



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:49 PM UTC

PDB ID : 5U68 / pdb_00005u68
Title : Structural basis for antibody cross-neutralization of respiratory syncytial virus and human metapneumovirus
Authors : Wen, X.; Jardetzky, T.S.
Deposited on : 2016-12-07
Resolution : 3.08 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:

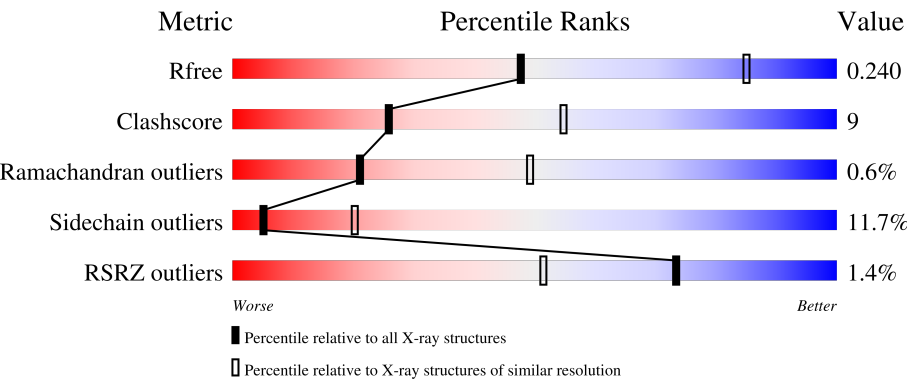
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.08 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	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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	562	% 51%23%6%20%
1	B	562	% 50%26%.20%
1	C	562	% 55%21%.20%
2	E	294	60%18%.21%
2	F	294	% 55%22%.21%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	294	% 66% 12% • 21%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 31169 atoms, of which 15527 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 Chimera protein of Fusion glycoprotein F0 and Envelope glycoprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	448	Total	C	H	N	O	S	0	0	0
			6971	2191	3503	573	681	23			
1	B	448	Total	C	H	N	O	S	0	0	0
			6966	2191	3498	573	681	23			
1	C	448	Total	C	H	N	O	S	0	0	0
			6972	2191	3504	573	681	23			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	PRO	conflict	UNP P03420
A	155	CYS	SER	conflict	UNP P03420
A	190	PHE	SER	conflict	UNP P03420
A	207	LEU	VAL	conflict	UNP P03420
A	290	CYS	SER	conflict	UNP P03420
A	379	VAL	ILE	conflict	UNP P03420
A	447	VAL	MET	conflict	UNP P03420
A	514	SER	-	linker	UNP P03420
A	515	ALA	-	linker	UNP P03420
A	516	ILE	-	linker	UNP P03420
A	517	GLY	-	linker	UNP P03420
A	546	GLY	-	expression tag	UNP M1E1E4
A	547	LEU	-	expression tag	UNP M1E1E4
A	548	VAL	-	expression tag	UNP M1E1E4
A	549	PRO	-	expression tag	UNP M1E1E4
A	550	ARG	-	expression tag	UNP M1E1E4
A	551	GLY	-	expression tag	UNP M1E1E4
A	552	SER	-	expression tag	UNP M1E1E4
A	553	SER	-	expression tag	UNP M1E1E4
A	554	ALA	-	expression tag	UNP M1E1E4
A	555	HIS	-	expression tag	UNP M1E1E4
A	556	HIS	-	expression tag	UNP M1E1E4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	557	HIS	-	expression tag	UNP M1E1E4
A	558	HIS	-	expression tag	UNP M1E1E4
A	559	HIS	-	expression tag	UNP M1E1E4
A	560	HIS	-	expression tag	UNP M1E1E4
A	561	HIS	-	expression tag	UNP M1E1E4
A	562	HIS	-	expression tag	UNP M1E1E4
B	102	ALA	PRO	conflict	UNP P03420
B	155	CYS	SER	conflict	UNP P03420
B	190	PHE	SER	conflict	UNP P03420
B	207	LEU	VAL	conflict	UNP P03420
B	290	CYS	SER	conflict	UNP P03420
B	379	VAL	ILE	conflict	UNP P03420
B	447	VAL	MET	conflict	UNP P03420
B	514	SER	-	linker	UNP P03420
B	515	ALA	-	linker	UNP P03420
B	516	ILE	-	linker	UNP P03420
B	517	GLY	-	linker	UNP P03420
B	546	GLY	-	expression tag	UNP M1E1E4
B	547	LEU	-	expression tag	UNP M1E1E4
B	548	VAL	-	expression tag	UNP M1E1E4
B	549	PRO	-	expression tag	UNP M1E1E4
B	550	ARG	-	expression tag	UNP M1E1E4
B	551	GLY	-	expression tag	UNP M1E1E4
B	552	SER	-	expression tag	UNP M1E1E4
B	553	SER	-	expression tag	UNP M1E1E4
B	554	ALA	-	expression tag	UNP M1E1E4
B	555	HIS	-	expression tag	UNP M1E1E4
B	556	HIS	-	expression tag	UNP M1E1E4
B	557	HIS	-	expression tag	UNP M1E1E4
B	558	HIS	-	expression tag	UNP M1E1E4
B	559	HIS	-	expression tag	UNP M1E1E4
B	560	HIS	-	expression tag	UNP M1E1E4
B	561	HIS	-	expression tag	UNP M1E1E4
B	562	HIS	-	expression tag	UNP M1E1E4
C	102	ALA	PRO	conflict	UNP P03420
C	155	CYS	SER	conflict	UNP P03420
C	190	PHE	SER	conflict	UNP P03420
C	207	LEU	VAL	conflict	UNP P03420
C	290	CYS	SER	conflict	UNP P03420
C	379	VAL	ILE	conflict	UNP P03420
C	447	VAL	MET	conflict	UNP P03420
C	514	SER	-	linker	UNP P03420

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	515	ALA	-	linker	UNP P03420
C	516	ILE	-	linker	UNP P03420
C	517	GLY	-	linker	UNP P03420
C	546	GLY	-	expression tag	UNP M1E1E4
C	547	LEU	-	expression tag	UNP M1E1E4
C	548	VAL	-	expression tag	UNP M1E1E4
C	549	PRO	-	expression tag	UNP M1E1E4
C	550	ARG	-	expression tag	UNP M1E1E4
C	551	GLY	-	expression tag	UNP M1E1E4
C	552	SER	-	expression tag	UNP M1E1E4
C	553	SER	-	expression tag	UNP M1E1E4
C	554	ALA	-	expression tag	UNP M1E1E4
C	555	HIS	-	expression tag	UNP M1E1E4
C	556	HIS	-	expression tag	UNP M1E1E4
C	557	HIS	-	expression tag	UNP M1E1E4
C	558	HIS	-	expression tag	UNP M1E1E4
C	559	HIS	-	expression tag	UNP M1E1E4
C	560	HIS	-	expression tag	UNP M1E1E4
C	561	HIS	-	expression tag	UNP M1E1E4
C	562	HIS	-	expression tag	UNP M1E1E4

