Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 11:13 PM EDT

PDB ID	:	5JTV
Title	:	USP7CD-UBL45 in complex with Ubiquitin
Authors	:	Murray, J.M.; Rouge, L.
Deposited on	:	2016-05-09
Resolution	:	3.31 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:

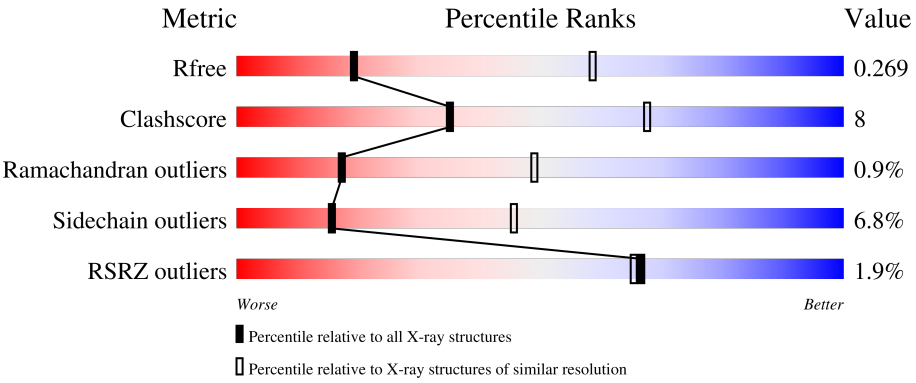
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.31 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	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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	594	2% 70% 23% • 5%
1	C	594	% 74% 19% • 5%
1	E	594	2% 72% 20% • • 5%
1	G	594	2% 72% 20% • 5%
2	B	76	84% 16%

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Mol	Chain	Length	Quality of chain
2	D	76	84% 16%
2	F	76	4% 89% 11%
2	H	76	68% 30%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 20520 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 Ubiquitin carboxyl-terminal hydrolase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	564	Total	C	N	O	S	2	0	0
			4562	2899	784	854	25			
1	C	564	Total	C	N	O	S	26	0	0
			4533	2878	784	846	25			
1	E	565	Total	C	N	O	S	11	0	0
			4530	2881	778	846	25			
1	G	563	Total	C	N	O	S	0	0	0
			4507	2861	776	845	25			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	MET	-	initiating methionine	UNP Q93009
A	193	HIS	-	expression tag	UNP Q93009
A	194	HIS	-	expression tag	UNP Q93009
A	195	HIS	-	expression tag	UNP Q93009
A	196	HIS	-	expression tag	UNP Q93009
A	197	HIS	-	expression tag	UNP Q93009
A	198	HIS	-	expression tag	UNP Q93009
A	199	GLY	-	expression tag	UNP Q93009
A	200	GLU	-	expression tag	UNP Q93009
A	201	ASN	-	expression tag	UNP Q93009
A	202	LEU	-	expression tag	UNP Q93009
A	203	TYR	-	expression tag	UNP Q93009
A	204	PHE	-	expression tag	UNP Q93009
A	205	GLN	-	expression tag	UNP Q93009
A	206	GLY	-	expression tag	UNP Q93009
A	872	GLY	-	linker	UNP Q93009
A	873	GLY	-	linker	UNP Q93009
A	874	SER	-	linker	UNP Q93009
A	875	GLY	-	linker	UNP Q93009
A	876	GLY	-	linker	UNP Q93009
A	877	SER	-	linker	UNP Q93009

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Chain	Residue	Modelled	Actual	Comment	Reference
A	878	GLY	-	linker	UNP Q93009
A	879	GLY	-	linker	UNP Q93009
A	880	SER	-	linker	UNP Q93009
A	881	GLY	-	linker	UNP Q93009
C	192	MET	-	initiating methionine	UNP Q93009
C	193	HIS	-	expression tag	UNP Q93009
C	194	HIS	-	expression tag	UNP Q93009
C	195	HIS	-	expression tag	UNP Q93009
C	196	HIS	-	expression tag	UNP Q93009
C	197	HIS	-	expression tag	UNP Q93009
C	198	HIS	-	expression tag	UNP Q93009
C	199	GLY	-	expression tag	UNP Q93009
C	200	GLU	-	expression tag	UNP Q93009
C	201	ASN	-	expression tag	UNP Q93009
C	202	LEU	-	expression tag	UNP Q93009
C	203	TYR	-	expression tag	UNP Q93009
C	204	PHE	-	expression tag	UNP Q93009
C	205	GLN	-	expression tag	UNP Q93009
C	206	GLY	-	expression tag	UNP Q93009
C	872	GLY	-	linker	UNP Q93009
C	873	GLY	-	linker	UNP Q93009
C	874	SER	-	linker	UNP Q93009
C	875	GLY	-	linker	UNP Q93009
C	876	GLY	-	linker	UNP Q93009
C	877	SER	-	linker	UNP Q93009
C	878	GLY	-	linker	UNP Q93009
C	879	GLY	-	linker	UNP Q93009
C	880	SER	-	linker	UNP Q93009
C	881	GLY	-	linker	UNP Q93009
E	192	MET	-	initiating methionine	UNP Q93009
E	193	HIS	-	expression tag	UNP Q93009
E	194	HIS	-	expression tag	UNP Q93009
E	195	HIS	-	expression tag	UNP Q93009
E	196	HIS	-	expression tag	UNP Q93009
E	197	HIS	-	expression tag	UNP Q93009
E	198	HIS	-	expression tag	UNP Q93009
E	199	GLY	-	expression tag	UNP Q93009
E	200	GLU	-	expression tag	UNP Q93009
E	201	ASN	-	expression tag	UNP Q93009
E	202	LEU	-	expression tag	UNP Q93009
E	203	TYR	-	expression tag	UNP Q93009
E	204	PHE	-	expression tag	UNP Q93009

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Chain	Residue	Modelled	Actual	Comment	Reference
E	205	GLN	-	expression tag	UNP Q93009
E	206	GLY	-	expression tag	UNP Q93009
E	872	GLY	-	linker	UNP Q93009
E	873	GLY	-	linker	UNP Q93009
E	874	SER	-	linker	UNP Q93009
E	875	GLY	-	linker	UNP Q93009
E	876	GLY	-	linker	UNP Q93009
E	877	SER	-	linker	UNP Q93009
E	878	GLY	-	linker	UNP Q93009
E	879	GLY	-	linker	UNP Q93009
E	880	SER	-	linker	UNP Q93009
E	881	GLY	-	linker	UNP Q93009
G	192	MET	-	initiating methionine	UNP Q93009
G	193	HIS	-	expression tag	UNP Q93009
G	194	HIS	-	expression tag	UNP Q93009
G	195	HIS	-	expression tag	UNP Q93009
G	196	HIS	-	expression tag	UNP Q93009
G	197	HIS	-	expression tag	UNP Q93009
G	198	HIS	-	expression tag	UNP Q93009
G	199	GLY	-	expression tag	UNP Q93009
G	200	GLU	-	expression tag	UNP Q93009
G	201	ASN	-	expression tag	UNP Q93009
G	202	LEU	-	expression tag	UNP Q93009
G	203	TYR	-	expression tag	UNP Q93009
G	204	PHE	-	expression tag	UNP Q93009
G	205	GLN	-	expression tag	UNP Q93009
G	206	GLY	-	expression tag	UNP Q93009
G	872	GLY	-	linker	UNP Q93009
G	873	GLY	-	linker	UNP Q93009
G	874	SER	-	linker	UNP Q93009
G	875	GLY	-	linker	UNP Q93009
G	876	GLY	-	linker	UNP Q93009
G	877	SER	-	linker	UNP Q93009
G	878	GLY	-	linker	UNP Q93009
G	879	GLY	-	linker	UNP Q93009
G	880	SER	-	linker	UNP Q93009
G	881	GLY	-	linker	UNP Q93009

