARG:HD3	3:G:95:ARG:NH2	2.03	0.74
3:G:27:ASP:H	3:G:28:SER:CA	2.01	0.73
2:D:172:THR:CG2	2:D:185:THR:HG22	2.19	0.73
3:G:176:ASN:HD22	3:G:177:SER:H	1.36	0.73
1:A:33:LEU:HD21	2:B:-24:ARG:NH2	2.04	0.72
1:C:96:LYS:HA	2:D:156:GLN:HE22	1.53	0.72
1:C:166:LYS:HE3	1:C:177:LEU:HD21	1.72	0.72
1:C:16:GLN:CB	2:D:9:VAL:HG22	2.20	0.72
3:G:112:LEU:HB2	3:G:113:THR:HA	1.73	0.71
1:C:34:PHE:CD2	1:C:43:THR:HG23	2.26	0.70
4:H:200:ASN:HD21	4:H:202:ARG:HH12	1.38	0.70
1:C:110:PHE:HB2	1:C:150:LEU:HD23	1.73	0.70
3:G:176:ASN:HD22	3:G:177:SER:N	1.90	0.70
2:B:68:GLU:O	2:B:70:THR:N	2.25	0.70
1:A:89:PRO:HD3	1:A:169:HIS:HD2	1.55	0.69
1:C:99:VAL:CG1	1:C:157:PRO:HB3	2.22	0.69
1:C:101:LEU:O	1:C:103:GLN:N	2.26	0.69
1:C:24:TYR:CD2	1:C:61:GLY:HA2	2.27	0.68
3:G:27:ASP:HB3	3:G:30:SER:OG	1.93	0.68
1:A:140:LEU:HB2	1:A:148:HIS:CD2	2.29	0.68
1:C:26:HIS:CD2	1:C:34:PHE:CZ	2.82	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:120:PRO:HG2	4:F:209:VAL:HG11	1.75	0.68
1:C:59:GLN:NE2	1:C:63:GLN:NE2	2.42	0.68
3:E:27:ASP:H	3:E:28:SER:CA	2.06	0.67
3:E:31:ASN:ND2	3:E:95:ARG:CG	2.56	0.67
4:H:142:CYS:HB2	4:H:156:TRP:CZ2	2.29	0.67
1:A:96:LYS:HA	2:B:156:GLN:HE22	1.59	0.67
2:D:-19:CYS:HB2	2:D:12:PHE:CD2	2.29	0.67
4:F:142:CYS:HB2	4:F:156:TRP:CZ2	2.29	0.66
1:A:33:LEU:HD21	2:B:-24:ARG:HH21	1.59	0.66
3:G:31:ASN:OD1	3:G:95:ARG:HB3	1.95	0.66
1:A:59[A]:GLN:CA	1:A:59[A]:GLN:NE2	2.44	0.66
1:A:27:GLU:OE2	1:A:140:LEU:HD23	1.97	0.65
2:B:101:ILE:HD11	2:B:173:CYS:HB3	1.77	0.65
3:G:104:LEU:HA	3:G:105:THR:HB	1.79	0.65
1:C:94:PHE:O	1:C:108:ILE:HB	1.97	0.65
2:B:147:LEU:HG	2:B:147:LEU:O	1.95	0.65
2:D:144:SER:HB2	2:D:159:VAL:HG13	1.78	0.64
4:F:33:TRP:CD1	4:F:75:LEU:HB2	2.32	0.64
4:H:124:VAL:HG23	4:H:234:ALA:HB3	1.78	0.64
1:A:39:ASP:HB2	1:A:40:LYS:HE3	1.78	0.64
1:A:34:PHE:CD2	1:A:43:THR:HG23	2.33	0.64
2:B:174:HIS:CE1	2:B:183:PRO:HB3	2.33	0.64
3:E:58:GLN:HG3	3:E:63:ILE:HG23	1.80	0.64
3:G:147:GLN:O	3:G:147:GLN:NE2	2.31	0.63
1:C:13:THR:HB	1:C:68:GLU:HG3	1.80	0.63
1:C:112[B]:ASP:OD1	1:C:112[B]:ASP:C	2.42	0.63
3:E:31:ASN:ND2	3:E:95:ARG:HG2	2.14	0.63
1:A:16:GLN:HB3	2:B:9:VAL:HG22	1.80	0.63
2:B:18:PHE:CZ	2:B:82:TYR:HB2	2.33	0.63
2:B:174:HIS:HE1	2:B:183:PRO:HB3	1.64	0.63
1:C:97:SER:O	1:C:105:ASN:ND2	2.26	0.63
1:A:115:PHE:CD2	2:B:35:ARG:HD3	2.33	0.63
2:B:129:VAL:HG11	2:B:159:VAL:CG2	2.28	0.63
2:B:167:GLN:HE21	2:B:169:GLU:CG	2.12	0.62
3:G:8:PRO:HG2	3:G:11:LEU:HD12	1.81	0.62
1:A:59[A]:GLN:CD	1:A:59[A]:GLN:H	2.04	0.62
4:F:85:THR:HG23	4:F:109:THR:HA	1.81	0.62
1:C:74:ILE:CD1	1:C:74:ILE:CB	2.75	0.62
1:A:15:TYR:CZ	1:A:69:LYS:HG2	2.35	0.61
1:C:75:LEU:HB3	2:D:33:TYR:CD1	2.35	0.61
1:A:112[A]:ASP:CG	1:A:148:HIS:HB3	2.25	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:TYR:HD2	1:C:152:TYR:HD2	1.48	0.61
2:D:179:SER:CB	2:D:179:SER:HG	2.07	0.61
3:G:165:VAL:HG13	3:G:166:LEU:H	1.64	0.61
2:B:-22:TYR:CD2	3:E:97:SER:HB2	2.36	0.61
2:B:94:LEU:HD13	2:B:179:SER:HA	1.83	0.61
1:A:15:TYR:CE2	1:A:69:LYS:HG2	2.36	0.61
2:B:69:ARG:HB2	3:E:51:ARG:CZ	2.31	0.61
1:A:17:SER:HG	1:A:18:PRO:HA	1.65	0.60
1:C:77:LYS:HA	1:C:81:PHE:CE1	2.36	0.60
1:C:147:PHE:CZ	2:D:11:GLN:OE1	2.54	0.60
4:F:158:VAL:HA	4:F:204:HIS:O	2.01	0.60
