Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2023 – 02:51 PM JST

PDB ID	:	5GG4
Title	:	Crystal structure of USP7 with RNF169 peptide
Authors	:	Jiang, Y.; Gong, Q.
Deposited on	:	2016-06-15
Resolution	:	3.11 Å(reported)

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

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

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

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

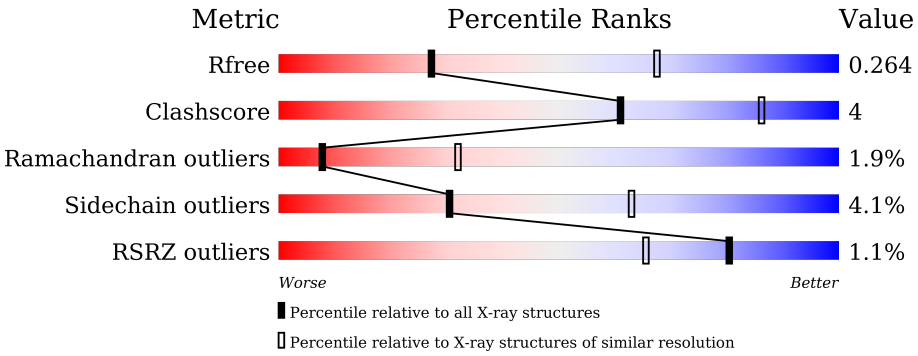
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.11 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	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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	334	79% 13% • 6%
1	B	334	86% 9% 5%
1	C	334	63% 5% • 31%
1	D	334	61% 7% • 32%
2	E	13	8% 54% 15% 8% 8% 15%
2	F	13	8% 54% 8% 8% 31%

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Mol	Chain	Length	Quality of chain
2	G	13	
2	H	13	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8632 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	313	Total	C	N	O	S	0	0	0
			2393	1524	390	462	17			
1	B	317	Total	C	N	O	S	0	0	0
			2391	1527	389	457	18			
1	C	231	Total	C	N	O	S	0	0	0
			1744	1109	281	340	14			
1	D	228	Total	C	N	O	S	0	0	0
			1743	1109	282	338	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	557	SER	-	expression tag	UNP Q93009
A	558	HIS	-	expression tag	UNP Q93009
A	559	MET	-	expression tag	UNP Q93009
B	557	SER	-	expression tag	UNP Q93009
B	558	HIS	-	expression tag	UNP Q93009
B	559	MET	-	expression tag	UNP Q93009
C	557	SER	-	expression tag	UNP Q93009
C	558	HIS	-	expression tag	UNP Q93009
C	559	MET	-	expression tag	UNP Q93009
D	557	SER	-	expression tag	UNP Q93009
D	558	HIS	-	expression tag	UNP Q93009
D	559	MET	-	expression tag	UNP Q93009

- Molecule 2 is a protein called Peptide from E3 ubiquitin-protein ligase RNF169.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	11	Total	C	N	O	S	0	0	0
			94	57	24	12	1			
2	F	9	Total	C	N	O	S	0	0	0
			76	45	20	10	1			

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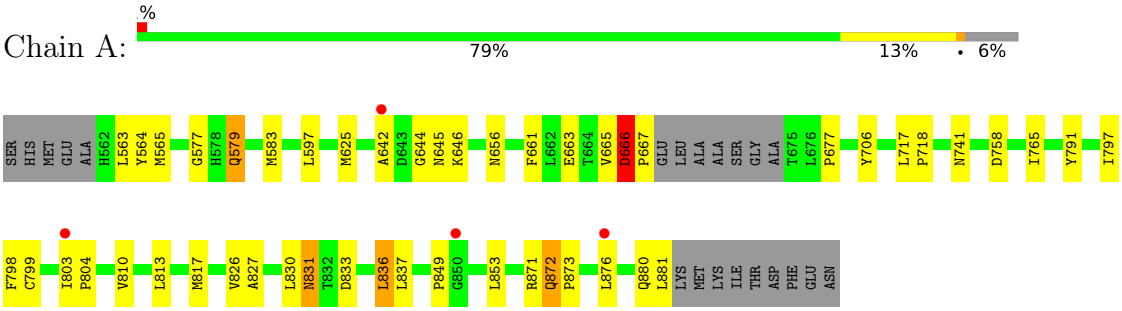
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	10	Total	C	N	O	S	0	0	0
			86	51	23	11	1			
2	H	12	Total	C	N	O	S	0	0	0
			105	63	28	13	1			

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.