- Molecule 2 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	76	Total	C	N	O	S	0	0	0
			597	375	104	117	1			

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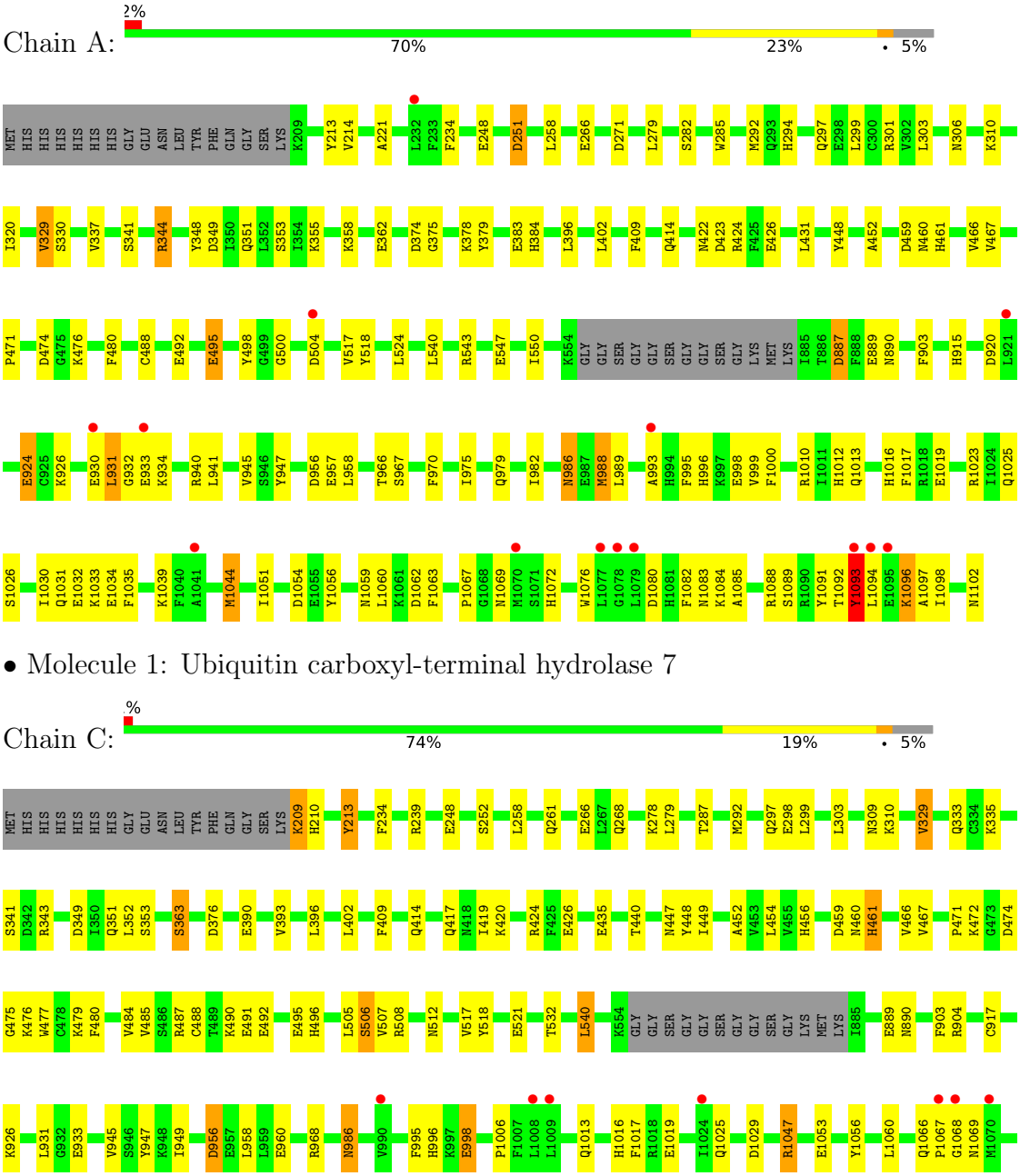
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	76	Total	C	N	O	S	0	0	0
			597	375	104	117	1			
2	F	76	Total	C	N	O	S	0	0	0
			597	375	104	117	1			
2	H	76	Total	C	N	O	S	0	0	0
			597	375	104	117	1			

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.

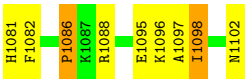
• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7

Chain A:



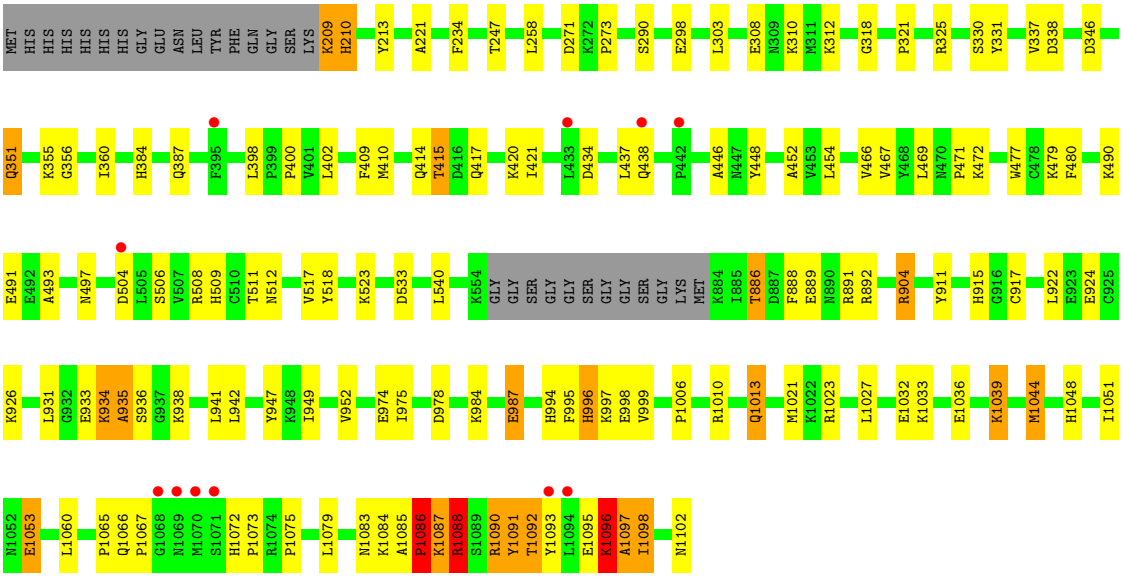
• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7

Chain C:



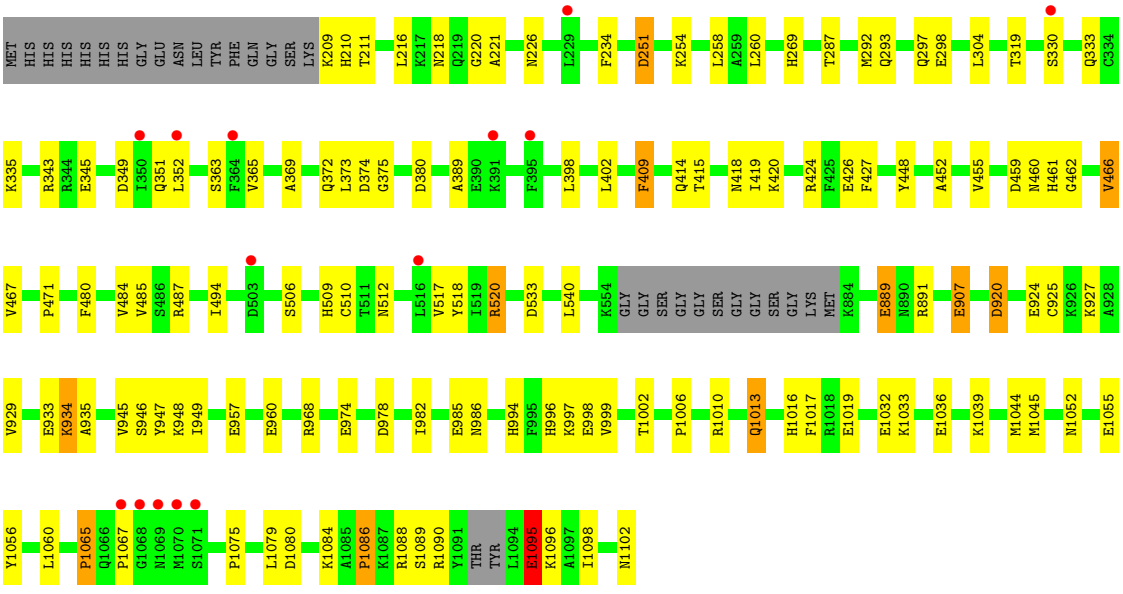
• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7

Chain E:



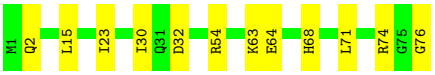
• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7

Chain G:



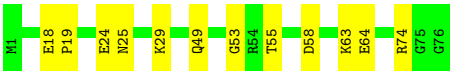
• Molecule 2: Polyubiquitin-B

Chain B:



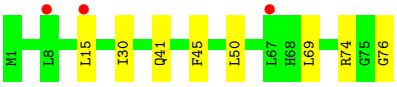
• Molecule 2: Polyubiquitin-B

Chain D:



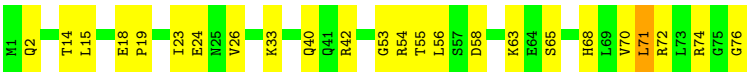
• Molecule 2: Polyubiquitin-B

Chain F:



• Molecule 2: Polyubiquitin-B

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	113.61Å 115.52Å 257.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.95 – 3.31 46.95 – 3.31	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.95-3.31) 92.6 (46.95-3.31)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 3.32Å)	Xtriage
Refinement program	PHENIX dev_2210	Depositor
R, R_{free}	0.239 , 0.269 0.239 , 0.269	Depositor DCC
R_{free} test set	2596 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	94.0	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 28.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.036 for k,h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	20520	wwPDB-VP
Average B, all atoms (Å^2)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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	0.34	3/4663 (0.1%)	0.53	1/6290 (0.0%)
1	C	0.26	0/4634	0.49	1/6254 (0.0%)
1	E	0.28	0/4630	0.54	4/6249 (0.1%)
1	G	0.29	0/4605	0.54	4/6215 (0.1%)
2	B	0.32	0/603	0.68	1/812 (0.1%)
2	D	0.27	0/603	0.52	0/812
2	F	0.28	0/603	0.60	0/812
2	H	0.30	0/603	0.67	1/812 (0.1%)
All	All	0.29	3/20944 (0.0%)	0.54	12/28256 (0.0%)

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	E	0	2
1	G	0	2
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	498	TYR	CD2-CE2	-7.40	1.28	1.39
1	A	498	TYR	CD1-CE1	-6.54	1.29	1.39
1	A	498	TYR	CE2-CZ	-5.01	1.32	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	506	SER	CB-CA-C	13.36	135.49	110.10
1	E	1088	ARG	N-CA-C	8.57	134.13	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	1096	LYS	CD-CE-NZ	-8.38	92.44	111.70
2	B	71	LEU	CB-CA-C	-7.57	95.81	110.20
1	G	996	HIS	N-CA-C	-7.00	92.11	111.00
2	H	71	LEU	CB-CA-C	-6.43	97.98	110.20
1	G	1095	GLU	CB-CA-C	-5.87	98.66	110.40
1	G	506	SER	N-CA-C	-5.43	96.33	111.00
1	A	498	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	E	1086	PRO	C-N-CA	5.18	134.66	121.70
1	C	998	GLU	N-CA-C	-5.15	97.09	111.00
1	E	996	HIS	CB-CA-C	-5.14	100.12	110.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	504	ASP	Peptide
1	E	1092	THR	Peptide
1	E	504	ASP	Peptide
1	G	1090	ARG	Peptide
1	G	1095	GLU	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	4562	0	4423	91	1
1	C	4533	0	4370	71	0
1	E	4530	0	4366	86	0
1	G	4507	0	4335	88	1
2	B	597	0	618	12	0
2	D	597	0	618	8	0
2	F	597	0	618	12	0
2	H	597	0	618	21	0
All	All	20520	0	19966	330	1

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 8.