2:B:167:GLN:HE21	2:B:169:GLU:HG2	1.67	0.60
3:G:25:TYR:HD2	3:G:27:ASP:HB2	1.66	0.60
1:A:110:PHE:HB2	1:A:150:LEU:HD23	1.84	0.60
2:B:132:PHE:O	2:B:172:THR:N	2.35	0.60
1:A:72:LEU:HD13	2:B:10:HIS:HB2	1.83	0.60
1:C:143:ARG:HB2	1:C:143:ARG:HH11	1.66	0.60
3:E:34:PRO:HD2	3:E:91:ALA:O	2.01	0.59
1:A:121:ILE:HD12	1:A:149:LYS:HD2	1.84	0.59
1:A:89:PRO:HD3	1:A:169:HIS:CD2	2.37	0.59
1:C:145:HIS:HB3	2:D:11:GLN:NE2	2.16	0.59
1:C:72:LEU:HD13	2:D:10:HIS:HB2	1.84	0.59
3:E:27:ASP:N	3:E:28:SER:CA	2.64	0.59
1:C:24:TYR:CE2	1:C:61:GLY:HA2	2.38	0.58
4:H:95:LEU:N	4:H:96:GLY:HA2	2.18	0.58
1:C:119:ILE:HD11	1:C:167:VAL:HG11	1.86	0.58
1:C:135:TYR:HD2	1:C:152:TYR:CD2	2.20	0.58
1:A:9:PHE:HB2	1:A:27:GLU:HB2	1.86	0.58
1:C:24:TYR:CD2	1:C:61:GLY:CA	2.87	0.58
3:G:35:TRP:CZ3	3:G:90:CYS:HB2	2.39	0.58
1:A:54:ILE:HG22	2:B:-26:VAL:HG13	1.85	0.57
1:A:86:ASN:ND2	1:A:170:TRP:HB2	2.19	0.57
1:A:166:LYS:HB2	1:A:177:LEU:CD2	2.35	0.57
4:H:161:LYS:HD2	4:H:162:GLU:N	2.20	0.57
1:A:112[B]:ASP:HB2	1:A:148:HIS:HB3	1.85	0.57
4:H:158:VAL:HA	4:H:204:HIS:O	2.05	0.57
3:G:166:LEU:HD13	4:H:166:GLY:HA2	1.87	0.57
1:C:93:VAL:HG13	1:C:107:LEU:HD22	1.87	0.57
2:D:74:LEU:HA	2:D:78:CYS:HB2	1.86	0.57
1:A:60:GLY:HA3	2:B:-22:TYR:CE2	2.40	0.57
1:A:17:SER:OG	1:A:18:PRO:CA	2.45	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:ALA:HB3	4:H:29:ASN:HD21	1.71	0.56
1:C:109:CYS:O	1:C:150:LEU:HA	2.05	0.56
2:D:149:ARG:O	2:D:151:GLY:N	2.38	0.56
2:D:174:HIS:CE1	2:D:183:PRO:HB3	2.40	0.56
3:G:32:TYR:CE2	3:G:34:PRO:HG3	2.40	0.56
4:H:120:PRO:CG	4:H:209:VAL:HG11	2.35	0.56
3:E:96:GLY:HA2	3:E:97:SER:C	2.31	0.56
2:D:94:LEU:HD13	2:D:179:SER:HA	1.88	0.56
3:G:96:GLY:HA2	3:G:97:SER:C	2.29	0.56
3:G:104:LEU:HA	3:G:105:THR:CB	2.35	0.56
1:A:116:PRO:HG2	1:A:170:TRP:HZ3	1.69	0.56
1:C:84:ALA:HB2	2:D:34:ASN:ND2	2.20	0.56
1:A:112[B]:ASP:OD1	1:A:112[B]:ASP:C	2.48	0.56
2:B:101:ILE:HD11	2:B:173:CYS:CB	2.36	0.56
1:C:35:TYR:CZ	1:C:44:VAL:HG11	2.41	0.56
1:A:26:HIS:CD2	1:A:34:PHE:CZ	2.93	0.56
1:C:93:VAL:HG21	1:C:165:CYS:HB2	1.87	0.55
1:A:16:GLN:CB	2:B:9:VAL:HG22	2.36	0.55
1:A:35:TYR:CZ	1:A:44:VAL:HG11	2.42	0.55
1:C:143:ARG:HB2	1:C:143:ARG:NH1	2.21	0.55
3:G:103:LYS:HB3	3:G:104:LEU:HD22	1.88	0.55
4:F:124:VAL:HG23	4:F:234:ALA:HB3	1.89	0.55
1:A:13:THR:HB	1:A:68:GLU:HG3	1.89	0.55
1:A:143:ARG:C	1:A:145:HIS:H	2.15	0.54
4:H:33:TRP:CD1	4:H:75:LEU:HB2	2.42	0.54
1:A:94:PHE:CZ	1:A:108:ILE:HG21	2.42	0.54
4:F:35:ARG:HH21	4:F:86:SER:HB2	1.73	0.54
1:A:54:ILE:HD13	2:B:85:THR:HB	1.90	0.54
1:C:89:PRO:HD3	1:C:169:HIS:CD2	2.38	0.54
1:A:98:PRO:HG3	2:B:118:SER:CB	2.38	0.54
3:E:32:TYR:CE2	3:E:34:PRO:HG3	2.42	0.54
4:H:159:ASN:N	4:H:160:GLY:HA2	2.23	0.54
1:A:37:ASP:OD2	1:A:40:LYS:HB2	2.08	0.54
1:A:101:LEU:H	1:A:101:LEU:CD2	2.20	0.53
2:B:-19:CYS:HB2	2:B:12:PHE:CD2	2.43	0.53
1:A:59[B]:GLN:OE1	1:A:62:LEU:HD12	2.07	0.53
3:E:93:SER:OG	3:E:104:LEU:N	2.39	0.53
1:C:119:ILE:HD11	1:C:167:VAL:CG1	2.39	0.53
1:A:178:LYS:HE2	1:A:178:LYS:HA	1.90	0.53
2:B:139:THR:O	2:B:142:VAL:HG23	2.09	0.53
4:F:90:CYS:O	4:F:103:GLY:N	2.30	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:LEU:O	1:C:101:LEU:O	2.27	0.53
