



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 26, 2023 – 09:28 PM EDT

PDB ID : 6CRN
Title : Structure of the USP15 deubiquitinase domain in complex with a high-affinity first-generation Ubv
Authors : Singer, A.U.; Teyra, J.; Boehmelt, G.; Lenter, M.; Sicheri, F.; Sidhu, S.S.
Deposited on : 2018-03-19
Resolution : 2.50 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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

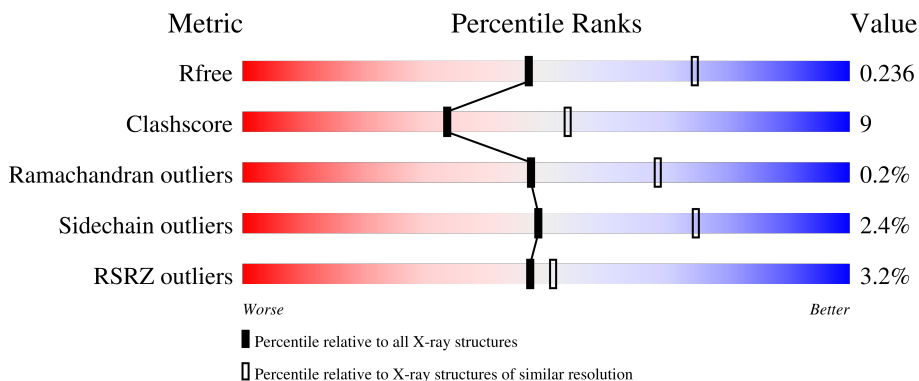
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	360	2% 80% 13% • 5%
1	B	360	% 80% 11% • 8%
1	C	360	% 78% 12% • 7%
1	D	360	2% 77% 17% • 5%
2	E	81	2% 80% 11% 9%

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Mol	Chain	Length	Quality of chain
2	F	81	
2	G	81	
2	H	81	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 13451 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 15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	343	2767	1772	462	515	18	0	2	0
1	B	332	2673	1717	445	495	16	0	1	0
1	C	334	2687	1727	449	495	16	0	1	0
1	D	343	2738	1755	454	511	18	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	270	SER	-	expression tag	UNP Q9Y4E8
A	271	GLY	-	expression tag	UNP Q9Y4E8
A	272	ALA	-	expression tag	UNP Q9Y4E8
A	273	ALA	-	expression tag	UNP Q9Y4E8
A	274	ALA	-	expression tag	UNP Q9Y4E8
A	625	SER	-	expression tag	UNP Q9Y4E8
A	626	SER	-	expression tag	UNP Q9Y4E8
A	627	GLY	-	expression tag	UNP Q9Y4E8
A	628	GLX	-	expression tag	UNP Q9Y4E8
A	629	ASN	-	expression tag	UNP Q9Y4E8
B	270	SER	-	expression tag	UNP Q9Y4E8
B	271	GLY	-	expression tag	UNP Q9Y4E8
B	272	ALA	-	expression tag	UNP Q9Y4E8
B	273	ALA	-	expression tag	UNP Q9Y4E8
B	274	ALA	-	expression tag	UNP Q9Y4E8
B	625	SER	-	expression tag	UNP Q9Y4E8
B	626	SER	-	expression tag	UNP Q9Y4E8
B	627	GLY	-	expression tag	UNP Q9Y4E8
B	628	GLX	-	expression tag	UNP Q9Y4E8
B	629	ASN	-	expression tag	UNP Q9Y4E8
C	270	SER	-	expression tag	UNP Q9Y4E8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	271	GLY	-	expression tag	UNP Q9Y4E8
C	272	ALA	-	expression tag	UNP Q9Y4E8
C	273	ALA	-	expression tag	UNP Q9Y4E8
C	274	ALA	-	expression tag	UNP Q9Y4E8
C	625	SER	-	expression tag	UNP Q9Y4E8
C	626	SER	-	expression tag	UNP Q9Y4E8
C	627	GLY	-	expression tag	UNP Q9Y4E8
C	628	GLX	-	expression tag	UNP Q9Y4E8
C	629	ASN	-	expression tag	UNP Q9Y4E8
D	270	SER	-	expression tag	UNP Q9Y4E8
D	271	GLY	-	expression tag	UNP Q9Y4E8
D	272	ALA	-	expression tag	UNP Q9Y4E8
D	273	ALA	-	expression tag	UNP Q9Y4E8
D	274	ALA	-	expression tag	UNP Q9Y4E8
D	625	SER	-	expression tag	UNP Q9Y4E8
D	626	SER	-	expression tag	UNP Q9Y4E8
D	627	GLY	-	expression tag	UNP Q9Y4E8
D	628	GLX	-	expression tag	UNP Q9Y4E8
D	629	ASN	-	expression tag	UNP Q9Y4E8