All (330) 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)
2:B:74:ARG:NH1	1:E:1096:LYS:HB2	1.64	1.12
1:A:1096:LYS:HB3	2:F:74:ARG:NH1	1.69	1.08
1:C:292:MET:HE1	1:G:1095:GLU:O	1.59	1.03
1:E:934:LYS:HZ3	1:E:934:LYS:H	1.03	1.01
1:C:292:MET:CE	1:G:1095:GLU:O	2.09	1.00
1:A:1096:LYS:HE2	2:F:74:ARG:HH11	1.41	0.85
1:C:996:HIS:O	1:C:996:HIS:ND1	2.08	0.85
1:E:891:ARG:NH1	1:E:911:TYR:O	2.09	0.85
1:A:1096:LYS:HB3	2:F:74:ARG:HH12	1.41	0.85
1:E:936:SER:OG	1:E:975:ILE:O	1.97	0.83
1:E:1091:TYR:HB2	1:E:1092:THR:HA	1.60	0.83
1:A:306:ASN:OD1	1:A:310:LYS:NZ	2.13	0.82
2:B:74:ARG:HH11	1:E:1096:LYS:HB2	1.42	0.82
1:E:420:LYS:NZ	1:E:512:ASN:OD1	2.13	0.81
1:A:467:VAL:HG13	1:A:480:PHE:HB2	1.61	0.80
2:H:14:THR:O	2:H:33:LYS:NZ	2.14	0.78
1:E:308:GLU:OE1	1:E:312:LYS:NZ	2.17	0.77
1:C:986:ASN:OD1	1:C:986:ASN:N	2.18	0.77
1:C:299:LEU:HD23	1:G:1098:ILE:HD11	1.68	0.76
1:A:299:LEU:HD23	1:E:1098:ILE:HD11	1.67	0.76
1:C:420:LYS:NZ	1:C:512:ASN:OD1	2.16	0.75
1:E:926:LYS:HG3	1:E:931:LEU:HD21	1.68	0.75
1:A:422:ASN:O	1:A:500:GLY:HA2	1.86	0.74
1:G:467:VAL:HG13	1:G:480:PHE:HB2	1.70	0.73
2:D:55:THR:OG1	2:D:58:ASP:OD2	2.06	0.72
1:A:1096:LYS:CE	2:F:74:ARG:HH11	2.01	0.72
1:A:1083:ASN:OD1	1:A:1084:LYS:N	2.24	0.71
1:G:398:LEU:O	1:G:520:ARG:NH1	2.22	0.71
1:E:1088:ARG:HA	1:G:907:GLU:O	1.90	0.71
1:G:418:ASN:O	1:G:460:ASN:ND2	2.22	0.71
1:G:934:LYS:HB2	1:G:934:LYS:NZ	2.04	0.71
1:G:409:PHE:HE1	2:H:71:LEU:O	1.73	0.70
1:A:424:ARG:NH1	1:A:426:GLU:OE2	2.24	0.70
1:G:343:ARG:NH2	2:H:63:LYS:O	2.21	0.70
2:B:2:GLN:HB3	2:B:63:LYS:HE2	1.71	0.70
1:E:1013:GLN:HG2	1:E:1060:LEU:HG	1.74	0.70
1:E:933:GLU:HB2	1:E:934:LYS:NZ	2.06	0.70
1:C:474:ASP:O	1:C:476:LYS:N	2.25	0.70
1:A:1096:LYS:HB3	2:F:74:ARG:HH11	1.54	0.69
1:G:209:LYS:N	1:G:960:GLU:OE2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:TYR:OH	2:B:64:GLU:OE2	2.11	0.69
1:G:1013:GLN:HG2	1:G:1060:LEU:HG	1.73	0.68
1:G:409:PHE:CE1	2:H:71:LEU:O	2.46	0.68
1:C:926:LYS:HG3	1:C:931:LEU:HD21	1.76	0.68
1:G:448:TYR:OH	1:G:520:ARG:NH1	2.26	0.68
1:C:459:ASP:OD1	1:C:460:ASN:N	2.24	0.67
1:E:934:LYS:HZ3	1:E:934:LYS:N	1.85	0.67
1:A:1039:LYS:HB2	1:A:1080:ASP:HB3	1.76	0.67
1:E:934:LYS:H	1:E:934:LYS:NZ	1.86	0.66
1:A:995:PHE:HD2	1:A:998:GLU:O	1.78	0.66
1:C:1098:ILE:HG21	1:G:298:GLU:CD	2.17	0.65
1:A:1092:THR:O	1:A:1093:TYR:HB2	1.95	0.64
1:A:926:LYS:O	1:A:931:LEU:HD11	1.97	0.64
1:G:424:ARG:NH1	1:G:426:GLU:OE2	2.31	0.63
1:C:1017:PHE:H	1:C:1056:TYR:HA	1.63	0.63
1:E:493:ALA:O	1:E:497:ASN:ND2	2.31	0.63
1:E:213:TYR:HE2	1:E:472:LYS:HZ3	1.47	0.63
1:A:1069:ASN:HB3	1:A:1072:HIS:HB3	1.80	0.62
2:H:40:GLN:O	2:H:71:LEU:HD23	2.00	0.62
1:A:1010:ARG:O	1:A:1023:ARG:NH1	2.32	0.62
1:C:1102:ASN:HD22	1:G:254:LYS:HD2	1.65	0.61
1:A:459:ASP:OD1	1:A:460:ASN:N	2.32	0.61
1:A:1098:ILE:HG21	1:E:298:GLU:HG2	1.82	0.61
1:C:209:LYS:HG2	1:C:210:HIS:H	1.66	0.61
1:C:297:GLN:NE2	1:C:349:ASP:OD1	2.34	0.61
1:C:329:VAL:HG13	1:C:396:LEU:HD11	1.83	0.61
1:G:216:LEU:HD12	1:G:226:ASN:HA	1.83	0.61
1:G:297:GLN:NE2	1:G:349:ASP:OD1	2.34	0.60
1:A:889:GLU:HG2	1:A:890:ASN:H	1.67	0.60
1:G:298:GLU:OE1	2:H:72:ARG:NH2	2.34	0.60
1:C:452:ALA:HB3	1:C:517:VAL:HB	1.84	0.60
1:E:1086:PRO:HA	1:E:1087:LYS:CB	2.30	0.60
1:E:325:ARG:NH1	1:E:346:ASP:OD1	2.32	0.60
1:G:948:LYS:HE3	1:G:1002:THR:HG21	1.83	0.60
1:G:420:LYS:NZ	1:G:512:ASN:OD1	2.29	0.59
1:A:986:ASN:OD1	1:A:986:ASN:N	2.32	0.59
1:E:1083:ASN:OD1	1:E:1084:LYS:N	2.35	0.59
1:C:491:GLU:O	1:C:496:HIS:ND1	2.35	0.59
1:C:1086:PRO:HD2	1:G:414:GLN:O	2.03	0.59
1:G:269:HIS:NE2	1:G:533:ASP:OD2	2.29	0.58
1:C:926:LYS:HE3	1:C:931:LEU:HD22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:374:ASP:OD1	1:G:375:GLY:N	2.35	0.58
2:B:74:ARG:HH12	1:E:1096:LYS:HB2	1.62	0.58
2:D:63:LYS:HG2	2:D:64:GLU:HG3	1.85	0.58
1:E:1095:GLU:HB3	1:E:1096:LYS:HB3	1.84	0.58
1:A:297:GLN:NE2	1:A:349:ASP:OD1	2.36	0.58
1:C:209:LYS:NZ	1:C:485:VAL:O	2.37	0.58
1:A:1096:LYS:CB	2:F:74:ARG:NH1	2.58	0.57
1:A:543:ARG:O	1:A:547:GLU:HB2	2.04	0.57
1:C:335:LYS:HD2	1:C:390:GLU:HG3	1.86	0.57
1:G:420:LYS:HD2	1:G:459:ASP:HA	1.86	0.57
1:A:996:HIS:HE1	1:A:1082:PHE:CZ	2.22	0.57
1:C:449:ILE:HG12	1:C:521:GLU:HG2	1.87	0.57
1:A:986:ASN:HD22	1:A:1012:HIS:HE1	1.52	0.57
1:G:1044:MET:HG3	1:G:1075:PRO:HG3	1.85	0.56
1:G:1044:MET:SD	1:G:1045:MET:HG2	2.45	0.56
1:A:1031:GLN:NE2	1:C:1029:ASP:OD1	2.38	0.56
1:C:292:MET:HE3	1:G:1095:GLU:O	2.03	0.56
1:A:251:ASP:OD2	1:A:251:ASP:N	2.39	0.56
1:A:452:ALA:HB3	1:A:517:VAL:HB	1.87	0.56
1:A:986:ASN:HD22	1:A:1012:HIS:CE1	2.23	0.56
1:C:917:CYS:HA	1:C:958:LEU:HA	1.87	0.56
1:E:1033:LYS:H	1:E:1033:LYS:HD2	1.71	0.56
1:E:247:THR:HB	1:E:258:LEU:HD23	1.87	0.56
2:H:23:ILE:HG12	2:H:54:ARG:O	2.05	0.56
1:A:358:LYS:HE2	1:A:362:GLU:OE2	2.06	0.56
1:A:488:CYS:HB2	1:A:492:GLU:OE2	2.06	0.56
1:C:461:HIS:HA	2:D:74:ARG:HB2	1.88	0.56
1:G:380:ASP:H	2:H:2:GLN:HE22	1.55	0.55
1:E:1039:LYS:HB3	1:E:1039:LYS:HZ2	1.71	0.55