1:A:121:ILE:CD1	1:A:149:LYS:HD2	2.38	0.53
1:C:11:GLY:H	1:C:26:HIS:CE1	2.26	0.53
3:E:20:SER:HA	3:E:75:LEU:O	2.09	0.53
1:C:84:ALA:HB2	2:D:34:ASN:CG	2.33	0.53
2:D:87:VAL:HG12	2:D:88:PRO:HD3	1.89	0.53
2:B:80:HIS:C	2:B:80:HIS:CD2	2.87	0.52
2:D:-22:TYR:CD2	3:G:97:SER:HB2	2.44	0.52
1:C:5:ASP:OD1	1:C:5:ASP:N	2.42	0.52
4:H:214:LEU:HD23	4:H:218:ASP:HB3	1.91	0.52
3:G:188:ALA:HB3	3:G:191:ASN:HB2	1.92	0.52
2:B:152:ASP:O	2:B:153:TRP:HB2	2.10	0.52
1:C:141:VAL:HB	2:D:13:LYS:HE2	1.92	0.52
1:A:68:GLU:OE2	1:A:68:GLU:HA	2.09	0.52
1:A:156:ILE:O	1:A:157:PRO:O	2.28	0.52
1:C:68:GLU:OE1	2:D:10:HIS:ND1	2.43	0.52
2:D:24:ARG:HB2	2:D:24:ARG:NH1	2.25	0.52
2:D:147:LEU:HD11	2:D:155:PHE:CD2	2.45	0.52
4:H:159:ASN:ND2	4:H:204:HIS:H	2.08	0.52
4:H:200:ASN:HD21	4:H:202:ARG:NH1	2.07	0.51
2:B:132:PHE:HB2	2:B:172:THR:HB	1.91	0.51
2:B:87:VAL:HG12	2:B:88:PRO:HD3	1.92	0.51
4:F:24:GLN:NE2	4:F:28:HIS:O	2.43	0.51
1:C:99:VAL:CG1	1:C:157:PRO:CB	2.88	0.51
4:H:3:VAL:O	4:H:23:ASP:O	2.27	0.51
2:D:101:ILE:HD12	2:D:186:VAL:HG12	1.91	0.51
4:H:156:TRP:O	4:H:162:GLU:HA	2.11	0.51
2:B:129:VAL:HG12	2:B:159:VAL:HG21	1.89	0.51
3:E:27:ASP:HB3	3:E:30:SER:OG	2.09	0.51
1:A:77:LYS:O	1:A:79:SER:N	2.44	0.51
2:B:29:THR:OG1	2:B:41:PHE:HB3	2.11	0.51
1:C:87:GLU:O	1:C:171:GLY:HA3	2.11	0.51
2:D:127:ILE:HD12	2:D:177:HIS:CD2	2.46	0.51
1:A:143:ARG:HH11	1:A:143:ARG:HB2	1.76	0.51
3:G:105:THR:HG22	3:G:106:PHE:N	2.25	0.51
2:B:41:PHE:CE2	2:B:70:THR:HG22	2.46	0.50
1:A:106:THR:HA	1:A:153:LEU:O	2.11	0.50
1:A:115:PHE:CE2	2:B:35:ARG:HD3	2.46	0.50
1:C:59:GLN:HE21	1:C:63:GLN:NE2	2.08	0.50
2:D:172:THR:HG22	2:D:185:THR:HG22	1.90	0.50
1:A:135:TYR:HD2	1:A:152:TYR:CD2	2.29	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:33:PHE:HB3	3:E:73:PHE:CE2	2.46	0.50
1:A:180:TRP:CZ3	1:A:182:PRO:HD3	2.46	0.50
3:E:35:TRP:CZ3	3:E:90:CYS:HB2	2.47	0.50
1:C:86:ASN:HD21	1:C:170:TRP:HE3	1.59	0.50
1:A:119:ILE:HD11	1:A:167:VAL:HG11	1.94	0.50
3:G:58:GLN:HG2	3:G:62:LEU:O	2.12	0.50
3:E:94:ARG:HG3	3:E:94:ARG:HH11	1.76	0.50
1:A:83:PRO:HB3	2:B:8:PHE:CE1	2.47	0.49
3:E:95:ARG:CG	3:E:96:GLY:N	2.75	0.49
1:A:162:ILE:HG23	1:A:181:GLU:CG	2.42	0.49
2:B:144:SER:HB2	2:B:159:VAL:HG13	1.94	0.49
3:E:104:LEU:HA	3:E:105:THR:CB	2.42	0.49
1:A:35:TYR:CD1	1:A:35:TYR:C	2.91	0.49
4:F:3:VAL:O	4:F:23:ASP:O	2.31	0.49
3:G:13:VAL:CG2	3:G:17:SER:HB2	2.43	0.49
3:G:87:MET:HA	3:G:110:THR:O	2.12	0.49
4:H:37:ASP:OD1	4:H:37:ASP:N	2.44	0.49
1:A:98:PRO:HG3	2:B:118:SER:HB3	1.93	0.49
1:C:9:PHE:HB2	1:C:27:GLU:HB2	1.93	0.49
2:B:74:LEU:HA	2:B:78:CYS:HB2	1.95	0.49
2:D:69:ARG:HG2	3:G:51:ARG:NH1	2.28	0.49
1:A:109:CYS:O	1:A:150:LEU:HA	2.13	0.48
2:D:119:VAL:HG21	2:D:129:VAL:HG21	1.94	0.48
4:F:124:VAL:CG2	4:F:207:CYS:HB3	2.43	0.48
1:A:178:LYS:HA	1:A:178:LYS:CE	2.43	0.48
1:A:47:LEU:HD12	1:A:50:PHE:CE2	2.48	0.48
1:A:136:GLU:CD	1:A:149:LYS:HE3	2.38	0.48
1:C:126:ASN:OD1	1:C:162:ILE:HD12	2.14	0.48
1:C:138:SER:O	1:C:149:LYS:HG2	2.12	0.48
4:H:28:HIS:HE1	4:H:101:TYR:CD2	2.30	0.48
3:E:105:THR:O	3:E:106:PHE:HB2	2.13	0.48
2:D:18:PHE:CZ	2:D:82:TYR:HB2	2.49	0.48
3:E:26:GLU:CB	3:E:27:ASP:HA	2.43	0.48
4:H:159:ASN:HD22	4:H:204:HIS:HB3	1.79	0.48
1:C:14:VAL:O	1:C:22:GLY:HA2	2.13	0.48