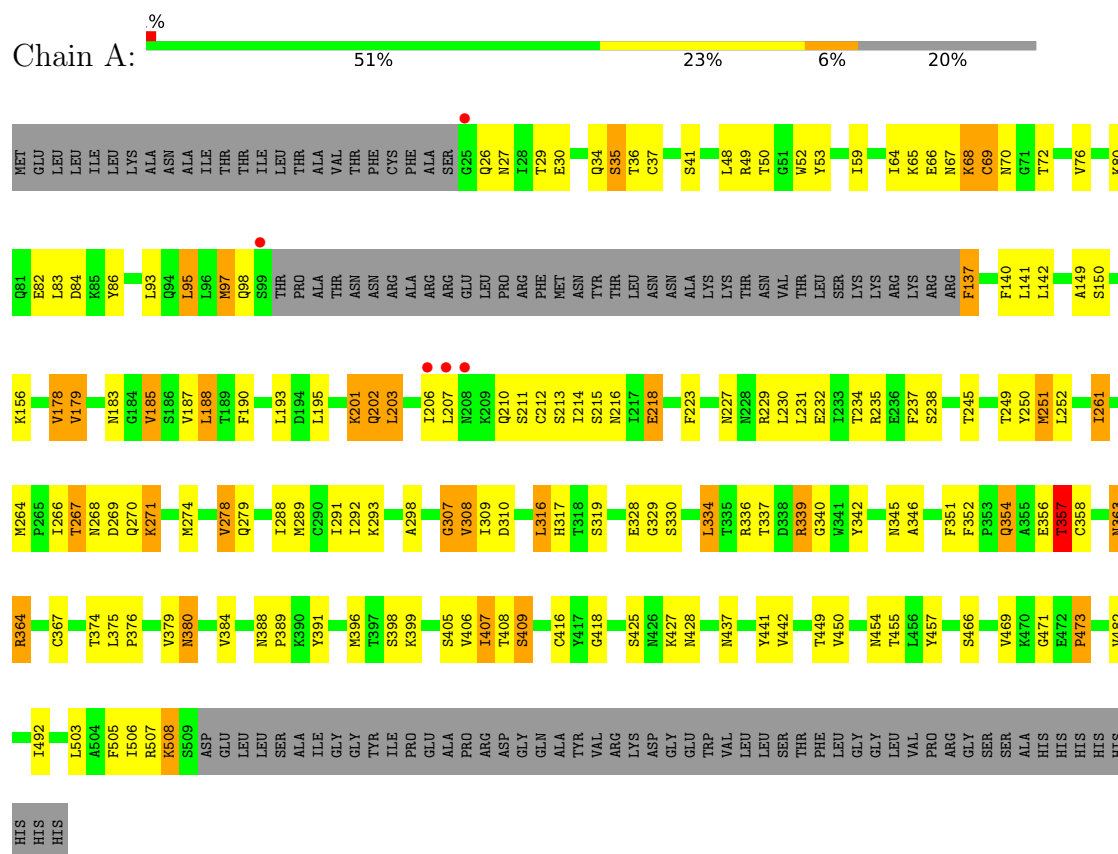
- Molecule 2 is a protein called MPE8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	233	Total	C	H	N	O	S	0	0	0
			3420	1090	1674	298	352	6			
2	F	233	Total	C	H	N	O	S	0	0	0
			3420	1090	1674	298	352	6			
2	G	233	Total	C	H	N	O	S	0	0	0
			3420	1090	1674	298	352	6			

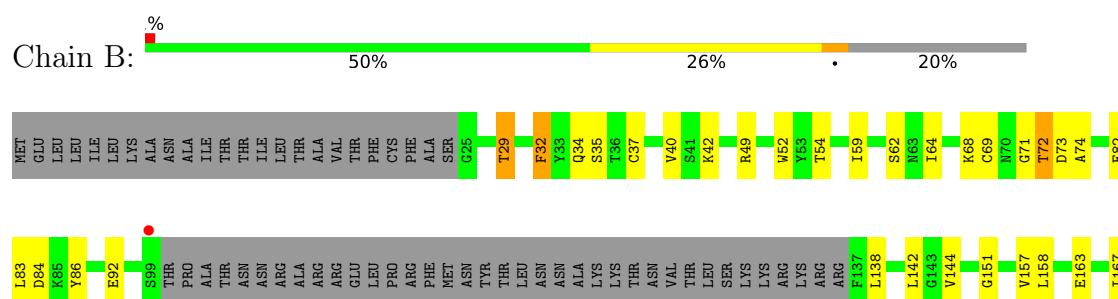
3 Residue-property plots [i](#)

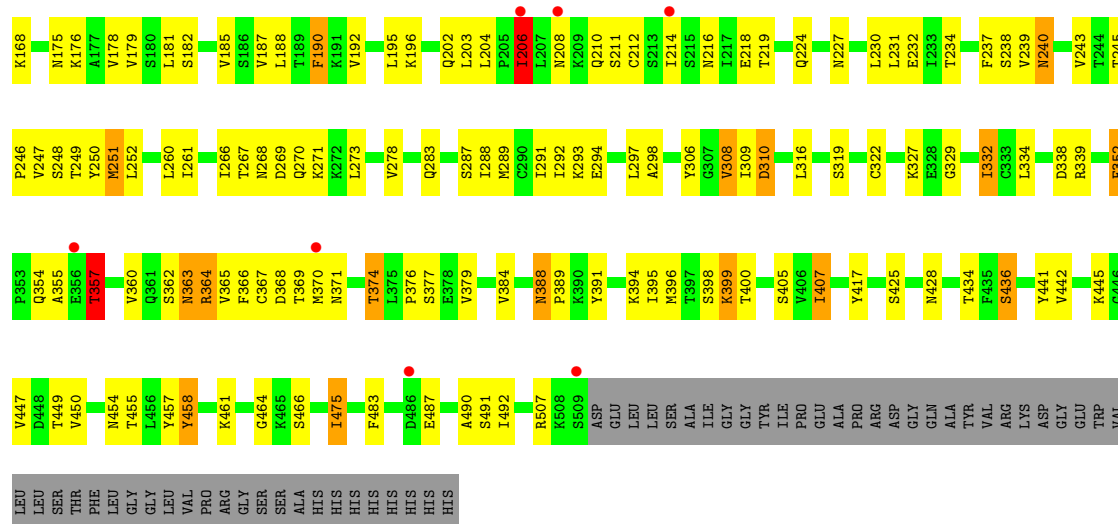
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Chimera protein of Fusion glycoprotein F0 and Envelope glycoprotein

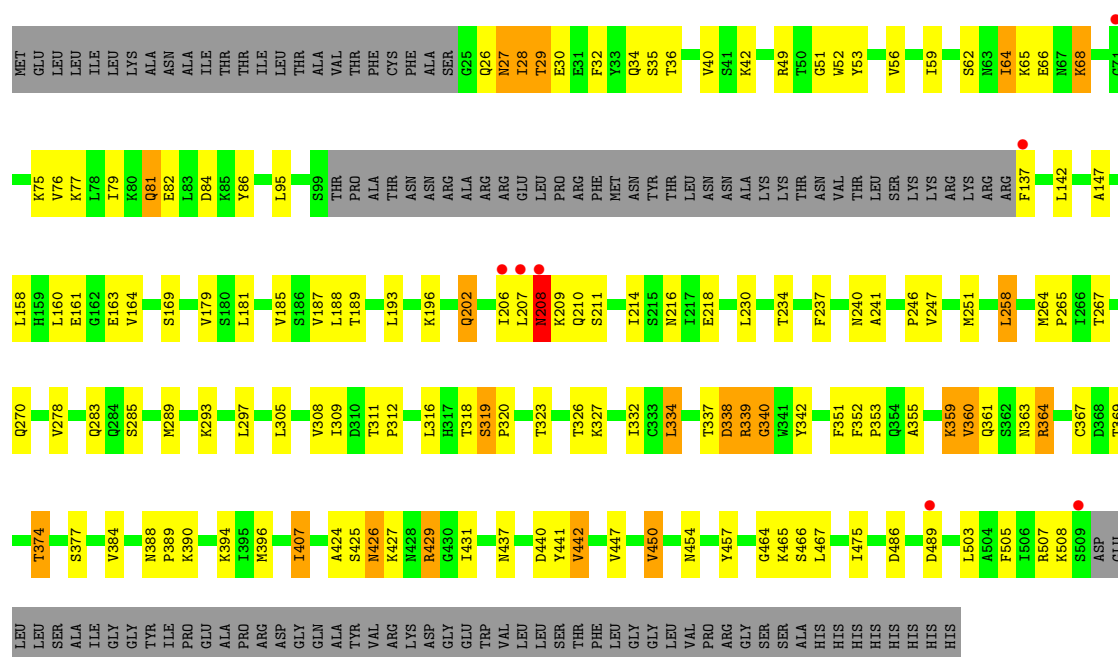


- Molecule 1: Chimera protein of Fusion glycoprotein F0 and Envelope glycoprotein