1:A:996:HIS:HE1	1:A:1082:PHE:CE2	2.23	0.55
1:A:1085:ALA:HB1	1:E:414:GLN:O	2.07	0.55
1:C:491:GLU:HG3	1:C:495:GLU:HG3	1.89	0.55
1:A:930:GLU:HG2	1:A:932:GLY:H	1.70	0.55
1:E:410:MET:HB3	1:E:421:ILE:HD11	1.87	0.55
1:C:261:GLN:HB3	1:C:540:LEU:HD11	1.88	0.55
1:A:1030:ILE:HD12	1:A:1034:GLU:OE2	2.07	0.54
1:A:355:LYS:NZ	1:A:423:ASP:OD2	2.41	0.54
2:F:45:PHE:HB3	2:F:50:LEU:HD21	1.89	0.54
1:G:1052:ASN:HB3	1:G:1055:GLU:HB2	1.88	0.54
2:H:24:GLU:OE1	2:H:53:GLY:N	2.38	0.54
1:E:400:PRO:HG3	1:E:523:LYS:HD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:477:TRP:CD1	1:E:490:LYS:HG2	2.43	0.53
1:G:452:ALA:HB3	1:G:517:VAL:HB	1.89	0.53
1:G:933:GLU:HG3	1:G:934:LYS:H	1.73	0.53
1:G:345:GLU:OE2	2:H:65:SER:HA	2.08	0.53
1:A:341:SER:OG	2:B:64:GLU:OE1	2.25	0.53
1:G:949:ILE:HG13	1:G:1006:PRO:HB2	1.91	0.53
1:C:1102:ASN:ND2	1:G:254:LYS:HD2	2.23	0.53
2:H:26:VAL:HG21	2:H:56:LEU:HD11	1.90	0.53
2:B:15:LEU:HD11	2:B:30:ILE:HG13	1.90	0.53
1:C:234:PHE:CD2	1:C:471:PRO:HB3	2.43	0.53
2:B:2:GLN:H	2:B:63:LYS:HD2	1.73	0.53
1:C:420:LYS:HE3	1:C:456:HIS:ND1	2.24	0.53
1:G:986:ASN:O	1:G:1013:GLN:N	2.38	0.53
1:E:384:HIS:O	1:E:387:GLN:NE2	2.42	0.52
1:A:461:HIS:HA	2:B:74:ARG:HB2	1.92	0.52
1:C:1066:GLN:OE1	1:C:1069:ASN:ND2	2.43	0.52
1:G:455:VAL:HB	1:G:466:VAL:HG23	1.90	0.52
1:C:956:ASP:OD1	1:C:956:ASP:N	2.42	0.52
1:C:1095:GLU:HA	1:G:292:MET:SD	2.50	0.52
1:A:1102:ASN:OXT	1:E:310:LYS:NZ	2.35	0.52
1:C:467:VAL:HG13	1:C:480:PHE:HB2	1.91	0.52
1:G:933:GLU:HG3	1:G:934:LYS:N	2.25	0.52
2:H:18:GLU:HG3	2:H:19:PRO:HD2	1.92	0.52
1:C:466:VAL:HG11	1:C:479:LYS:HE3	1.91	0.51
1:E:234:PHE:CD2	1:E:471:PRO:HB3	2.45	0.51
1:E:995:PHE:HD2	1:E:996:HIS:O	1.92	0.51
2:H:40:GLN:HB3	2:H:71:LEU:HD21	1.90	0.51
1:A:214:VAL:HG11	1:A:271:ASP:HA	1.91	0.51
1:C:298:GLU:HG3	2:D:49:GLN:OE1	2.09	0.51
1:E:213:TYR:HE2	1:E:472:LYS:NZ	2.07	0.51
1:E:904:ARG:NH1	1:G:1084:LYS:HB3	2.26	0.51
1:G:920:ASP:N	1:G:920:ASP:OD1	2.44	0.51
1:E:933:GLU:HB2	1:E:934:LYS:HZ3	1.75	0.51
2:H:42:ARG:HB2	2:H:70:VAL:HG23	1.92	0.51
1:E:221:ALA:HB1	2:F:76:GLY:HA3	1.92	0.51
1:G:1016:HIS:HA	1:G:1056:TYR:HB3	1.93	0.50
1:G:933:GLU:CG	1:G:934:LYS:H	2.24	0.50
1:E:452:ALA:HB3	1:E:517:VAL:HB	1.94	0.50
1:G:365:VAL:O	1:G:369:ALA:N	2.44	0.50
1:A:920:ASP:O	1:A:924:GLU:HB2	2.11	0.50
1:A:1096:LYS:CB	2:F:74:ARG:HH12	2.17	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:SER:OG	1:C:507:VAL:N	2.45	0.50
1:G:448:TYR:HB3	1:G:518:TYR:HB3	1.93	0.49
1:G:380:ASP:H	2:H:2:GLN:NE2	2.08	0.49
1:C:889:GLU:HG2	1:C:890:ASN:H	1.76	0.49
1:A:329:VAL:HG13	1:A:396:LEU:HD11	1.93	0.49
1:A:890:ASN:HD21	1:A:915:HIS:HE1	1.61	0.49
1:E:933:GLU:HB2	1:E:934:LYS:HZ1	1.76	0.49
1:E:1044:MET:HG3	1:E:1075:PRO:HG3	1.95	0.49
1:E:415:THR:HB	1:E:417:GLN:HG2	1.93	0.49
1:E:888:PHE:O	1:E:889:GLU:HG3	2.12	0.49
2:F:15:LEU:HD11	2:F:30:ILE:HG13	1.94	0.49
1:G:398:LEU:HB2	1:G:520:ARG:HH22	1.78	0.49
1:C:1016:HIS:HA	1:C:1056:TYR:HB3	1.95	0.49
1:A:329:VAL:HG13	1:A:344:ARG:HG3	1.96	0.48
1:A:1084:LYS:HG3	1:C:904:ARG:HD2	1.95	0.48
1:E:1072:HIS:ND1	1:E:1073:PRO:HD2	2.28	0.48
1:E:448:TYR:HB3	1:E:518:TYR:HB3	1.95	0.48
2:D:24:GLU:OE1	2:D:53:GLY:N	2.45	0.48
1:G:924:GLU:HA	1:G:927:LYS:HE2	1.95	0.48
1:C:417:GLN:HE21	1:C:419:ILE:HD11	1.79	0.48
1:E:1083:ASN:ND2	1:E:1085:ALA:HB2	2.28	0.48
1:E:1096:LYS:O	1:E:1097:ALA:HB3	2.14	0.48
1:C:414:GLN:HG2	1:G:947:TYR:OH	2.13	0.48
1:G:1032:GLU:O	1:G:1036:GLU:HG3	2.14	0.48
1:E:949:ILE:HG13	1:E:1006:PRO:HB2	1.96	0.48
1:E:942:LEU:HD23	1:E:952:VAL:HG22	1.96	0.47
1:G:211:THR:HB	1:G:487:ARG:NH2	2.29	0.47
1:C:1081:HIS:ND1	1:C:1082:PHE:O	2.47	0.47
1:G:461:HIS:HA	2:H:74:ARG:HB2	1.96	0.47
1:E:994:HIS:CE1	1:E:1079:LEU:HD12	2.49	0.47
1:G:935:ALA:HB3	1:G:974:GLU:OE2	2.14	0.47
1:C:1013:GLN:HG2	1:C:1060:LEU:HG	1.96	0.47
1:A:474:ASP:OD2	1:A:476:LYS:HG2	2.15	0.47
1:A:431:LEU:HB3	1:A:448:TYR:HB2	1.96	0.47
1:C:209:LYS:CG	1:C:210:HIS:H	2.27	0.47
1:C:488:CYS:HB2	1:C:492:GLU:OE2	2.14	0.47
1:G:945:VAL:HG21	1:G:968:ARG:NH1	2.30	0.47
1:A:448:TYR:HB3	1:A:518:TYR:HB3	1.96	0.47
1:C:448:TYR:HB3	1:C:518:TYR:HB3	1.96	0.46
1:G:335:LYS:NZ	1:G:372:GLN:OE1	2.44	0.46
1:G:1016:HIS:HB3	1:G:1056:TYR:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:GLU:HG2	1:G:1098:ILE:HG21	1.97	0.46
2:H:42:ARG:HD3	2:H:72:ARG:CZ	2.45	0.46
1:G:211:THR:HB	1:G:487:ARG:HH22	1.79	0.46
1:G:352:LEU:HB3	1:G:363:SER:OG	2.15	0.46
1:G:459:ASP:OD1	1:G:510:CYS:HB2	2.15	0.46
1:C:995:PHE:HD2	1:C:998:GLU:O	1.97	0.46
1:G:409:PHE:N	1:G:409:PHE:CD2	2.82	0.46
1:A:1084:LYS:HG3	1:C:904:ARG:CD	2.46	0.46
1:G:218:ASN:OD1	1:G:220:GLY:N	2.45	0.46
1:C:472:LYS:HB2	1:C:474:ASP:OD2	2.16	0.46
1:E:398:LEU:HG	1:E:437:LEU:HD21	1.98	0.46
1:A:979:GLN:HB3	1:A:989:LEU:HD11	1.98	0.46
1:E:273:PRO:HG2	1:E:915:HIS:CD2	2.51	0.46
1:A:887:ASP:OD1	1:A:887:ASP:N	2.49	0.45
1:E:209:LYS:HG3	1:E:210:HIS:N	2.31	0.45
1:E:355:LYS:HD3	1:E:421:ILE:HD13	1.98	0.45