1:C:101:LEU:HA	1:C:157:PRO:O	2.13	0.48
1:A:135:TYR:HD2	1:A:152:TYR:HD2	1.59	0.48
2:B:95:GLU:OE1	2:B:95:GLU:N	2.46	0.48
3:E:13:VAL:HG22	3:E:17:SER:HB2	1.95	0.48
1:A:145:HIS:HA	2:B:13:LYS:HZ1	1.78	0.48
2:B:96:GLN:O	2:B:97:PRO:O	2.31	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:PRO:C	1:C:60:GLY:N	2.72	0.48
1:A:109:CYS:HB2	1:A:123:TRP:CH2	2.49	0.48
1:A:118:VAL:O	1:A:169:HIS:ND1	2.47	0.48
1:C:68:GLU:OE2	1:C:68:GLU:HA	2.14	0.47
4:H:157:TRP:HA	4:H:161:LYS:O	2.12	0.47
1:A:143:ARG:HB2	1:A:143:ARG:NH1	2.29	0.47
4:F:23:ASP:HA	4:F:71:LYS:O	2.14	0.47
1:C:66:ALA:HB3	4:H:29:ASN:ND2	2.29	0.47
2:D:36:GLU:OE2	2:D:54:LEU:HD22	2.13	0.47
2:D:119:VAL:HB	2:D:157:VAL:HG13	1.95	0.47
2:D:177:HIS:CG	2:D:178:PRO:HD2	2.49	0.47
4:F:132:ILE:HD11	4:F:198:TRP:HD1	1.79	0.47
1:C:11:GLY:HA2	1:C:24:TYR:OH	2.13	0.47
2:D:101:ILE:HD11	2:D:173:CYS:HB3	1.96	0.47
1:C:26:HIS:HB2	1:C:34:PHE:CE1	2.49	0.47
2:D:80:HIS:CD2	2:D:80:HIS:C	2.92	0.47
1:A:162:ILE:HG23	1:A:181:GLU:HG3	1.96	0.47
4:H:99:GLU:CD	4:H:101:TYR:CE1	2.93	0.47
4:F:200:ASN:HD21	4:F:202:ARG:NH2	2.12	0.47
4:F:156:TRP:CZ3	4:F:207:CYS:HB2	2.50	0.47
3:G:93:SER:OG	3:G:104:LEU:N	2.48	0.47
4:F:142:CYS:HB2	4:F:156:TRP:CH2	2.50	0.47
3:G:121:PRO:O	3:G:123:PRO:HD3	2.15	0.47
2:B:66:TYR:O	2:B:68:GLU:N	2.49	0.46
1:C:116:PRO:O	1:C:118:VAL:N	2.46	0.46
3:E:50:ILE:HD12	3:E:57:LYS:HB2	1.97	0.46
3:E:97:SER:OG	3:E:98:GLY:N	2.45	0.46
4:F:35:ARG:HG3	4:F:37:ASP:OD1	2.15	0.46
1:A:4:ALA:HB1	2:B:18:PHE:O	2.14	0.46
1:C:112[A]:ASP:CG	1:C:148:HIS:HB3	2.40	0.46
2:D:12:PHE:HE1	2:D:29:THR:HG23	1.80	0.46
1:A:115:PHE:CD1	1:A:116:PRO:HA	2.51	0.46
4:F:156:TRP:CH2	4:F:207:CYS:HB2	2.50	0.46
1:C:147:PHE:HZ	2:D:11:GLN:OE1	1.98	0.46
1:C:178:LYS:CE	1:C:178:LYS:HA	2.46	0.46
2:D:136:GLN:HE21	2:D:136:GLN:N	2.14	0.46
1:A:93:VAL:HG13	1:A:107:LEU:HD22	1.96	0.46
2:B:67:LEU:C	2:B:68:GLU:O	2.59	0.46
2:D:56:ARG:HH11	2:D:56:ARG:CB	2.28	0.46
4:H:122:VAL:HG21	4:H:209:VAL:HB	1.96	0.46
4:H:142:CYS:HB2	4:H:156:TRP:CH2	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:ILE:HG21	1:C:179:HIS:HE1	1.80	0.46
3:E:38:GLN:HE21	3:E:44:PRO:HD3	1.80	0.46
3:E:91:ALA:HB2	3:E:106:PHE:CD1	2.51	0.46
2:D:164:THR:HA	2:D:165:PRO:HD2	1.75	0.46
1:A:103:GLN:O	1:A:157:PRO:HD2	2.15	0.45
1:A:159:ASP:HA	1:A:160:ASP:HA	1.53	0.45
3:G:2:GLU:O	3:G:26:GLU:HG2	2.15	0.45
1:A:107:LEU:HB2	1:A:153:LEU:HB3	1.97	0.45
2:B:167:GLN:HE21	2:B:169:GLU:HG3	1.80	0.45
1:C:77:LYS:O	1:C:80:ASN:N	2.47	0.45
1:C:159:ASP:HA	1:C:160:ASP:HA	1.72	0.45
2:D:52:THR:O	2:D:54:LEU:N	2.49	0.45
1:A:111:VAL:HG21	1:A:121:ILE:HD11	1.98	0.45
3:E:104:LEU:HA	3:E:105:THR:HB	1.98	0.45
3:E:181:TRP:CZ2	4:F:143:LEU:HD21	2.51	0.45
4:F:37:ASP:OD1	4:F:37:ASP:N	2.50	0.45
1:C:10:TYR:HA	1:C:26:HIS:ND1	2.31	0.45
1:C:74:ILE:H	1:C:74:ILE:HD13	1.81	0.45
3:G:8:PRO:CG	3:G:11:LEU:HD12	2.45	0.45
2:B:125:ALA:HB1	2:B:147:LEU:HD21	1.99	0.45
1:C:143:ARG:C	1:C:145:HIS:H	2.24	0.45
2:D:56:ARG:HH11	2:D:56:ARG:HB2	1.82	0.45
2:B:-24:ARG:NH1	2:B:85:THR:OG1	2.50	0.45
4:H:161:LYS:HD2	4:H:162:GLU:O	2.17	0.45
3:E:95:ARG:HG3	3:E:96:GLY:N	2.32	0.45
3:G:91:ALA:HB2	3:G:106:PHE:HA	1.99	0.45