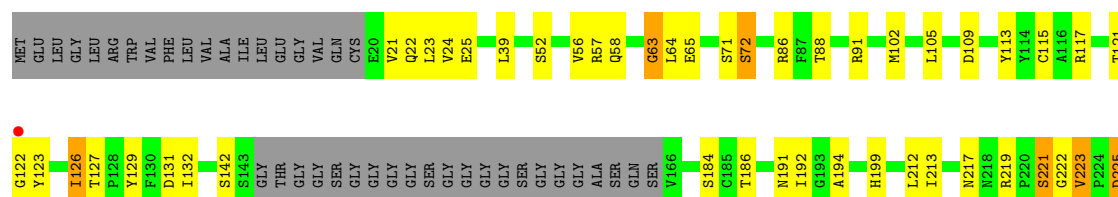


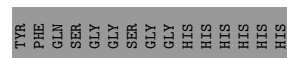


- Molecule 1: Chimera protein of Fusion glycoprotein F0 and Envelope glycoprotein



- Molecule 2: MPE8





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	155.54Å 155.54Å 275.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.19 – 3.08 48.19 – 3.08	Depositor EDS
% Data completeness (in resolution range)	74.6 (48.19-3.08) 74.6 (48.19-3.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.184 , 0.239 0.189 , 0.240	Depositor DCC
R_{free} test set	2687 reflections (3.44%)	wwPDB-VP
Wilson B-factor (Å ²)	67.5	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	31169	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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	1.21	4/3518 (0.1%)	1.28	19/4764 (0.4%)
1	B	1.30	13/3518 (0.4%)	1.29	17/4764 (0.4%)
1	C	1.06	5/3518 (0.1%)	1.20	18/4764 (0.4%)
2	E	0.98	0/1783	1.17	8/2423 (0.3%)
2	F	1.43	8/1783 (0.4%)	1.31	13/2423 (0.5%)
2	G	0.75	0/1783	0.99	3/2423 (0.1%)
All	All	1.16	30/15903 (0.2%)	1.23	78/21561 (0.4%)

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	1
1	B	0	2
1	C	0	1
All	All	0	4

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	239	ALA	CA-CB	-8.13	1.40	1.53
1	B	357	THR	CA-CB	7.93	1.66	1.53
2	F	121	THR	CA-C	7.54	1.62	1.53
1	A	407	ILE	CA-CB	-7.25	1.45	1.54
1	B	357	THR	CA-C	6.58	1.61	1.52
1	B	308	VAL	CA-CB	6.37	1.62	1.54
1	A	149	ALA	CA-CB	-6.34	1.43	1.53
1	B	32	PHE	CA-C	-6.34	1.45	1.52
2	F	67	VAL	CA-CB	-6.33	1.49	1.55
1	A	357	THR	CA-CB	6.28	1.64	1.53
1	C	431	ILE	CA-CB	-6.28	1.46	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	206	ILE	CA-CB	6.27	1.62	1.54
2	F	272	VAL	CA-CB	-6.26	1.47	1.54
1	B	243	VAL	C-O	-5.90	1.17	1.24
1	B	288	ILE	CA-CB	-5.88	1.47	1.53
1	C	424	ALA	CA-CB	-5.71	1.44	1.53
1	B	407	ILE	CA-CB	-5.64	1.47	1.54
1	B	208	ASN	CB-CG	5.59	1.66	1.52
2	F	59	ALA	CA-CB	-5.44	1.44	1.53
1	B	196	LYS	CA-C	-5.42	1.46	1.52
1	A	206	ILE	CA-CB	5.40	1.61	1.54
2	F	116	ALA	CA-CB	-5.28	1.44	1.53
1	C	147	ALA	CA-CB	-5.24	1.44	1.53
1	C	285	SER	CA-C	-5.16	1.46	1.52
1	B	208	ASN	CA-CB	5.13	1.62	1.53
1	B	376	PRO	CA-C	-5.09	1.46	1.52
1	B	37	CYS	CA-C	-5.02	1.46	1.53
2	F	77	ILE	CA-CB	-5.01	1.48	1.54
2	F	186	THR	CA-CB	-5.01	1.46	1.53
1	B	247	VAL	CA-C	-5.00	1.48	1.53