- Molecule 2 is a protein called Ubiquitin variant 15.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	74	Total	C	N	O	S	0	0	0
			581	372	94	114	1			
2	F	74	Total	C	N	O	S	0	0	0
			585	373	97	114	1			
2	G	72	Total	C	N	O	S	0	0	0
			569	364	92	112	1			
2	H	69	Total	C	N	O	S	0	0	0
			530	340	84	105	1			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Zn	0	0
			1	1		

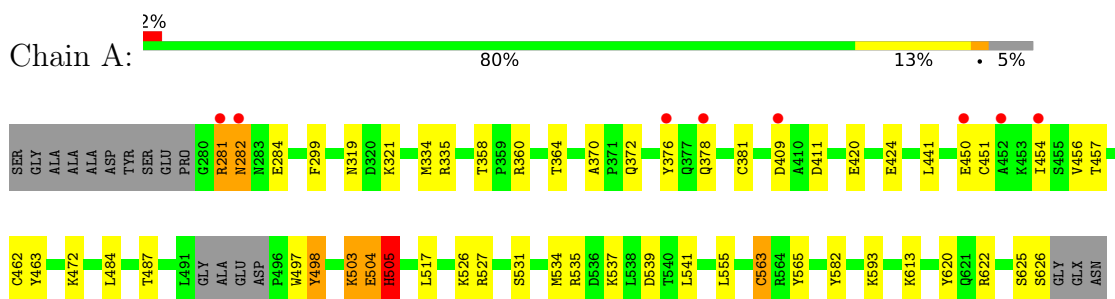
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	73	Total	O	0	0
			73	73		
4	B	82	Total	O	0	0
			82	82		
4	C	74	Total	O	0	0
			74	74		
4	D	79	Total	O	0	0
			79	79		
4	E	5	Total	O	0	0
			5	5		
4	F	3	Total	O	0	0
			3	3		
4	H	1	Total	O	0	0
			1	1		

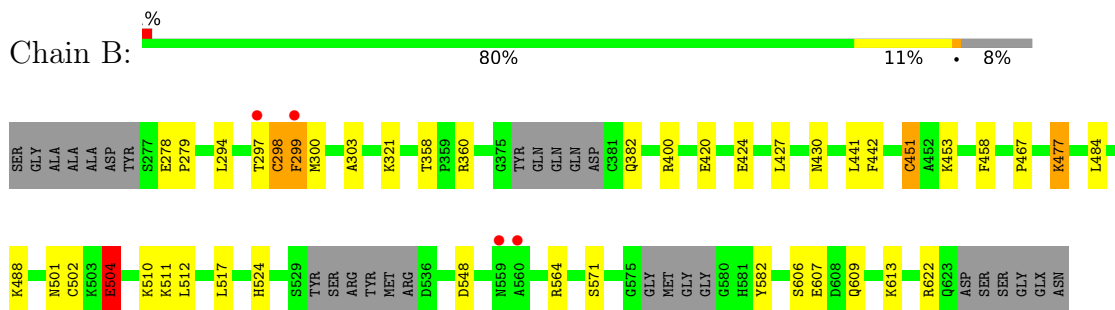
3 Residue-property plots [i](#)

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.