1:A:55:LEU:HB3	2:B:-27:LEU:HD22	1.98	0.45
1:C:100:LEU:O	1:C:103:GLN:HB2	2.16	0.45
4:H:214:LEU:HB2	4:H:227:PRO:O	2.17	0.45
1:A:162:ILE:HG23	1:A:181:GLU:CD	2.42	0.44
3:E:35:TRP:CD1	3:E:75:LEU:HD13	2.52	0.44
1:C:74:ILE:CD1	1:C:74:ILE:N	2.79	0.44
1:C:145:HIS:HB3	2:D:11:GLN:HE22	1.81	0.44
2:D:149:ARG:O	2:D:149:ARG:HG2	2.16	0.44
2:D:174:HIS:HE1	2:D:183:PRO:HB3	1.79	0.44
3:G:7:LEU:HA	3:G:8:PRO:C	2.42	0.44
3:E:12:ARG:CZ	3:E:12:ARG:HB3	2.47	0.44
4:F:67:ARG:HG3	4:F:72:GLU:O	2.17	0.44
1:A:64:ASN:OD1	2:B:-19:CYS:HB3	2.17	0.44
2:D:93:ARG:NH1	2:D:153:TRP:O	2.50	0.44
1:C:90:GLN:O	1:C:111:VAL:HA	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112[B]:ASP:OD1	1:A:113:ASN:N	2.51	0.44
1:C:32:GLU:HB2	1:C:140:LEU:HD21	1.98	0.44
1:A:80:ASN:O	1:A:81:PHE:C	2.60	0.44
4:F:182:ASP:CB	4:F:183:SER:CA	2.90	0.44
1:C:152:TYR:OH	2:D:151:GLY:O	2.36	0.44
2:D:139:THR:O	2:D:142:VAL:HG23	2.18	0.44
4:H:28:HIS:HE1	4:H:101:TYR:HD2	1.65	0.44
1:A:96:LYS:HA	2:B:156:GLN:NE2	2.30	0.44
4:F:27:ASN:ND2	4:F:70:GLN:OE1	2.51	0.44
2:D:134:ASN:HD21	2:D:169:GLU:HG2	1.82	0.44
2:D:155:PHE:O	2:D:156:GLN:HB3	2.18	0.44
3:G:26:GLU:CB	3:G:27:ASP:HA	2.48	0.44
4:H:33:TRP:CE3	4:H:89:PHE:O	2.71	0.44
4:H:35:ARG:HH21	4:H:86:SER:HB2	1.83	0.44
2:B:-22:TYR:CD2	3:E:97:SER:CB	3.01	0.44
2:B:69:ARG:NH2	2:B:70:THR:OG1	2.48	0.43
1:C:18:PRO:HD3	2:D:6:ARG:O	2.18	0.43
1:A:116:PRO:HG2	1:A:170:TRP:CZ3	2.51	0.43
3:G:147:GLN:HE21	3:G:147:GLN:C	2.26	0.43
1:A:116:PRO:C	1:A:118:VAL:H	2.25	0.43
2:B:90:SER:C	2:B:92:ARG:H	2.25	0.43
3:E:36:TYR:CE1	3:E:46:LEU:HB2	2.53	0.43
2:D:41:PHE:CE2	2:D:70:THR:HG22	2.53	0.43
4:H:35:ARG:HB3	4:H:45:ILE:HD11	2.00	0.43
2:B:38:TYR:CD1	2:B:39:LEU:HB3	2.53	0.43
2:B:122:PHE:O	2:B:154:THR:HA	2.18	0.43
1:A:32:GLU:OE1	1:A:138:SER:HB2	2.17	0.43
1:A:72:LEU:O	1:A:76:THR:OG1	2.32	0.43
1:A:114:ILE:CD1	1:A:119:ILE:HD13	2.49	0.43
1:C:19:GLY:O	1:C:21:ILE:HD12	2.19	0.43
1:C:115:PHE:CZ	2:D:9:VAL:HG11	2.54	0.43
2:D:41:PHE:HB2	2:D:48:TYR:CE2	2.54	0.43
2:D:94:LEU:HD13	2:D:178:PRO:O	2.19	0.43
3:G:128:LEU:HD13	3:G:138:VAL:HG23	2.01	0.43
4:F:28:HIS:HE1	4:F:101:TYR:CD2	2.37	0.43
2:D:174:HIS:HB2	2:D:185:THR:HG23	1.99	0.43
3:G:177:SER:OG	4:H:190:ARG:HD2	2.19	0.43
4:H:157:TRP:NE1	4:H:208:GLN:OE1	2.51	0.43
1:A:119:ILE:HD11	1:A:167:VAL:CG1	2.48	0.43
1:C:116:PRO:C	1:C:118:VAL:H	2.27	0.43
4:F:63:TYR:HD1	4:F:75:LEU:HD11	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:LEU:HD12	1:C:150:LEU:N	2.33	0.43
2:D:120:THR:O	2:D:122:PHE:HD1	2.02	0.43
4:H:58:ASP:C	4:H:60:PRO:HD3	2.44	0.43
2:B:30:ARG:HG2	2:B:40:ARG:HG3	2.00	0.43
2:B:94:LEU:O	2:B:123:TYR:O	2.37	0.43
1:A:84:ALA:HB2	2:B:34:ASN:CG	2.44	0.42
4:F:35:ARG:HB3	4:F:45:ILE:HD11	2.01	0.42
1:C:114:ILE:HD13	1:C:119:ILE:HD13	2.00	0.42
2:B:142:VAL:HA	2:B:160:MET:O	2.19	0.42
3:G:35:TRP:CD1	3:G:75:LEU:HD13	2.54	0.42
3:E:8:PRO:O	3:E:110:THR:HG23	2.20	0.42
1:C:70:HIS:CE1	4:H:95:LEU:HD21	2.55	0.42
4:H:67:ARG:HB2	4:H:73:PHE:CD1	2.54	0.42
2:B:-22:TYR:H	3:E:97:SER:HB2	1.84	0.42
3:E:26:GLU:HB2	3:E:27:ASP:HA	2.00	0.42
4:F:33:TRP:HE3	4:F:89:PHE:O	2.01	0.42
3:E:34:PRO:CD	3:E:91:ALA:O	2.66	0.42
4:F:107:ARG:HG2	4:F:151:HIS:NE2	2.35	0.42