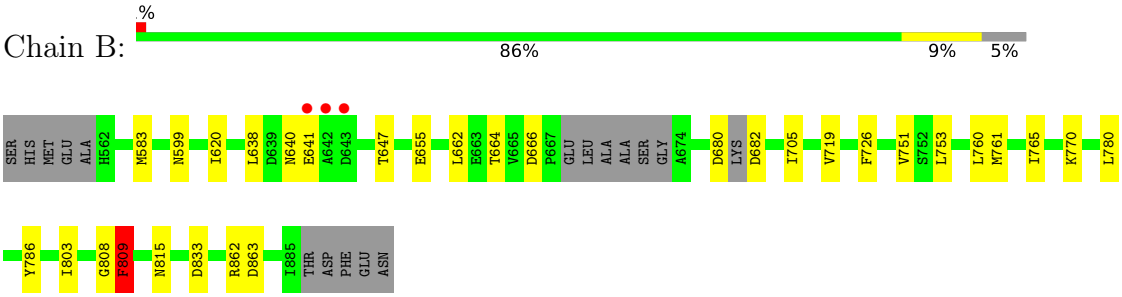
• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7

Chain A:



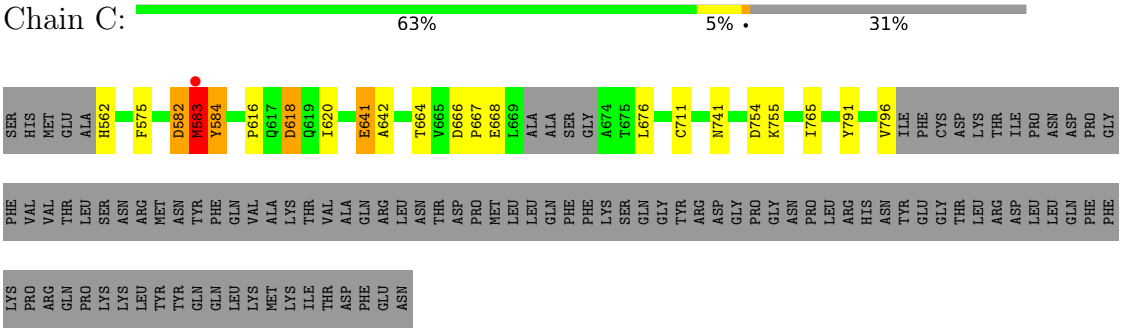
• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7

Chain B:



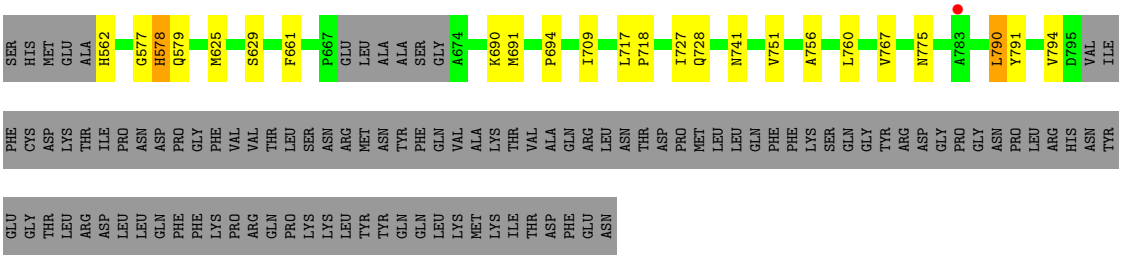
• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7

Chain C:

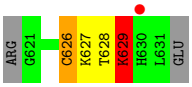


• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7

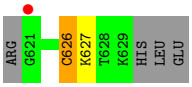
Chain D:



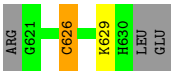
• Molecule 2: Peptide from E3 ubiquitin-protein ligase RNF169