1:E:491:GLU:H	1:E:491:GLU:CD	2.19	0.45
1:E:936:SER:O	1:E:938:LYS:HG3	2.17	0.45
1:G:925:CYS:O	1:G:929:VAL:HG22	2.16	0.45
1:C:1066:GLN:O	1:C:1068:GLY:N	2.49	0.45
1:A:988:MET:SD	1:A:1060:LEU:HD22	2.57	0.45
1:A:996:HIS:CE1	1:A:1082:PHE:CZ	3.03	0.45
1:C:996:HIS:O	1:C:996:HIS:CG	2.70	0.45
1:A:234:PHE:CD2	1:A:471:PRO:HB3	2.52	0.45
1:A:996:HIS:O	1:A:996:HIS:CD2	2.70	0.45
1:C:1088:ARG:NH2	1:G:419:ILE:HD11	2.31	0.45
1:C:209:LYS:N	1:C:213:TYR:O	2.50	0.45
1:E:434:ASP:CG	1:E:446:ALA:H	2.20	0.45
1:A:1016:HIS:HA	1:A:1056:TYR:HB3	1.99	0.45
1:A:1069:ASN:HB3	1:A:1072:HIS:CB	2.46	0.45
1:C:424:ARG:NH1	1:C:426:GLU:OE2	2.50	0.45
2:H:55:THR:OG1	2:H:58:ASP:OD2	2.25	0.45
1:E:935:ALA:HB3	1:E:974:GLU:OE2	2.17	0.44
1:C:947:TYR:OH	1:G:414:GLN:HG2	2.17	0.44
1:C:1098:ILE:HG23	1:C:1098:ILE:O	2.17	0.44
1:E:331:TYR:OH	1:E:438:GLN:NE2	2.47	0.44
1:G:427:PHE:CE1	1:G:494:ILE:HG23	2.52	0.44
1:A:375:GLY:O	1:A:378:LYS:HG3	2.17	0.44
1:A:996:HIS:CE1	1:A:1082:PHE:CE2	3.06	0.44
1:E:1090:ARG:O	1:E:1091:TYR:O	2.36	0.44
1:G:234:PHE:CD2	1:G:471:PRO:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:293:GLN:OE1	1:G:462:GLY:HA2	2.17	0.44
1:A:285:TRP:CZ2	1:E:1098:ILE:HG13	2.53	0.44
1:A:933:GLU:HG3	1:A:934:LYS:H	1.83	0.44
2:B:23:ILE:HG12	2:B:54:ARG:O	2.18	0.44
1:G:373:LEU:HD12	1:G:389:ALA:HB3	2.00	0.44
1:A:320:ILE:HG22	1:A:348:TYR:HE2	1.82	0.44
1:E:996:HIS:O	1:E:997:LYS:C	2.56	0.44
1:E:904:ARG:HE	1:E:904:ARG:HB3	1.57	0.44
1:A:1000:PHE:CE2	1:E:356:GLY:HA3	2.53	0.43
1:E:466:VAL:HG11	1:E:479:LYS:HE3	2.00	0.43
1:E:987:GLU:HG2	1:E:1010:ARG:HG3	1.99	0.43
1:A:524:LEU:HD23	1:A:524:LEU:HA	1.88	0.43
1:E:1091:TYR:CB	1:E:1092:THR:HA	2.34	0.43
1:E:922:LEU:HD11	1:E:941:LEU:HB2	2.00	0.43
1:A:495:GLU:H	1:A:495:GLU:HG2	1.51	0.43
1:E:467:VAL:HG13	1:E:480:PHE:HB2	2.01	0.43
1:A:1017:PHE:H	1:A:1056:TYR:HA	1.83	0.43
1:E:337:VAL:HG12	1:E:338:ASP:H	1.82	0.43
1:G:251:ASP:N	1:G:251:ASP:OD2	2.51	0.43
1:A:945:VAL:HG23	1:A:967:SER:HB2	1.99	0.43
2:F:41:GLN:HB3	2:F:69:LEU:HD11	2.01	0.43
1:G:934:LYS:HB2	1:G:934:LYS:HZ3	1.81	0.43
1:A:1098:ILE:HG21	1:E:298:GLU:CG	2.46	0.43
2:D:18:GLU:HG3	2:D:19:PRO:HD2	2.00	0.43
1:G:1017:PHE:N	1:G:1056:TYR:HD1	2.16	0.43
1:E:506:SER:O	1:E:509:HIS:N	2.46	0.42
1:E:1021:MET:SD	1:E:1053:GLU:HG2	2.59	0.42
1:A:282:SER:O	1:E:1102:ASN:HB2	2.19	0.42
1:A:374:ASP:OD1	1:A:375:GLY:N	2.50	0.42
1:A:1032:GLU:HA	1:A:1035:PHE:HD2	1.84	0.42
1:C:414:GLN:O	1:G:1086:PRO:HD2	2.19	0.42
2:F:41:GLN:CB	2:F:69:LEU:HD11	2.48	0.42
1:G:409:PHE:CE1	2:H:71:LEU:C	2.93	0.42
1:A:940:ARG:NH1	1:A:975:ILE:HG23	2.34	0.42
1:C:949:ILE:HG13	1:C:1006:PRO:HB2	2.01	0.42
1:C:209:LYS:HE2	1:C:960:GLU:OE2	2.20	0.42
1:C:310:LYS:NZ	1:G:1102:ASN:OXT	2.52	0.42
1:C:1047:ARG:HH11	1:C:1047:ARG:HB3	1.85	0.42
1:G:997:LYS:HA	1:G:998:GLU:C	2.39	0.42
1:A:301:ARG:NH1	1:A:349:ASP:OD1	2.52	0.42
1:C:310:LYS:HA	1:C:310:LYS:HD3	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:351:GLN:H	1:E:351:GLN:HG2	1.61	0.42
1:A:337:VAL:HG11	1:A:384:HIS:CD2	2.55	0.42
1:A:414:GLN:HG2	1:E:947:TYR:OH	2.19	0.42
1:E:337:VAL:HG11	1:E:384:HIS:CG	2.54	0.42
1:E:996:HIS:O	1:E:998:GLU:N	2.53	0.42
2:H:15:LEU:HD23	2:H:15:LEU:HA	1.89	0.42
1:A:285:TRP:HZ2	1:E:1098:ILE:HG13	1.85	0.42
1:E:318:GLY:C	1:E:321:PRO:HD2	2.40	0.42
1:E:508:ARG:HA	1:E:511:THR:HB	2.02	0.41
1:A:1091:TYR:N	1:A:1091:TYR:CD2	2.88	0.41
1:C:933:GLU:O	1:C:933:GLU:HG3	2.20	0.41
1:G:459:ASP:OD1	1:G:510:CYS:CB	2.68	0.41
1:G:889:GLU:HB2	1:G:891:ARG:HG2	2.01	0.41
1:A:941:LEU:HD11	1:A:970:PHE:HB3	2.02	0.41
2:D:74:ARG:NH1	1:G:1096:LYS:HA	2.35	0.41
1:G:994:HIS:CE1	1:G:1079:LEU:HD12	2.55	0.41
1:C:1017:PHE:HD2	1:C:1053:GLU:HA	1.84	0.41
1:E:1032:GLU:O	1:E:1036:GLU:HG3	2.21	0.41
1:A:292:MET:HB3	1:A:294:HIS:CE1	2.56	0.41
1:C:352:LEU:HB3	1:C:363:SER:OG	2.21	0.41
1:C:477:TRP:CD1	1:C:490:LYS:HG2	2.56	0.41
1:G:304:LEU:HD23	1:G:304:LEU:HA	1.93	0.41
1:A:993:ALA:HB3	1:A:1076:TRP:CZ3	2.56	0.41
1:G:1039:LYS:HB2	1:G:1080:ASP:HB3	2.01	0.41
1:G:1065:PRO:HB3	1:G:1075:PRO:HD3	2.03	0.41
1:C:239:ARG:NH1	1:C:268:GLN:OE1	2.43	0.41
1:A:422:ASN:O	1:A:500:GLY:CA	2.63	0.41
1:A:1044:MET:O	1:A:1044:MET:HG2	2.20	0.41
2:D:25:ASN:O	2:D:29:LYS:HG3	2.21	0.41
1:E:978:ASP:OD1	1:E:978:ASP:N	2.49	0.41
1:A:221:ALA:HB1	2:B:76:GLY:HA3	2.01	0.41
1:A:947:TYR:OH	1:E:414:GLN:HG2	2.21	0.41
1:A:996:HIS:HE1	1:A:1082:PHE:CE1	2.38	0.41
1:G:978:ASP:O	1:G:1010:ARG:HD3	2.20	0.41
1:A:1062:ASP:C	1:A:1063:PHE:HD2	2.25	0.40
1:C:447:ASN:O	1:C:521:GLU:HG3	2.21	0.40
1:E:1010:ARG:O	1:E:1023:ARG:NH1	2.54	0.40
1:G:221:ALA:HB1	2:H:76:GLY:HA3	2.02	0.40
1:G:260:LEU:HD23	1:G:260:LEU:HA	1.89	0.40
1:A:934:LYS:CB	1:A:934:LYS:NZ	2.84	0.40
1:A:1088:ARG:CD	1:A:1089:SER:H	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:GLN:H	2:B:63:LYS:CD	2.35	0.40
1:E:886:THR:O	1:E:888:PHE:N	2.46	0.40
1:G:292:MET:HE3	1:G:292:MET:HB3	1.81	0.40