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	GLN	N-CA-C	11.85	125.09	108.74
2	E	194	ALA	N-CA-C	-9.13	102.15	113.20
1	C	340	GLY	N-CA-C	7.79	121.59	110.46
2	F	59	ALA	CA-C-N	-7.63	110.58	119.05
2	F	59	ALA	C-N-CA	-7.63	110.58	119.05
1	A	64	ILE	N-CA-C	7.59	121.47	110.09
1	A	508	LYS	N-CA-C	7.38	121.30	109.79
1	A	142	LEU	N-CA-C	7.10	120.06	111.82
1	C	240	ASN	N-CA-C	7.09	120.49	112.97
1	C	207	LEU	N-CA-C	-6.99	103.64	112.93
2	F	67	VAL	CB-CA-C	-6.77	105.95	111.71
1	A	473	PRO	CA-C-O	-6.77	113.62	121.34
2	G	122	GLY	N-CA-C	6.72	129.10	113.18
1	C	142	LEU	N-CA-C	6.71	119.94	111.69
1	B	138	LEU	N-CA-C	6.60	124.86	110.80
2	F	207	THR	N-CA-C	6.56	120.53	110.36
2	E	223	VAL	CA-C-N	6.22	126.14	119.85
2	E	223	VAL	C-N-CA	6.22	126.14	119.85
2	F	273	LEU	N-CA-C	6.22	119.73	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	352	PHE	CA-C-N	-6.22	112.07	119.84
1	B	352	PHE	C-N-CA	-6.22	112.07	119.84
1	B	64	ILE	N-CA-C	6.21	119.60	109.78
2	G	67	VAL	CB-CA-C	-6.11	106.52	111.71
1	C	258	LEU	N-CA-C	-6.10	104.19	111.69
1	A	376	PRO	CA-C-O	-6.04	114.55	121.56
1	A	72	THR	N-CA-C	6.03	118.21	109.71
1	A	384	VAL	N-CA-C	6.03	116.22	110.74
2	F	226	ARG	N-CA-C	5.90	117.39	111.07
2	E	63	GLY	N-CA-C	5.88	127.10	113.18
1	A	207	LEU	N-CA-C	-5.86	105.13	112.93
1	C	407	ILE	N-CA-C	5.83	116.59	108.89
2	F	221	SER	N-CA-C	5.83	118.11	111.11
1	B	362	SER	CB-CA-C	-5.83	109.30	117.23
1	C	359	LYS	N-CA-C	-5.72	99.86	109.07
1	C	208	ASN	N-CA-C	5.71	117.68	107.80
1	B	384	VAL	CB-CA-C	-5.61	104.63	111.87
1	A	492	ILE	CB-CA-C	-5.60	104.65	111.87
1	A	271	LYS	N-CA-C	-5.59	105.28	111.71
1	C	384	VAL	N-CA-C	5.59	116.25	110.82
1	A	288	ILE	N-CA-C	5.57	115.81	107.51
1	A	375	LEU	CA-C-N	5.57	125.52	119.78
1	A	375	LEU	C-N-CA	5.57	125.52	119.78
1	B	72	THR	N-CA-C	-5.57	107.07	112.97
1	B	271	LYS	N-CA-C	-5.55	105.33	111.71
1	B	360	VAL	N-CA-C	5.50	117.25	108.89
1	B	37	CYS	N-CA-C	-5.49	103.81	111.39
2	G	217	ASN	N-CA-C	5.49	116.89	110.41
1	C	247	VAL	CB-CA-C	-5.45	105.34	111.23
2	E	249	ALA	N-CA-C	5.43	116.40	108.14
1	A	384	VAL	CB-CA-C	-5.43	104.78	111.94
1	A	203	LEU	N-CA-C	-5.42	107.67	114.56
2	F	28	GLY	N-CA-C	-5.42	105.61	112.54
1	C	64	ILE	CB-CA-C	-5.38	104.29	111.13
2	F	24	VAL	N-CA-C	5.35	116.43	107.18
1	C	64	ILE	N-CA-C	5.34	118.10	110.09
1	B	142	LEU	N-CA-C	5.32	118.93	112.23
1	B	211	SER	N-CA-C	5.27	117.08	110.91
2	E	72	SER	N-CA-C	5.27	117.10	111.36
1	B	248	SER	N-CA-C	5.25	116.87	110.41
1	B	507	ARG	N-CA-C	-5.24	98.86	108.02
1	C	390	LYS	N-CA-C	5.24	117.41	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	163	GLU	N-CA-C	-5.23	105.70	111.71
2	E	21	VAL	N-CA-C	5.22	116.27	108.54
1	B	436	SER	N-CA-C	-5.21	102.35	110.42
2	F	204	LEU	CA-C-N	5.18	124.63	119.24
2	F	204	LEU	C-N-CA	5.18	124.63	119.24
2	F	134	GLY	N-CA-C	-5.17	104.28	112.66
1	C	27	ASN	N-CA-C	5.17	118.87	111.02
1	B	458	TYR	N-CA-C	-5.16	101.55	109.76
1	C	81	GLN	N-CA-C	-5.16	105.73	111.36
1	A	329	GLY	N-CA-C	-5.16	105.12	112.55
1	B	206	ILE	N-CA-C	-5.15	107.28	112.17
1	A	469	VAL	N-CA-C	5.14	114.70	106.88
1	A	307	GLY	N-CA-C	5.11	121.00	114.66
1	C	464	GLY	N-CA-C	5.11	117.96	111.37
1	C	450	VAL	N-CA-C	-5.09	100.73	108.17
2	E	105	LEU	N-CA-C	5.09	117.09	110.43
2	F	229	ALA	N-CA-C	5.00	116.42	108.96

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	67	ASN	Peptide
1	B	355	ALA	Peptide
1	B	72	THR	Peptide
1	C	26	GLN	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	3468	3503	3510	94	0
1	B	3468	3498	3510	77	0
1	C	3468	3504	3510	58	0
2	E	1746	1674	1676	32	0
2	F	1746	1674	1676	36	0
2	G	1746	1674	1676	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15642	15527	15558	296	0