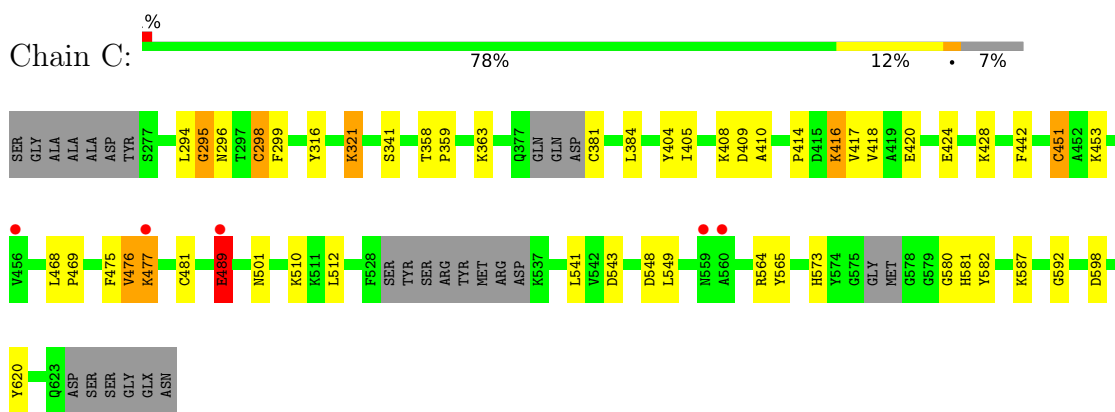
- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 15



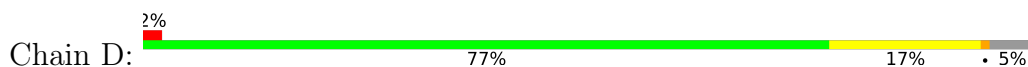
- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 15

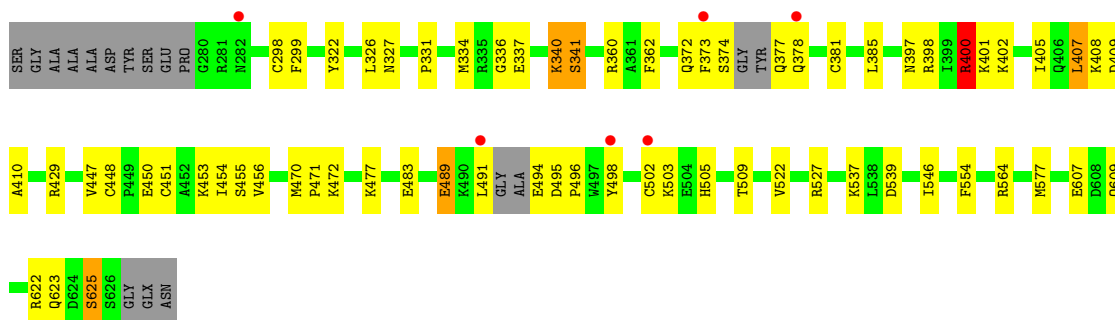


- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 15

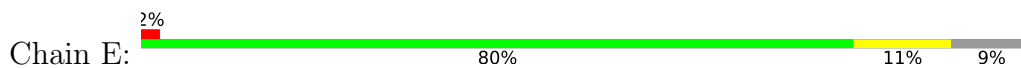


- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 15

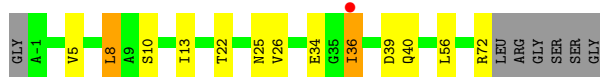
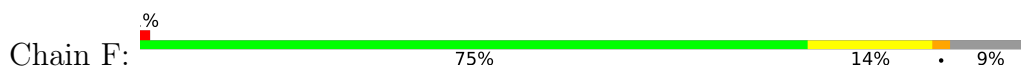