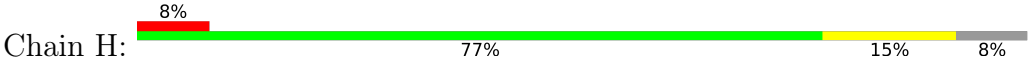
• Molecule 2: Peptide from E3 ubiquitin-protein ligase RNF169

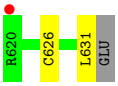


• Molecule 2: Peptide from E3 ubiquitin-protein ligase RNF169



• Molecule 2: Peptide from E3 ubiquitin-protein ligase RNF169





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	162.19Å 99.97Å 124.30Å 90.00° 95.54° 90.00°	Depositor
Resolution (Å)	46.97 – 3.11 49.98 – 3.11	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.97-3.11) 99.5 (49.98-3.11)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	50.00 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.226 , 0.268 0.228 , 0.264	Depositor DCC
R_{free} test set	1783 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	83.1	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 46.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8632	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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	0.32	0/2449	0.54	0/3343
1	B	0.31	0/2447	0.53	0/3343
1	C	0.30	0/1783	0.52	0/2438
1	D	0.29	0/1782	0.52	0/2430
2	E	0.58	0/95	0.85	0/122
2	F	0.72	0/76	0.51	0/96
2	G	0.46	0/87	0.61	0/111
2	H	0.41	0/106	0.60	0/136
All	All	0.32	0/8825	0.54	0/12019

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
2	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	629	LYS	Peptide

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	2393	0	2183	28	0
1	B	2391	0	2148	14	0
1	C	1744	0	1559	11	0
1	D	1743	0	1591	10	0
2	E	94	0	104	9	0
2	F	76	0	86	9	0
2	G	86	0	93	4	0
2	H	105	0	117	4	0
All	All	8632	0	7881	74	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 4.