1:C:94:PHE:CZ	1:C:108:ILE:HG21	2.54	0.42
4:H:212:TYR:HA	4:H:229:THR:HG23	2.01	0.42
4:F:33:TRP:CE3	4:F:89:PHE:O	2.72	0.42
1:A:60:GLY:HA3	2:B:-22:TYR:HE2	1.84	0.42
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.88	0.42
3:E:26:GLU:O	3:E:71:LYS:HE2	2.19	0.42
1:A:86:ASN:HD22	1:A:170:TRP:HB2	1.85	0.41
1:A:99:VAL:HG11	1:A:182:PRO:HB3	2.01	0.41
1:A:158:SER:OG	1:A:159:ASP:N	2.50	0.41
2:B:79:ARG:O	2:B:82:TYR:N	2.53	0.41
4:F:214:LEU:HD13	4:F:227:PRO:HG2	2.02	0.41
1:C:69:LYS:O	1:C:70:HIS:C	2.62	0.41
2:D:41:PHE:CD2	2:D:70:THR:HG22	2.55	0.41
4:H:122:VAL:HG21	4:H:232:VAL:HB	2.01	0.41
1:A:83:PRO:CG	2:B:6:ARG:HG2	2.50	0.41
1:C:59:GLN:HE21	1:C:63:GLN:HE21	1.67	0.41
1:C:156:ILE:O	1:C:158:SER:N	2.53	0.41
2:D:22:THR:HG21	2:D:83:GLU:CG	2.49	0.41
1:A:107:LEU:HD23	1:A:107:LEU:HA	1.79	0.41
4:F:67:ARG:HB2	4:F:73:PHE:CD1	2.55	0.41
1:C:64:ASN:OD1	2:D:-19:CYS:HB3	2.20	0.41
1:C:123:TRP:CD1	1:C:134:VAL:HG11	2.56	0.41
4:F:124:VAL:HG22	4:F:207:CYS:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:127:PRO:HD3	4:F:140:LEU:HA	2.02	0.41
2:D:52:THR:O	2:D:53:GLU:C	2.62	0.41
2:D:66:TYR:O	2:D:68:GLU:N	2.54	0.41
4:H:23:ASP:HA	4:H:71:LYS:O	2.21	0.41
1:A:16:GLN:HE21	1:A:21:ILE:HB	1.86	0.41
1:A:60:GLY:CA	2:B:-22:TYR:CE2	3.03	0.41
1:A:2:ILE:HD11	2:B:26:ARG:HD3	2.03	0.41
3:E:51:ARG:HD3	3:E:95:ARG:HH12	1.84	0.41
1:C:31:ASP:OD1	2:D:149:ARG:NH1	2.54	0.41
1:A:98:PRO:HD3	2:B:120:THR:HG21	2.02	0.41
1:A:164:ASP:HA	1:A:178:LYS:O	2.21	0.41
2:B:-17:GLY:HA3	4:F:95:LEU:O	2.20	0.41
2:B:97:PRO:HG3	2:B:122:PHE:HB3	2.02	0.41
2:B:97:PRO:HD3	2:B:179:SER:OG	2.21	0.41
2:B:163:MET:SD	2:B:165:PRO:HD3	2.61	0.41
1:C:158:SER:OG	1:C:159:ASP:N	2.51	0.41
2:D:131:TRP:CD1	2:D:161:LEU:HB2	2.56	0.41
1:C:57:GLU:HA	1:C:58:PRO:HD3	1.95	0.41
3:G:24:SER:HB3	3:G:72:ARG:HD3	2.01	0.41
1:A:77:LYS:O	1:A:78:ARG:C	2.64	0.40
2:B:79:ARG:O	2:B:80:HIS:C	2.65	0.40
4:F:34:TYR:CE1	4:F:44:LEU:HD22	2.57	0.40
4:F:156:TRP:CE3	4:F:191:LEU:HD22	2.56	0.40
1:C:48:PRO:O	1:C:51:GLY:N	2.51	0.40
1:C:99:VAL:HG13	1:C:157:PRO:HB3	2.01	0.40
1:C:47:LEU:HD12	1:C:50:PHE:CE2	2.56	0.40
2:B:123:TYR:CD2	2:B:124:PRO:HD3	2.57	0.40
1:C:74:ILE:CD1	1:C:74:ILE:H	2.33	0.40
1:A:166:LYS:HB2	1:A:177:LEU:HD23	2.04	0.40
3:E:37:LYS:HB2	3:E:47:ILE:HD13	2.04	0.40
4:F:157:TRP:NE1	4:F:208:GLN:OE1	2.55	0.40
2:D:171:TYR:O	2:D:187:GLU:HA	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	182/183 (100%)	141 (78%)	29 (16%)	12 (7%)	1	7
1	C	181/183 (99%)	144 (80%)	27 (15%)	10 (6%)	1	11
2	B	186/221 (84%)	144 (77%)	26 (14%)	16 (9%)	0	3
2	D	186/221 (84%)	143 (77%)	32 (17%)	11 (6%)	1	10
3	E	131/210 (62%)	104 (79%)	16 (12%)	11 (8%)	0	4
3	G	164/210 (78%)	126 (77%)	24 (15%)	14 (8%)	0	3
4	F	235/241 (98%)	205 (87%)	23 (10%)	7 (3%)	3	23
4	H	231/241 (96%)	198 (86%)	29 (13%)	4 (2%)	7	35
All	All	1496/1710 (88%)	1205 (80%)	206 (14%)	85 (6%)	1	11

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	ASP
1	A	78	ARG
2	B	67	LEU
2	B	95	GLU
2	B	97	PRO
2	B	98	ASN
2	B	178	PRO
3	E	34	PRO
3	E	102	TYR
3	E	104	LEU
3	E	105	THR
4	F	95	LEU
4	F	99	GLU
1	C	101	LEU
1	C	102	GLY
2	D	67	LEU
2	D	150	ASN
2	D	167	GLN
3	G	34	PRO
3	G	104	LEU
3	G	105	THR
4	H	99	GLU