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

All (296) 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:B:374:THR:HG21	1:C:454:ASN:H	1.53	0.73
1:A:266:ILE:HA	2:E:126:ILE:HG23	1.72	0.71
2:E:226:ARG:NH1	2:E:247:ASP:OD2	2.23	0.71
2:F:56:VAL:HG12	2:F:66:TRP:HA	1.71	0.71
1:A:407:ILE:HD11	1:A:457:TYR:HB3	1.74	0.68
2:E:129:TYR:HB3	2:E:199:HIS:CD2	2.29	0.68
1:A:418:GLY:N	1:A:437:ASN:OD1	2.29	0.65
1:C:340:GLY:HA2	1:C:355:ALA:HB2	1.79	0.65
1:A:374:THR:HG21	1:B:454:ASN:H	1.62	0.65
1:A:69:CYS:CB	1:A:212:CYS:HA	2.27	0.64
1:B:428:ASN:O	2:E:217:ASN:ND2	2.31	0.64
2:F:59:ALA:HB3	2:F:62:LYS:HB2	1.80	0.64
1:A:227:ASN:ND2	1:A:231:LEU:HD11	2.13	0.64
1:B:407:ILE:HD11	1:B:457:TYR:HB3	1.79	0.63
1:A:41:SER:OG	1:A:409:SER:OG	2.15	0.62
1:C:28:ILE:C	1:C:28:ILE:HD12	2.25	0.61
1:A:95:LEU:HD23	1:A:95:LEU:O	2.01	0.61
1:A:270:GLN:NE2	2:E:126:ILE:HD11	2.15	0.61
1:C:28:ILE:HD12	1:C:29:THR:N	2.16	0.61
1:B:332:ILE:HG23	1:B:475:ILE:HD11	1.83	0.61
1:A:363:ASN:OD1	1:A:363:ASN:N	2.33	0.60
1:C:267:THR:OG1	1:C:270:GLN:OE1	2.17	0.60
1:A:59:ILE:HG23	1:A:193:LEU:HB3	1.84	0.60
1:C:68:LYS:NZ	1:C:211:SER:O	2.33	0.59
1:A:428:ASN:O	2:G:217:ASN:ND2	2.36	0.59
1:B:309:ILE:HG22	1:B:310:ASP:HB2	1.83	0.59
1:B:270:GLN:NE2	2:F:126:ILE:HD11	2.18	0.59
2:F:23:LEU:HD22	2:F:132:ILE:HG22	1.85	0.58
1:A:310:ASP:OD1	1:A:364:ARG:NH2	2.35	0.58
1:C:246:PRO:HB3	1:C:283:GLN:HA	1.84	0.58
2:F:129:TYR:HB3	2:F:199:HIS:CD2	2.39	0.58
2:F:255:SER:OG	2:F:256:TYR:N	2.35	0.58
2:E:25:GLU:OE2	2:E:115:CYS:N	2.34	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:225:ASP:OD2	2:E:225:ASP:N	2.34	0.58
1:B:388:ASN:ND2	1:B:388:ASN:O	2.37	0.57
1:A:83:LEU:HD23	1:A:223:PHE:CE2	2.39	0.57
1:B:54:THR:HG21	1:B:151:GLY:HA2	1.87	0.57
1:A:30:GLU:OE2	1:A:441:TYR:OH	2.14	0.57
1:B:270:GLN:NE2	1:B:306:TYR:O	2.36	0.57
1:B:227:ASN:ND2	1:B:231:LEU:HD11	2.20	0.57
1:B:442:VAL:CG1	1:B:447:VAL:HG21	2.35	0.57
1:A:93:LEU:HD11	1:A:234:THR:HG22	1.87	0.57
1:A:345:ASN:HD21	1:B:454:ASN:HB3	1.70	0.57
1:B:266:ILE:HA	2:F:126:ILE:HG23	1.87	0.56
1:A:405:SER:OG	1:A:406:VAL:N	2.37	0.56
1:A:405:SER:HB3	1:A:457:TYR:CE2	2.40	0.56
1:B:379:VAL:HG23	1:B:391:TYR:CE1	2.41	0.56
2:E:226:ARG:HH12	2:E:247:ASP:CG	2.14	0.56
1:C:289:MET:HE1	1:C:297:LEU:HD11	1.85	0.56
1:C:364:ARG:CG	1:C:364:ARG:HH11	2.19	0.56
1:C:53:TYR:HB2	1:C:305:LEU:HD21	1.87	0.55
2:F:55:TRP:NE1	2:F:100:LEU:HB2	2.20	0.55
1:B:405:SER:HB3	1:B:457:TYR:CE2	2.42	0.55
1:A:398:SER:OG	1:A:399:LYS:N	2.39	0.55
2:F:126:ILE:O	2:F:126:ILE:HG12	2.05	0.55
1:A:356:GLU:N	1:A:356:GLU:OE2	2.40	0.55
1:B:364:ARG:HH11	1:B:364:ARG:CG	2.20	0.55
1:C:318:THR:O	1:C:339:ARG:NH1	2.40	0.55
1:A:68:LYS:O	1:A:70:ASN:N	2.41	0.54
1:C:59:ILE:HG23	1:C:193:LEU:HB3	1.89	0.54
1:B:230:LEU:O	1:B:234:THR:HG23	2.08	0.54
2:F:59:ALA:HB1	2:F:60:PRO:CD	2.38	0.54
1:B:62:SER:O	1:B:86:TYR:OH	2.21	0.54
2:G:57:ARG:NH2	2:G:65:GLU:OE2	2.33	0.53
1:A:507:ARG:NH1	1:A:507:ARG:HB2	2.23	0.53
1:C:237:PHE:CE2	1:C:289:MET:HE2	2.44	0.53
2:E:129:TYR:HB3	2:E:199:HIS:NE2	2.23	0.53
1:B:487:GLU:HG2	1:B:490:ALA:HB3	1.90	0.53
1:B:445:LYS:NZ	1:B:464:GLY:O	2.33	0.52
1:B:352:PHE:CE2	1:B:367:CYS:HB3	2.44	0.52
1:B:239:VAL:HG13	1:C:246:PRO:HG2	1.91	0.52
1:A:229:ARG:NE	1:A:250:TYR:O	2.38	0.52
2:G:129:TYR:HB3	2:G:199:HIS:CD2	2.44	0.52
2:G:112:VAL:HG22	2:G:138:LEU:HG	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:THR:HG21	1:B:371:ASN:HB3	1.90	0.52
1:B:29:THR:HG23	1:B:42:LYS:HG3	1.92	0.52
2:F:127:THR:HG21	2:F:197:ASP:H	1.73	0.52
1:B:447:VAL:O	1:B:461:LYS:NZ	2.35	0.52
2:E:191:ASN:OD1	2:E:192:ILE:N	2.40	0.52
1:A:380:ASN:ND2	1:A:380:ASN:O	2.39	0.51
1:A:354:GLN:O	1:A:357:THR:HG23	2.10	0.51
1:B:442:VAL:HG13	1:B:447:VAL:HG21	1.93	0.51
1:B:289:MET:HE1	1:B:297:LEU:HD11	1.93	0.51
1:C:334:LEU:HB3	1:C:475:ILE:HD13	1.93	0.51
1:B:388:ASN:ND2	1:B:388:ASN:C	2.68	0.51
2:G:256:TYR:HA	2:G:262:GLY:HA2	1.93	0.51
1:C:352:PHE:CE2	1:C:367:CYS:HB3	2.45	0.51
1:B:363:ASN:N	1:B:363:ASN:OD1	2.43	0.51
1:A:507:ARG:HB2	1:A:507:ARG:CZ	2.42	0.50
2:E:24:VAL:HG23	2:E:24:VAL:O	2.10	0.50
1:B:291:ILE:HG12	1:B:292:ILE:N	2.27	0.50
2:F:216:ASN:O	2:F:229:ALA:HB3	2.12	0.50
1:B:332:ILE:CG1	1:B:483:PHE:CD2	2.94	0.50
1:A:454:ASN:H	1:C:374:THR:HG21	1.75	0.50
1:C:86:TYR:CD1	1:C:86:TYR:C	2.90	0.50
1:C:429:ARG:HH11	1:C:429:ARG:HB2	1.76	0.50
1:A:86:TYR:CD1	1:A:86:TYR:C	2.89	0.50
1:A:379:VAL:HG23	1:A:391:TYR:CE1	2.46	0.50
1:C:62:SER:O	1:C:86:TYR:OH	2.25	0.49
1:A:82:GLU:HB3	1:A:223:PHE:CE2	2.47	0.49