All (74) 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:E:626:CYS:SG	2:F:626:CYS:HB2	1.97	1.04
2:E:626:CYS:HB2	2:F:626:CYS:HB3	1.36	1.04
2:G:626:CYS:HB2	2:H:626:CYS:SG	2.03	0.99
1:B:680:ASP:O	1:B:682:ASP:OD1	1.91	0.88
2:E:626:CYS:HB2	2:F:626:CYS:CB	2.12	0.79
2:E:626:CYS:CB	2:F:626:CYS:HB3	2.12	0.78
2:E:626:CYS:SG	2:F:626:CYS:CB	2.70	0.77
2:E:627:LYS:O	2:E:628:THR:OG1	2.06	0.74
2:G:626:CYS:CB	2:H:626:CYS:SG	2.84	0.64
1:B:808:GLY:HA2	1:B:809:PHE:HB2	1.81	0.62
1:A:836:LEU:HD23	1:A:881:LEU:HD22	1.82	0.62
2:E:626:CYS:CB	2:F:626:CYS:CB	2.76	0.62
1:C:583:MET:CE	1:C:765:ILE:HD11	2.30	0.60
1:C:620:ILE:HG22	1:C:664:THR:HG22	1.81	0.60
1:A:677:PRO:HB2	1:D:727:ILE:HD11	1.84	0.60
1:A:564:TYR:CE1	1:A:597:LEU:HD12	2.37	0.59
1:D:790:LEU:O	1:D:791:TYR:HB3	2.03	0.59
1:A:813:LEU:HD22	1:A:817:MET:HE1	1.84	0.58
1:A:758:ASP:OD2	2:E:629:LYS:NZ	2.29	0.57
1:B:808:GLY:HA2	1:B:809:PHE:CB	2.35	0.57
1:A:565:MET:HA	1:A:656:ASN:HD21	1.70	0.56
1:A:813:LEU:HB3	1:A:817:MET:HE2	1.87	0.56
1:A:625:MET:HE2	1:A:661:PHE:HB2	1.88	0.55
1:B:761:MET:HE3	2:F:627:LYS:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:761:MET:CE	2:F:627:LYS:HD3	2.37	0.54
2:G:626:CYS:HB2	2:H:626:CYS:HG	1.69	0.54
1:A:625:MET:CE	1:A:661:PHE:HB2	2.39	0.52
1:C:583:MET:HE2	1:C:765:ILE:HD11	1.91	0.52
1:B:705:ILE:HD12	1:B:719:VAL:HG11	1.91	0.52
1:A:803:ILE:N	1:A:804:PRO:HD3	2.26	0.51
1:C:618:ASP:N	1:C:618:ASP:OD1	2.43	0.50
1:A:666:ASP:CB	1:A:667:PRO:HD3	2.41	0.50
1:B:808:GLY:CA	1:B:809:PHE:CB	2.90	0.50
2:E:626:CYS:HG	2:F:626:CYS:HB2	1.76	0.50
1:D:625:MET:CE	1:D:661:PHE:HB2	2.42	0.49
1:B:620:ILE:HG22	1:B:664:THR:HG22	1.93	0.49
1:C:741:ASN:HB2	1:C:791:TYR:CG	2.48	0.49
1:C:666:ASP:O	1:C:668:GLU:N	2.46	0.49
1:A:872:GLN:CB	1:A:873:PRO:CA	2.91	0.48
1:D:690:LYS:HB2	1:D:767:VAL:HG22	1.94	0.48
1:D:709:ILE:HG23	1:D:760:LEU:CD2	2.43	0.48
1:A:872:GLN:CB	1:A:873:PRO:HA	2.44	0.48
1:B:815:ASN:HB3	1:B:862:ARG:CB	2.44	0.48
1:C:583:MET:O	1:C:584:TYR:CD2	2.67	0.48
2:G:626:CYS:CB	2:H:626:CYS:HG	2.27	0.47
1:A:830:LEU:O	1:A:831:ASN:CB	2.62	0.47
1:A:871:ARG:N	1:A:872:GLN:HA	2.29	0.47
1:B:780:LEU:HD22	1:B:786:TYR:HA	1.97	0.46
1:A:827:ALA:HA	1:A:837:LEU:HD11	1.97	0.46
1:A:583:MET:HE1	1:A:765:ILE:HG12	1.98	0.45
1:A:663:GLU:OE1	1:A:706:TYR:OH	2.35	0.45
1:B:726:PHE:CE1	1:B:770:LYS:HE3	2.52	0.45
1:C:582:ASP:O	1:C:583:MET:C	2.54	0.45
1:A:880:GLN:N	1:A:881:LEU:HA	2.31	0.45
1:A:577:GLY:O	1:A:579:GLN:NE2	2.50	0.45
1:A:798:PHE:CZ	1:A:826:VAL:HG21	2.51	0.45
1:A:717:LEU:N	1:A:718:PRO:CD	2.80	0.44
1:C:754:ASP:OD1	1:C:755:LYS:N	2.51	0.44
1:A:813:LEU:HB3	1:A:817:MET:CE	2.49	0.43
1:A:565:MET:HA	1:A:656:ASN:ND2	2.33	0.42
1:A:836:LEU:HD23	1:A:881:LEU:CD2	2.49	0.42
1:B:583:MET:HE1	1:B:765:ILE:HG12	2.01	0.42
1:D:625:MET:HE2	1:D:661:PHE:HB2	2.02	0.42
1:C:641:GLU:O	1:C:642:ALA:HB3	2.19	0.42
1:C:575:PHE:N	1:C:575:PHE:CD1	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:694:PRO:CB	1:D:775:ASN:HB2	2.50	0.41
1:A:666:ASP:HB3	1:A:667:PRO:HD3	2.02	0.41
1:B:803:ILE:N	1:B:803:ILE:HD12	2.36	0.41
1:A:797:ILE:HA	1:A:810:VAL:HA	2.02	0.41
1:A:741:ASN:HB2	1:A:791:TYR:CG	2.55	0.40
1:D:717:LEU:HB2	1:D:718:PRO:HD3	2.03	0.40
1:D:751:VAL:HG23	1:D:756:ALA:HB2	2.03	0.40
1:B:599:ASN:HA	1:B:647:THR:OG1	2.22	0.40
1:D:577:GLY:O	1:D:578:HIS:C	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	309/334 (92%)	279 (90%)	21 (7%)	9 (3%)	4 23
1	B	311/334 (93%)	288 (93%)	20 (6%)	3 (1%)	15 48
1	C	227/334 (68%)	210 (92%)	12 (5%)	5 (2%)	6 28
1	D	224/334 (67%)	208 (93%)	14 (6%)	2 (1%)	17 51
2	E	9/13 (69%)	7 (78%)	1 (11%)	1 (11%)	0 2
2	F	7/13 (54%)	7 (100%)	0	0	100 100
2	G	8/13 (62%)	6 (75%)	1 (12%)	1 (12%)	0 1
2	H	10/13 (77%)	8 (80%)	2 (20%)	0	100 100
All	All	1105/1388 (80%)	1013 (92%)	71 (6%)	21 (2%)	8 32