1	A	73	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	77	LYS
2	B	34	ASN
2	B	121	ASP
2	B	153	TRP
3	E	79	ASP
4	F	216	GLU
1	C	59	GLN
1	C	77	LYS
1	C	78	ARG
1	C	157	PRO
2	D	34	ASN
2	D	121	ASP
2	D	153	TRP
3	G	102	TYR
3	G	147	GLN
3	G	165	VAL
1	A	70	HIS
1	A	146	SER
2	B	53	GLU
2	B	167	GLN
3	E	15	GLU
1	C	117	PRO
1	C	158	SER
3	G	6	GLN
3	G	15	GLU
3	G	79	ASP
3	G	99	GLY
4	H	51	ALA
4	H	216	GLU
1	A	49	GLU
1	A	158	SER
2	B	77	ALA
2	B	79	ARG
3	E	6	GLN
3	E	176	ASN
4	F	184	ARG
1	C	146	SER
3	G	161	THR
3	G	190	ALA
1	A	95	PRO
2	B	68	GLU
3	E	53	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	F	5	GLN
4	F	219	GLU
2	D	53	GLU
2	D	100	ALA
2	D	178	PRO
3	G	106	PHE
1	A	11	GLY
1	A	157	PRO
3	E	7	LEU
1	A	117	PRO
3	E	81	GLN
1	C	11	GLY
2	B	-17	GLY
2	B	183	PRO
4	F	120	PRO
3	G	7	LEU
4	H	97	GLY
2	B	87	VAL
2	D	87	VAL
2	D	124	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	166/165 (101%)	118 (71%)	48 (29%)	0	1
1	C	164/165 (99%)	117 (71%)	47 (29%)	0	1
2	B	174/191 (91%)	145 (83%)	29 (17%)	2	11
2	D	172/191 (90%)	143 (83%)	29 (17%)	2	11
3	E	118/189 (62%)	98 (83%)	20 (17%)	2	11
3	G	155/189 (82%)	121 (78%)	34 (22%)	1	5
4	F	185/205 (90%)	162 (88%)	23 (12%)	4	21
4	H	186/205 (91%)	160 (86%)	26 (14%)	3	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1320/1500 (88%)	1064 (81%)	256 (19%)	1 8

All (256) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	13	THR
1	A	14	VAL
1	A	16	GLN
1	A	20	ASP
1	A	33	LEU
1	A	40	LYS
1	A	41	LYS
1	A	44	VAL
1	A	52	GLN
1	A	53	LEU
1	A	55	LEU
1	A	59[A]	GLN
1	A	59[B]	GLN
1	A	74	ILE
1	A	76	THR
1	A	82	THR
1	A	85	THR
1	A	92	THR
1	A	96	LYS
1	A	97	SER
1	A	100	LEU
1	A	101	LEU
1	A	103	GLN
1	A	106	THR
1	A	108	ILE
1	A	111	VAL
1	A	114	ILE
1	A	118	VAL
1	A	122	THR
1	A	124	LEU
1	A	128	LYS
1	A	134	VAL
1	A	136	GLU
1	A	137	THR
1	A	140	LEU
1	A	141	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	143	ARG
1	A	146	SER
1	A	149	LYS
1	A	150	LEU
1	A	154	THR
1	A	159	ASP
1	A	162	ILE
1	A	166	LYS
1	A	173	GLU
1	A	176	VAL
1	A	178	LYS
2	B	-25	GLU
2	B	6	ARG
2	B	23	GLN
2	B	24	ARG
2	B	39	LEU
2	B	45	VAL
2	B	51	VAL
2	B	56	ARG
2	B	68	GLU
2	B	69	ARG
2	B	78	CYS
2	B	93	ARG
2	B	95	GLU
2	B	98	ASN
2	B	104	SER
2	B	112	HIS
2	B	120	THR
2	B	136	GLN
2	B	138	GLU
2	B	142	VAL
2	B	146	GLN
2	B	159	VAL
2	B	162	GLU
2	B	163	MET
2	B	164	THR
2	B	176	GLU
2	B	181	LYS
2	B	185	THR
2	B	189	ARG
3	E	7	LEU
3	E	10	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	12	ARG
3	E	17	SER
3	E	20	SER
3	E	23	CYS
3	E	27	ASP
3	E	31	ASN
3	E	47	ILE
3	E	63	ILE
3	E	68	LYS
3	E	74	SER
3	E	78	THR
3	E	79	ASP
3	E	84	ASP
3	E	95	ARG
3	E	104	LEU
3	E	136	LYS
3	E	144	PHE
3	E	181	TRP
4	F	6	SER
4	F	9	ASN
4	F	27	ASN
4	F	30	ASN
4	F	32	TYR
4	F	35	ARG
4	F	37	ASP
4	F	44	LEU
4	F	53	SER
4	F	54	THR
4	F	70	GLN
4	F	72	GLU
4	F	76	ILE
4	F	92	SER
4	F	95	LEU
4	F	100	GLN
4	F	109	THR
4	F	170	ASP
4	F	174	LEU
4	F	190	ARG
4	F	193	VAL
4	F	196	THR
4	F	233	SER
1	C	2	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	5	ASP
1	C	13	THR
1	C	16	GLN
1	C	20	ASP
1	C	33	LEU
1	C	37	ASP
1	C	39	ASP
1	C	40	LYS
1	C	41	LYS
1	C	44	VAL
1	C	52	GLN
1	C	53	LEU
1	C	55	LEU
1	C	59	GLN
1	C	65	ILE
1	C	68	GLU