All (1) 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)
1:A:383:GLU:OE2	1:G:287:THR:OG1[4_545]	2.08	0.12

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	560/594 (94%)	523 (93%)	33 (6%)	4 (1%)	22	55
1	C	560/594 (94%)	522 (93%)	31 (6%)	7 (1%)	12	40
1	E	561/594 (94%)	516 (92%)	37 (7%)	8 (1%)	11	39
1	G	557/594 (94%)	517 (93%)	37 (7%)	3 (0%)	29	61
2	B	74/76 (97%)	74 (100%)	0	0	100	100
2	D	74/76 (97%)	74 (100%)	0	0	100	100
2	F	74/76 (97%)	74 (100%)	0	0	100	100
2	H	74/76 (97%)	74 (100%)	0	0	100	100
All	All	2534/2680 (95%)	2374 (94%)	138 (5%)	22 (1%)	17	49

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1093	TYR
1	A	1097	ALA

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Mol	Chain	Res	Type
1	E	1087	LYS
1	C	475	GLY
1	C	1096	LYS
1	E	1086	PRO
1	E	1088	ARG
1	E	1091	TYR
1	A	1067	PRO
1	A	1094	LEU
1	C	508	ARG
1	C	1097	ALA
1	E	935	ALA
1	G	1086	PRO
1	C	1098	ILE
1	E	1065	PRO
1	E	1097	ALA
1	G	1065	PRO
1	C	1067	PRO
1	C	1086	PRO
1	E	1067	PRO
1	G	1067	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	494/535 (92%)	453 (92%)	41 (8%)	11 37
1	C	487/535 (91%)	447 (92%)	40 (8%)	11 37
1	E	484/535 (90%)	448 (93%)	36 (7%)	13 41
1	G	483/535 (90%)	453 (94%)	30 (6%)	18 49
2	B	67/68 (98%)	65 (97%)	2 (3%)	41 69
2	D	67/68 (98%)	67 (100%)	0	100 100
2	F	67/68 (98%)	67 (100%)	0	100 100
2	H	67/68 (98%)	66 (98%)	1 (2%)	65 81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2216/2412 (92%)	2066 (93%)	150 (7%)	16 46