1:A:237:PHE:CZ	1:A:251:MET:HE1	2.46	0.49
1:B:163:GLU:OE2	1:B:182:SER:N	2.45	0.49
2:F:214:TYR:CE1	2:F:218:ASN:HB3	2.47	0.49
1:C:426:ASN:C	1:C:426:ASN:OD1	2.55	0.49
1:A:505:PHE:O	1:A:505:PHE:CD1	2.66	0.49
1:C:339:ARG:HH11	1:C:339:ARG:HG2	1.78	0.48
1:C:265:PRO:HA	2:G:196:TYR:CZ	2.48	0.48
2:F:199:HIS:CE1	2:F:215:ASP:H	2.31	0.48
1:B:379:VAL:HG23	1:B:391:TYR:CZ	2.48	0.48
1:B:398:SER:OG	1:B:399:LYS:N	2.47	0.48
1:C:29:THR:OG1	1:C:30:GLU:N	2.44	0.48
2:F:110:THR:O	2:F:111:ALA:HB2	2.13	0.48
1:A:345:ASN:OD1	1:A:346:ALA:N	2.47	0.48
2:G:127:THR:HG21	2:G:197:ASP:H	1.78	0.48
1:A:342:TYR:CZ	1:A:351:PHE:CD1	3.02	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:PRO:HB3	1:B:283:GLN:HA	1.96	0.47
1:B:395:ILE:HD13	1:B:492:ILE:HD13	1.96	0.47
2:G:53:MET:HB3	2:G:98:LEU:HD22	1.95	0.47
2:G:70:ILE:CD1	2:G:77:ILE:HD11	2.44	0.47
2:E:212:LEU:HD12	2:E:223:VAL:HG11	1.96	0.47
1:A:356:GLU:N	1:A:356:GLU:CD	2.71	0.47
2:F:127:THR:HG21	2:F:197:ASP:N	2.29	0.47
1:A:183:ASN:OD1	1:A:185:VAL:HG12	2.14	0.47
1:A:291:ILE:HG12	1:A:292:ILE:N	2.29	0.47
2:E:221:SER:OG	2:E:222:GLY:N	2.47	0.47
1:B:270:GLN:HG3	1:B:309:ILE:HD11	1.96	0.47
1:B:322:CYS:N	1:B:417:TYR:OH	2.44	0.47
2:E:217:ASN:HB3	2:E:229:ALA:O	2.15	0.47
2:G:183:ILE:HG12	2:G:268:THR:HG21	1.96	0.47
2:G:194:ALA:HB1	2:G:258:ARG:NH2	2.30	0.47
1:C:76:VAL:CG2	1:C:214:ILE:H	2.28	0.47
1:C:364:ARG:HH11	1:C:364:ARG:HG3	1.78	0.47
2:E:123:TYR:CD2	2:E:123:TYR:C	2.93	0.47
1:A:230:LEU:O	1:A:234:THR:HG23	2.15	0.47
1:C:237:PHE:CE2	1:C:289:MET:CE	2.97	0.47
2:E:71:SER:O	2:E:91:ARG:NH1	2.45	0.47
1:A:41:SER:CB	1:A:409:SER:OG	2.63	0.46
1:B:32:PHE:CD1	1:B:441:TYR:HB2	2.50	0.46
1:A:352:PHE:CE2	1:A:367:CYS:HB3	2.50	0.46
2:F:31:VAL:CG2	2:F:37:LEU:HD22	2.46	0.46
2:F:59:ALA:HB1	2:F:60:PRO:HD2	1.97	0.46
1:A:266:ILE:HG22	2:E:126:ILE:CG2	2.45	0.46
1:C:407:ILE:HD11	1:C:457:TYR:HB3	1.96	0.46
1:B:49:ARG:O	1:B:369:THR:HG23	2.15	0.46
1:B:240:ASN:OD1	1:B:240:ASN:N	2.48	0.46
1:A:264:MET:HB3	1:A:266:ILE:HG23	1.97	0.46
2:E:57:ARG:NH2	2:E:65:GLU:OE1	2.44	0.46
1:A:379:VAL:HA	1:A:391:TYR:CD1	2.50	0.46
1:C:230:LEU:O	1:C:234:THR:HG23	2.16	0.46
1:A:261:ILE:HG12	1:A:274:MET:HE2	1.98	0.46
1:B:266:ILE:HG22	2:F:126:ILE:CG2	2.46	0.46
2:F:31:VAL:HG12	2:F:32:LYS:N	2.30	0.45
1:A:35:SER:HA	1:A:473:PRO:HA	1.98	0.45
1:C:342:TYR:CZ	1:C:351:PHE:CD1	3.04	0.45
1:C:440:ASP:OD1	1:C:441:TYR:N	2.42	0.45
1:A:137:PHE:HD2	1:A:337:THR:HG22	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:257:ASP:OD1	2:G:258:ARG:N	2.49	0.45
1:C:79:ILE:O	1:C:82:GLU:N	2.49	0.45
2:F:142:SER:OG	2:F:143:SER:N	2.49	0.45
2:F:254:GLN:HG2	2:F:255:SER:N	2.32	0.45
1:A:316:LEU:HD11	1:A:336:ARG:NH2	2.31	0.45
1:B:268:ASN:O	1:B:269:ASP:C	2.60	0.45
1:C:56:VAL:HB	1:C:189:THR:HG22	1.98	0.45
2:G:25:GLU:OE1	2:G:25:GLU:N	2.42	0.45
2:G:71:SER:HB3	2:G:76:TYR:HB2	1.98	0.45
1:A:137:PHE:N	1:A:137:PHE:CD1	2.85	0.45
1:B:232:GLU:HB3	1:B:250:TYR:CD2	2.52	0.45
2:E:254:GLN:HG2	2:E:255:SER:N	2.32	0.45
1:A:308:VAL:HG11	1:A:345:ASN:HB2	1.99	0.45
1:C:360:VAL:HG23	1:C:361:GLN:N	2.31	0.45
2:F:83:VAL:HG11	2:F:87:PHE:CD2	2.52	0.45
1:B:332:ILE:HG23	1:B:475:ILE:CG1	2.46	0.45
1:A:337:THR:C	1:A:339:ARG:H	2.25	0.45
2:F:203:GLN:O	2:F:249:ALA:HB1	2.18	0.44
2:E:255:SER:OG	2:E:256:TYR:N	2.49	0.44
2:G:126:ILE:HD13	2:G:126:ILE:O	2.18	0.44
1:A:317:HIS:CG	1:A:408:THR:HG22	2.52	0.44
1:C:311:THR:HB	1:C:312:PRO:HD2	1.99	0.44
2:G:58:GLN:O	2:G:111:ALA:HB1	2.17	0.44
1:A:49:ARG:HD2	1:A:52:TRP:CH2	2.53	0.44
1:C:51:GLY:C	1:C:305:LEU:HD12	2.43	0.44
2:F:273:LEU:N	2:F:273:LEU:HD23	2.33	0.44
1:B:49:ARG:HD2	1:B:52:TRP:CH2	2.52	0.44
1:C:53:TYR:HB3	1:C:264:MET:HE3	1.99	0.44
1:C:338:ASP:HB2	1:C:342:TYR:OH	2.18	0.44
1:A:50:THR:HG23	1:A:307:GLY:H	1.82	0.44
1:A:235:ARG:NH1	1:B:250:TYR:CE1	2.86	0.44
1:A:267:THR:HG23	1:A:269:ASP:H	1.83	0.44
1:A:291:ILE:HG22	1:A:298:ALA:HB3	1.99	0.44
1:A:68:LYS:O	1:A:69:CYS:C	2.60	0.44
1:A:266:ILE:HD11	1:A:271:LYS:HG2	2.00	0.44
1:A:482:VAL:O	1:A:482:VAL:HG23	2.16	0.44
1:A:505:PHE:HE2	1:C:505:PHE:CE2	2.35	0.44
1:C:369:THR:O	1:C:369:THR:HG22	2.16	0.44
2:E:86:ARG:NH1	2:E:109:ASP:OD2	2.51	0.44
1:A:150:SER:HB3	1:B:458:TYR:CD2	2.52	0.44
1:B:370:MET:CG	1:C:457:TYR:CE1	3.01	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:LYS:HA	1:B:491:SER:HA	2.00	0.44
1:A:201:LYS:O	1:A:202:GLN:CB	2.65	0.43
1:A:330:SER:O	1:A:330:SER:OG	2.24	0.43
1:A:267:THR:HG23	1:A:268:ASN:N	2.32	0.43
2:F:56:VAL:HG21	2:F:133:TRP:CZ3	2.54	0.43