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	667	PRO

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Mol	Chain	Res	Type
1	A	642	ALA
1	A	644	GLY
1	A	872	GLN
1	C	583	MET
2	E	629	LYS
1	A	645	ASN
1	A	646	LYS
1	B	641	GLU
1	B	809	PHE
1	D	578	HIS
1	A	666	ASP
1	A	831	ASN
1	B	640	ASN
1	C	582	ASP
1	C	641	GLU
2	G	629	LYS
1	A	849	PRO
1	D	794	VAL
1	A	665	VAL
1	C	616	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	248/306 (81%)	240 (97%)	8 (3%)	39	69
1	B	240/306 (78%)	230 (96%)	10 (4%)	30	62
1	C	177/306 (58%)	170 (96%)	7 (4%)	31	64
1	D	181/306 (59%)	174 (96%)	7 (4%)	32	64
2	E	10/12 (83%)	9 (90%)	1 (10%)	7	28
2	F	8/12 (67%)	7 (88%)	1 (12%)	4	19
2	G	9/12 (75%)	8 (89%)	1 (11%)	6	24
2	H	11/12 (92%)	10 (91%)	1 (9%)	9	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	884/1272 (70%)	848 (96%)	36 (4%)	30 63

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	563	LEU
1	A	579	GLN
1	A	666	ASP
1	A	799	CYS
1	A	833	ASP
1	A	836	LEU
1	A	853	LEU
1	A	876	LEU
1	B	638	LEU
1	B	655	GLU
1	B	662	LEU
1	B	666	ASP
1	B	751	VAL
1	B	753	LEU
1	B	760	LEU
1	B	809	PHE
1	B	833	ASP
1	B	863	ASP
1	C	562	HIS
1	C	583	MET
1	C	584	TYR
1	C	618	ASP
1	C	676	LEU
1	C	711	CYS
1	C	796	VAL
1	D	562	HIS
1	D	579	GLN
1	D	629	SER
1	D	691	MET
1	D	728	GLN
1	D	741	ASN
1	D	790	LEU
2	E	626	CYS
2	F	626	CYS
2	G	626	CYS
2	H	631	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	630	HIS

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	313/334 (93%)	-0.06	4 (1%) 77 60	48, 76, 147, 170	0
1	B	317/334 (94%)	-0.15	3 (0%) 84 71	47, 76, 131, 174	0
1	C	231/334 (69%)	-0.20	1 (0%) 92 85	53, 86, 118, 138	0
1	D	228/334 (68%)	-0.16	1 (0%) 92 85	61, 86, 120, 161	0
2	E	11/13 (84%)	0.24	1 (9%) 9 3	55, 62, 86, 97	0
2	F	9/13 (69%)	0.31	1 (11%) 5 2	69, 71, 96, 104	0
2	G	10/13 (76%)	-0.06	0 100 100	68, 81, 94, 97	0
2	H	12/13 (92%)	0.30	1 (8%) 11 4	72, 85, 130, 140	0
All	All	1131/1388 (81%)	-0.12	12 (1%) 80 65	47, 81, 131, 174	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	642	ALA	5.8
1	B	643	ASP	5.1
1	A	850	GLY	4.0
2	H	620	ARG	3.4
1	A	642	ALA	3.2
1	D	783	ALA	3.1
2	F	621	GLY	2.6
1	B	641	GLU	2.4
1	A	876	LEU	2.1
1	C	583	MET	2.1
1	A	803	ILE	2.0
2	E	630	HIS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.