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	213	TYR
1	A	248	GLU
1	A	251	ASP
1	A	258	LEU
1	A	266	GLU
1	A	279	LEU
1	A	303	LEU
1	A	329	VAL
1	A	330	SER
1	A	344	ARG
1	A	351	GLN
1	A	353	SER
1	A	402	LEU
1	A	409	PHE
1	A	466	VAL
1	A	495	GLU
1	A	540	LEU
1	A	550	ILE
1	A	887	ASP
1	A	903	PHE
1	A	924	GLU
1	A	931	LEU
1	A	956	ASP
1	A	957	GLU
1	A	958	LEU
1	A	966	THR
1	A	982	ILE
1	A	986	ASN
1	A	988	MET
1	A	999	VAL
1	A	1013	GLN
1	A	1019	GLU
1	A	1025	GLN
1	A	1026	SER
1	A	1033	LYS
1	A	1044	MET
1	A	1051	ILE

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Mol	Chain	Res	Type
1	A	1054	ASP
1	A	1059	ASN
1	A	1093	TYR
1	A	1096	LYS
2	B	32	ASP
2	B	68	HIS
1	C	209	LYS
1	C	213	TYR
1	C	248	GLU
1	C	252	SER
1	C	258	LEU
1	C	266	GLU
1	C	278	LYS
1	C	279	LEU
1	C	287	THR
1	C	303	LEU
1	C	309	ASN
1	C	329	VAL
1	C	333	GLN
1	C	341	SER
1	C	343	ARG
1	C	351	GLN
1	C	353	SER
1	C	363	SER
1	C	376	ASP
1	C	393	VAL
1	C	402	LEU
1	C	409	PHE
1	C	435	GLU
1	C	440	THR
1	C	454	LEU
1	C	461	HIS
1	C	484	VAL
1	C	487	ARG
1	C	505	LEU
1	C	506	SER
1	C	532	THR
1	C	540	LEU
1	C	903	PHE
1	C	945	VAL
1	C	956	ASP
1	C	968	ARG

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Mol	Chain	Res	Type
1	C	986	ASN
1	C	1019	GLU
1	C	1025	GLN
1	C	1047	ARG
1	E	209	LYS
1	E	210	HIS
1	E	271	ASP
1	E	290	SER
1	E	303	LEU
1	E	330	SER
1	E	351	GLN
1	E	360	ILE
1	E	402	LEU
1	E	409	PHE
1	E	415	THR
1	E	454	LEU
1	E	469	LEU
1	E	533	ASP
1	E	540	LEU
1	E	886	THR
1	E	892	ARG
1	E	904	ARG
1	E	917	CYS
1	E	924	GLU
1	E	934	LYS
1	E	984	LYS
1	E	987	GLU
1	E	999	VAL
1	E	1013	GLN
1	E	1027	LEU
1	E	1039	LYS
1	E	1044	MET
1	E	1048	HIS
1	E	1051	ILE
1	E	1053	GLU
1	E	1066	GLN
1	E	1090	ARG
1	E	1093	TYR
1	E	1096	LYS
1	E	1098	ILE
1	G	210	HIS
1	G	251	ASP

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Mol	Chain	Res	Type
1	G	258	LEU
1	G	319	THR
1	G	330	SER
1	G	333	GLN
1	G	351	GLN
1	G	402	LEU
1	G	409	PHE
1	G	415	THR
1	G	466	VAL
1	G	484	VAL
1	G	485	VAL
1	G	509	HIS
1	G	520	ARG
1	G	540	LEU
1	G	889	GLU
1	G	907	GLU
1	G	920	ASP
1	G	934	LYS
1	G	946	SER
1	G	957	GLU
1	G	982	ILE
1	G	985	GLU
1	G	999	VAL
1	G	1013	GLN
1	G	1019	GLU
1	G	1033	LYS
1	G	1088	ARG
1	G	1089	SER
2	H	68	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	351	GLN
1	A	996	HIS
1	A	1012	HIS
1	C	210	HIS
1	C	333	GLN
1	C	417	GLN
1	E	230	GLN
1	E	387	GLN
1	E	915	HIS

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Mol	Chain	Res	Type
1	E	1025	GLN
1	G	219	GLN
1	G	294	HIS
1	G	915	HIS
1	G	1012	HIS
1	G	1083	ASN
2	H	2	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

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, 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	564/594 (94%)	-0.05	14 (2%) 57 55	91, 114, 145, 166	1 (0%)
1	C	562/594 (94%)	-0.12	7 (1%) 79 79	88, 109, 137, 161	1 (0%)
1	E	565/594 (95%)	-0.13	11 (1%) 66 65	89, 110, 144, 168	2 (0%)
1	G	563/594 (94%)	-0.10	14 (2%) 57 55	88, 114, 153, 181	0
2	B	76/76 (100%)	-0.07	0 100 100	94, 105, 115, 123	0
2	D	76/76 (100%)	-0.08	0 100 100	89, 104, 113, 118	0
2	F	76/76 (100%)	-0.01	3 (3%) 39 38	103, 124, 139, 155	0
2	H	76/76 (100%)	-0.12	0 100 100	105, 135, 152, 162	0
All	All	2558/2680 (95%)	-0.10	49 (1%) 66 65	88, 112, 145, 181	4 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1094	LEU	11.2
1	E	504	ASP	6.6
1	E	1094	LEU	5.2
1	G	1070	MET	5.0
1	A	504	ASP	4.8
1	E	1068	GLY	4.8
1	E	1071	SER	4.6
1	A	1078	GLY	4.1
1	A	1077	LEU	3.9
1	A	1093	TYR	3.8
2	F	15	LEU	3.6
1	E	1070	MET	3.4
1	C	1067	PRO	3.4
1	A	1070	MET	3.3
1	C	1009	LEU	3.1
1	G	503	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	1068	GLY	3.0
1	A	993	ALA	3.0
2	F	67	LEU	2.9
1	G	1067	PRO	2.8
1	E	1093	TYR	2.7
1	E	1069	ASN	2.7
1	A	933	GLU	2.7
1	G	330	SER	2.6
1	G	1071	SER	2.6
1	A	232	LEU	2.6
1	A	921	LEU	2.5
1	E	395	PHE	2.5
1	A	1041	ALA	2.5
1	C	1070	MET	2.4
1	A	930	GLU	2.4
1	C	1024	ILE	2.4
1	C	1068	GLY	2.4
1	C	990	VAL	2.3
1	G	395	PHE	2.3
1	G	1069	ASN	2.3
1	E	438	GLN	2.3
1	G	364	PHE	2.3
1	G	516	LEU	2.2
1	A	1095	GLU	2.2
1	G	229	LEU	2.1
1	E	433	LEU	2.1
1	G	391	LYS	2.1
1	G	350	ILE	2.1
2	F	8	LEU	2.1
1	E	442	PRO	2.1
1	A	1079	LEU	2.1
1	G	352	LEU	2.0
1	C	1008	LEU	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.