1:A:183:ASN:OD1	1:A:185:VAL:CG1	2.67	0.43
1:A:278:VAL:HG11	1:C:95:LEU:HD21	1.99	0.43
1:B:293:LYS:O	1:B:294:GLU:C	2.62	0.43
1:C:208:ASN:HA	1:C:209:LYS:CG	2.49	0.43
1:C:270:GLN:HG3	1:C:309:ILE:HD11	2.01	0.43
2:G:56:VAL:HG21	2:G:264:PHE:CE2	2.53	0.43
1:A:345:ASN:OD1	1:A:345:ASN:C	2.62	0.43
1:B:398:SER:HG	1:B:400:THR:H	1.65	0.43
2:E:123:TYR:CD2	2:E:123:TYR:O	2.71	0.43
2:F:71:SER:HB3	2:F:76:TYR:HB2	2.01	0.43
2:F:72:SER:HA	2:F:91:ARG:NH1	2.34	0.43
1:A:232:GLU:HB3	1:A:250:TYR:CD2	2.54	0.43
1:B:73:ASP:CG	1:B:74:ALA:N	2.77	0.43
2:E:117:ARG:NH2	2:E:131:ASP:OD2	2.41	0.43
1:B:273:LEU:HD11	1:B:366:PHE:CZ	2.53	0.43
1:C:49:ARG:HD2	1:C:52:TRP:CH2	2.54	0.43
1:C:323:THR:HG23	1:C:332:ILE:HG13	2.01	0.43
1:B:86:TYR:CD1	1:B:86:TYR:C	2.96	0.42
1:C:77:LYS:O	1:C:81:GLN:HB2	2.19	0.42
2:E:72:SER:HA	2:E:91:ARG:NH1	2.34	0.42
2:E:213:ILE:CD1	2:E:219:ARG:HG2	2.49	0.42
1:A:279:GLN:HG3	1:C:241:ALA:HA	2.00	0.42
1:C:394:LYS:NZ	1:C:489:ASP:O	2.41	0.42
1:A:291:ILE:HD11	1:A:293:LYS:CD	2.49	0.42
1:B:92:GLU:OE2	1:B:238:SER:CB	2.67	0.42
1:B:190:PHE:CD2	1:B:260:LEU:HD13	2.54	0.42
2:F:129:TYR:HB3	2:F:199:HIS:NE2	2.34	0.42
2:F:174:SER:HB2	2:F:273:LEU:HD21	2.01	0.42
2:G:70:ILE:HG13	2:G:77:ILE:CG1	2.49	0.42
1:A:53:TYR:OH	1:A:188:LEU:HB2	2.19	0.42
1:B:32:PHE:CE1	1:B:441:TYR:HB2	2.54	0.42
2:F:58:GLN:O	2:F:111:ALA:HB1	2.20	0.42
2:G:56:VAL:HG23	2:G:66:TRP:HA	2.01	0.42
1:B:59:ILE:HB	1:B:297:LEU:HB3	2.02	0.42
1:A:270:GLN:O	1:A:271:LYS:C	2.60	0.42
1:B:49:ARG:HE	1:B:368:ASP:CG	2.28	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ILE:HG23	1:B:475:ILE:CD1	2.48	0.42
2:E:121:THR:O	2:E:121:THR:OG1	2.38	0.42
2:E:58:GLN:HB2	2:E:64:LEU:HD12	2.01	0.42
2:E:256:TYR:HA	2:E:262:GLY:HA2	2.02	0.42
1:A:69:CYS:HB2	1:A:212:CYS:HA	1.98	0.42
1:A:334:LEU:HD23	1:A:334:LEU:C	2.45	0.42
1:A:388:ASN:HB2	1:A:389:PRO:HD2	2.02	0.42
1:C:351:PHE:CE2	1:C:353:PRO:HB3	2.54	0.42
1:A:342:TYR:CE2	1:A:351:PHE:CD1	3.08	0.41
1:A:416:CYS:O	1:A:437:ASN:HA	2.20	0.41
1:B:32:PHE:CE2	1:B:34:GLN:HA	2.55	0.41
1:C:388:ASN:HB2	1:C:389:PRO:HD2	2.02	0.41
1:C:441:TYR:CD1	1:C:442:VAL:N	2.87	0.41
2:F:215:ASP:O	2:F:217:ASN:N	2.49	0.41
1:A:34:GLN:HE21	1:A:471:GLY:H	1.68	0.41
1:A:245:THR:O	1:A:245:THR:HG23	2.20	0.41
1:B:365:VAL:HG12	1:B:367:CYS:SG	2.60	0.41
1:C:32:PHE:CE2	1:C:34:GLN:HA	2.55	0.41
2:E:225:ASP:O	2:E:226:ARG:C	2.63	0.41
1:A:86:TYR:CE2	1:A:195:LEU:HD13	2.55	0.41
1:B:69:CYS:HB3	1:B:212:CYS:HA	2.02	0.41
2:F:129:TYR:C	2:F:129:TYR:CD2	2.99	0.41
1:A:214:ILE:CG2	1:A:215:SER:N	2.84	0.41
1:B:327:LYS:HG2	1:B:329:GLY:N	2.36	0.41
1:B:364:ARG:HH11	1:B:364:ARG:HG3	1.84	0.41
1:C:339:ARG:NH1	1:C:339:ARG:HG2	2.35	0.41
2:F:70:ILE:O	2:F:70:ILE:HG23	2.20	0.41
1:B:237:PHE:CZ	1:B:251:MET:HE1	2.56	0.41
1:B:292:ILE:HG23	1:B:292:ILE:O	2.20	0.41
1:A:216:ASN:HB3	1:A:218:GLU:HG2	2.02	0.41
1:A:356:GLU:C	1:A:358:CYS:N	2.77	0.41
1:A:36:THR:O	1:A:37:CYS:C	2.64	0.41
1:A:268:ASN:O	1:A:269:ASP:C	2.63	0.41
1:A:339:ARG:HG3	1:A:340:GLY:N	2.35	0.41
1:B:167:ILE:O	1:B:168:LYS:C	2.62	0.41
1:B:251:MET:HE2	1:B:287:SER:OG	2.20	0.41
1:C:164:VAL:HG21	1:C:293:LYS:HE2	2.03	0.41
2:E:102:MET:HE2	2:E:113:TYR:CE2	2.56	0.41
2:F:114:TYR:CE1	2:F:208:ALA:HB2	2.56	0.41
2:F:219:ARG:HD3	2:F:227:PHE:O	2.21	0.41
1:A:76:VAL:HG21	1:A:213:SER:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:LEU:C	1:B:204:LEU:HD23	2.46	0.41
1:C:319:SER:OG	1:C:320:PRO:HD2	2.21	0.41
1:A:237:PHE:CE2	1:A:289:MET:HE2	2.56	0.40
1:B:291:ILE:HG22	1:B:298:ALA:HB3	2.03	0.40
1:A:178:VAL:HG23	1:A:179:VAL:N	2.35	0.40
1:A:364:ARG:HH11	1:A:364:ARG:CG	2.34	0.40
2:E:22:GLN:O	2:E:23:LEU:HD12	2.21	0.40
1:A:48:LEU:HG	1:A:308:VAL:HG22	2.03	0.40
1:B:82:GLU:HG3	1:B:224:GLN:HB3	2.03	0.40
1:B:206:ILE:HG23	1:B:206:ILE:O	2.21	0.40
1:B:354:GLN:O	1:B:357:THR:HG22	2.21	0.40
1:C:62:SER:HB2	1:C:196:LYS:HA	2.04	0.40
1:A:97:MET:SD	1:A:97:MET:N	2.95	0.40
1:A:140:PHE:CE1	1:A:141:LEU:CD1	3.05	0.40
1:B:251:MET:HE3	1:B:251:MET:HA	2.02	0.40
2:E:229:ALA:HA	2:E:237:SER:O	2.21	0.40
1:C:137:PHE:CD2	1:C:337:THR:HG22	2.57	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	444/562 (79%)	404 (91%)	35 (8%)	5 (1%)	11	36
1	B	444/562 (79%)	396 (89%)	45 (10%)	3 (1%)	18	46
1	C	444/562 (79%)	404 (91%)	39 (9%)	1 (0%)	43	71
2	E	229/294 (78%)	211 (92%)	16 (7%)	2 (1%)	14	41
2	F	229/294 (78%)	209 (91%)	20 (9%)	0	100	100
2	G	229/294 (78%)	212 (93%)	16 (7%)	1 (0%)	30	58
All	All	2019/2568 (79%)	1836 (91%)	171 (8%)	12 (1%)	21	49