1	C	74	ILE
1	C	80	ASN
1	C	82	THR
1	C	85	THR
1	C	90	GLN
1	C	96	LYS
1	C	97	SER
1	C	100	LEU
1	C	106	THR
1	C	108	ILE
1	C	110	PHE
1	C	111	VAL
1	C	114	ILE
1	C	118	VAL
1	C	119	ILE
1	C	122	THR
1	C	124	LEU
1	C	128	LYS
1	C	134	VAL
1	C	136	GLU
1	C	137	THR
1	C	141	VAL
1	C	143	ARG
1	C	146	SER
1	C	149	LYS
1	C	150	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	162	ILE
1	C	173	GLU
1	C	176	VAL
1	C	178	LYS
2	D	-27	LEU
2	D	-25	GLU
2	D	-20	VAL
2	D	6	ARG
2	D	24	ARG
2	D	29	THR
2	D	39	LEU
2	D	51	VAL
2	D	64	LYS
2	D	69	ARG
2	D	74	LEU
2	D	95	GLU
2	D	99	VAL
2	D	103	LEU
2	D	104	SER
2	D	105	ARG
2	D	119	VAL
2	D	120	THR
2	D	127	ILE
2	D	136	GLN
2	D	142	VAL
2	D	146	GLN
2	D	150	ASN
2	D	157	VAL
2	D	162	GLU
2	D	163	MET
2	D	164	THR
2	D	183	PRO
2	D	185	THR
3	G	2	GLU
3	G	7	LEU
3	G	9	SER
3	G	10	ILE
3	G	17	SER
3	G	20	SER
3	G	22	ASN
3	G	23	CYS
3	G	27	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	31	ASN
3	G	47	ILE
3	G	48	ILE
3	G	58	GLN
3	G	63	ILE
3	G	74	SER
3	G	77	ILE
3	G	78	THR
3	G	79	ASP
3	G	104	LEU
3	G	110	THR
3	G	111	LEU
3	G	112	LEU
3	G	113	THR
3	G	146	SER
3	G	147	GLN
3	G	150	VAL
3	G	151	SER
3	G	160	ILE
3	G	166	LEU
3	G	176	ASN
3	G	194	ASN
3	G	196	SER
3	G	197	ILE
3	G	201	ASP
4	H	6	SER
4	H	9	ASN
4	H	13	VAL
4	H	27	ASN
4	H	37	ASP
4	H	53	SER
4	H	54	THR
4	H	55	GLU
4	H	70	GLN
4	H	72	GLU
4	H	76	ILE
4	H	95	LEU
4	H	109	THR
4	H	151	HIS
4	H	159	ASN
4	H	161	LYS
4	H	168	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	H	169	THR
4	H	170	ASP
4	H	174	LEU
4	H	193	VAL
4	H	196	THR
4	H	197	PHE
4	H	209	VAL
4	H	228	VAL
4	H	232	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	70	HIS
1	A	103	GLN
1	A	145	HIS
1	A	179	HIS
2	B	23	GLN
2	B	80	HIS
2	B	112	HIS
2	B	136	GLN
2	B	156	GLN
2	B	167	GLN
2	B	174	HIS
3	E	3	GLN
3	E	31	ASN
3	E	81	GLN
3	E	101	ASN
4	F	27	ASN
4	F	29	ASN
4	F	100	GLN
4	F	159	ASN
4	F	200	ASN
4	F	203	ASN
1	C	26	HIS
1	C	59	GLN
1	C	63	GLN
1	C	90	GLN
1	C	145	HIS
1	C	148	HIS
1	C	179	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	98	ASN
2	D	134	ASN
2	D	136	GLN
2	D	156	GLN
2	D	174	HIS
3	G	101	ASN
3	G	120	ASN
3	G	147	GLN
3	G	176	ASN
4	H	27	ASN
4	H	29	ASN
4	H	100	GLN
4	H	116	ASN
4	H	134	HIS
4	H	151	HIS
4	H	159	ASN
4	H	200	ASN
4	H	203	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	182/183 (99%)	-0.42	0 100 100	42, 93, 126, 142	2 (1%)
1	C	182/183 (99%)	-0.38	0 100 100	44, 98, 130, 149	1 (0%)
2	B	192/221 (86%)	-0.33	2 (1%) 79 63	80, 114, 147, 174	0
2	D	192/221 (86%)	-0.31	1 (0%) 87 76	87, 125, 154, 168	0
3	E	139/210 (66%)	0.07	0 100 100	126, 154, 195, 206	0
3	G	177/210 (84%)	0.06	5 (2%) 55 35	112, 156, 178, 192	1 (0%)
4	F	237/241 (98%)	-0.06	3 (1%) 75 55	120, 167, 208, 227	1 (0%)
4	H	235/241 (97%)	-0.13	3 (1%) 75 55	113, 151, 181, 193	0
All	All	1536/1710 (89%)	-0.19	14 (0%) 81 64	42, 136, 186, 227	5 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	98	GLY	3.9
4	F	154	LEU	3.6
4	H	124	VAL	3.0
3	G	22	ASN	2.9
4	H	123	ALA	2.8
4	H	205	PHE	2.8
2	B	129	VAL	2.7
2	B	173	CYS	2.6
2	D	-15	GLY	2.6
3	G	106	PHE	2.4
4	F	142	CYS	2.3
3	G	125	VAL	2.3
4	F	66	SER	2.2
3	G	97	SER	2.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.