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	69	CYS
1	A	202	GLN
1	B	357	THR
1	C	202	GLN
2	E	63	GLY
1	A	26	GLN
2	E	122	GLY
1	A	211	SER
2	G	62	LYS
1	B	71	GLY
1	B	389	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	408/504 (81%)	356 (87%)	52 (13%)	4	17
1	B	408/504 (81%)	350 (86%)	58 (14%)	3	13
1	C	408/504 (81%)	348 (85%)	60 (15%)	3	12
2	E	190/228 (83%)	176 (93%)	14 (7%)	13	38
2	F	190/228 (83%)	174 (92%)	16 (8%)	10	33
2	G	190/228 (83%)	180 (95%)	10 (5%)	20	48
All	All	1794/2196 (82%)	1584 (88%)	210 (12%)	5	20

All (210) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	35	SER
1	A	65	LYS
1	A	66	GLU
1	A	68	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	80	LYS
1	A	84	ASP
1	A	95	LEU
1	A	97	MET
1	A	137	PHE
1	A	156	LYS
1	A	178	VAL
1	A	179	VAL
1	A	185	VAL
1	A	187	VAL
1	A	188	LEU
1	A	190	PHE
1	A	201	LYS
1	A	203	LEU
1	A	210	GLN
1	A	218	GLU
1	A	238	SER
1	A	249	THR
1	A	251	MET
1	A	252	LEU
1	A	261	ILE
1	A	267	THR
1	A	278	VAL
1	A	308	VAL
1	A	309	ILE
1	A	316	LEU
1	A	319	SER
1	A	328	GLU
1	A	334	LEU
1	A	339	ARG
1	A	354	GLN
1	A	357	THR
1	A	363	ASN
1	A	364	ARG
1	A	380	ASN
1	A	396	MET
1	A	409	SER
1	A	425	SER
1	A	427	LYS
1	A	442	VAL
1	A	449	THR
1	A	450	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	455	THR
1	A	466	SER
1	A	503	LEU
1	A	506	ILE
1	A	508	LYS
1	B	29	THR
1	B	35	SER
1	B	40	VAL
1	B	68	LYS
1	B	83	LEU
1	B	84	ASP
1	B	144	VAL
1	B	157	VAL
1	B	158	LEU
1	B	175	ASN
1	B	176	LYS
1	B	178	VAL
1	B	179	VAL
1	B	181	LEU
1	B	185	VAL
1	B	187	VAL
1	B	188	LEU
1	B	190	PHE
1	B	192	VAL
1	B	195	LEU
1	B	202	GLN
1	B	206	ILE
1	B	210	GLN
1	B	214	ILE
1	B	216	ASN
1	B	218	GLU
1	B	219	THR
1	B	240	ASN
1	B	245	THR
1	B	249	THR
1	B	251	MET
1	B	252	LEU
1	B	261	ILE
1	B	267	THR
1	B	278	VAL
1	B	308	VAL
1	B	310	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	316	LEU
1	B	319	SER
1	B	332	ILE
1	B	334	LEU
1	B	338	ASP
1	B	339	ARG
1	B	363	ASN
1	B	364	ARG
1	B	374	THR
1	B	377	SER
1	B	388	ASN
1	B	396	MET
1	B	399	LYS
1	B	425	SER
1	B	434	THR
1	B	436	SER
1	B	449	THR
1	B	450	VAL
1	B	455	THR
1	B	466	SER
1	B	475	ILE
1	C	27	ASN
1	C	28	ILE
1	C	29	THR
1	C	35	SER
1	C	36	THR
1	C	40	VAL
1	C	42	LYS
1	C	64	ILE
1	C	65	LYS
1	C	66	GLU
1	C	68	LYS
1	C	75	LYS
1	C	84	ASP
1	C	158	LEU
1	C	160	LEU
1	C	161	GLU
1	C	169	SER
1	C	179	VAL
1	C	181	LEU
1	C	185	VAL
1	C	187	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	188	LEU
1	C	202	GLN
1	C	208	ASN
1	C	210	GLN
1	C	216	ASN
1	C	218	GLU
1	C	251	MET
1	C	258	LEU
1	C	278	VAL
1	C	308	VAL
1	C	316	LEU
1	C	319	SER
1	C	326	THR
1	C	327	LYS
1	C	334	LEU
1	C	338	ASP
1	C	339	ARG
1	C	359	LYS
1	C	360	VAL
1	C	363	ASN
1	C	364	ARG
1	C	374	THR
1	C	377	SER
1	C	396	MET
1	C	425	SER
1	C	426	ASN
1	C	427	LYS
1	C	429	ARG
1	C	437	ASN
1	C	442	VAL
1	C	447	VAL
1	C	450	VAL
1	C	465	LYS
1	C	466	SER
1	C	467	LEU
1	C	486	ASP
1	C	503	LEU
1	C	507	ARG
1	C	508	LYS
2	E	39	LEU
2	E	52	SER
2	E	56	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	88	THR
2	E	126	ILE
2	E	127	THR
2	E	132	ILE
2	E	142	SER
2	E	184	SER
2	E	186	THR
2	E	221	SER
2	E	225	ASP
2	E	246	GLU
2	E	273	LEU
2	F	23	LEU
2	F	24	VAL
2	F	49	SER
2	F	65	GLU
2	F	88	THR
2	F	123	TYR
2	F	124	ASN
2	F	125	SER
2	F	126	ILE
2	F	127	THR
2	F	169	GLN
2	F	188	SER
2	F	198	VAL
2	F	221	SER
2	F	259	SER
2	F	261	SER
2	G	22	GLN
2	G	65	GLU
2	G	88	THR
2	G	121	THR
2	G	125	SER
2	G	126	ILE
2	G	127	THR
2	G	186	THR
2	G	241	THR
2	G	273	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	159	HIS
1	A	227	ASN
1	A	268	ASN
1	B	380	ASN
1	C	216	ASN
1	C	277	ASN
1	C	388	ASN
1	C	428	ASN
2	E	103	ASN
2	F	103	ASN
2	F	124	ASN
2	G	103	ASN
2	G	135	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 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	448/562 (79%)	-0.49	5 (1%) 78 57	34, 56, 123, 168	0
1	B	448/562 (79%)	-0.48	8 (1%) 67 45	28, 49, 111, 182	0
1	C	448/562 (79%)	-0.30	7 (1%) 70 47	32, 66, 129, 180	0
2	E	233/294 (79%)	-0.43	1 (0%) 88 75	45, 71, 106, 127	0
2	F	233/294 (79%)	-0.59	4 (1%) 69 46	31, 45, 67, 103	0
2	G	233/294 (79%)	0.05	4 (1%) 69 46	62, 109, 147, 186	0
All	All	2043/2568 (79%)	-0.39	29 (1%) 73 51	28, 60, 127, 186	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	124	ASN	5.7
1	C	206	ILE	5.2
2	G	166	VAL	4.9
1	A	206	ILE	4.4
2	G	122	GLY	4.1
2	G	274	GLY	4.0
1	B	214	ILE	4.0
1	C	207	LEU	3.8
2	F	123	TYR	3.7
1	B	208	ASN	3.4
1	C	208	ASN	3.2
2	F	274	GLY	3.0
1	A	207	LEU	3.0
2	E	122	GLY	3.0
1	A	25	GLY	2.9
1	A	99	SER	2.7
1	B	486	ASP	2.7
1	C	137	PHE	2.6
1	C	71	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	99	SER	2.5
2	G	215	ASP	2.5
1	B	206	ILE	2.5
1	B	370	MET	2.3
1	B	356	GLU	2.3
2	F	143	SER	2.3
1	C	509	SER	2.3
1	B	509	SER	2.2
1	A	208	ASN	2.1
1	C	489	ASP	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 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.