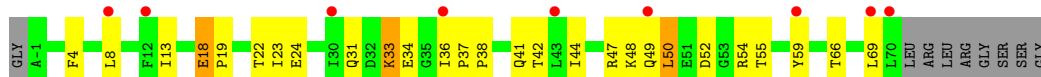
● Molecule 2: Ubiquitin variant 15.2



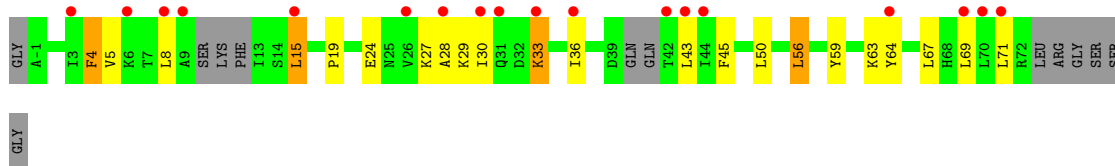
● Molecule 2: Ubiquitin variant 15.2



● Molecule 2: Ubiquitin variant 15.2



● Molecule 2: Ubiquitin variant 15.2



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	41.77Å 98.94Å 122.04Å 66.49° 88.31° 78.10°	Depositor
Resolution (Å)	111.72 – 2.50 111.72 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.8 (111.72-2.50) 92.8 (111.72-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.52Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.188 , 0.235 0.188 , 0.236	Depositor DCC
R_{free} test set	2878 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	40.6	Xtrriage
Anisotropy	0.222	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.095 for h,h-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13451	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.46	3/2840 (0.1%)	0.81	9/3847 (0.2%)
1	B	0.52	5/2742 (0.2%)	0.60	3/3713 (0.1%)
1	C	0.49	2/2757 (0.1%)	0.77	14/3732 (0.4%)
1	D	0.35	0/2809	0.65	7/3806 (0.2%)
2	E	0.31	0/589	0.56	0/795
2	F	0.32	0/593	0.65	1/800 (0.1%)
2	G	0.43	0/577	0.85	3/779 (0.4%)
2	H	0.52	0/535	0.85	3/723 (0.4%)
All	All	0.45	10/13442 (0.1%)	0.72	40/18195 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	3
1	D	0	1
All	All	0	6

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	477	LYS	CE-NZ	12.23	1.79	1.49
1	C	489	GLU	CD-OE1	10.24	1.36	1.25
1	B	477	LYS	CD-CE	10.15	1.76	1.51
1	A	335	ARG	CD-NE	10.04	1.63	1.46
1	A	335	ARG	CZ-NH2	8.38	1.44	1.33

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	ARG	NE-CZ-NH2	20.68	130.64	120.30
1	A	335	ARG	NE-CZ-NH1	-14.28	113.16	120.30
1	A	411	ASP	CB-CG-OD1	-13.71	105.96	118.30
1	C	298	CYS	CA-CB-SG	13.46	138.23	114.00
2	G	50	LEU	CB-CG-CD2	-12.07	90.47	111.00

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	281	ARG	Peptide
1	A	503	LYS	Peptide
1	C	295	GLY	Peptide
1	C	296	ASN	Peptide
1	C	489	GLU	Sidechain

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	2767	0	2670	41	0
1	B	2673	0	2605	31	0
1	C	2687	0	2621	34	0
1	D	2738	0	2640	50	0
2	E	581	0	597	8	0
2	F	585	0	598	8	0
2	G	569	0	583	34	0
2	H	530	0	534	21	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	73	0	0	3	0
4	B	82	0	0	3	0
4	C	74	0	0	1	0
4	D	79	0	0	2	0
4	E	5	0	0	0	0
4	F	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1	0	0	0	0
All	All	13451	0	12848	222	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.

The worst 5 of 222 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:477:LYS:CE	1:B:477:LYS:CD	1.76	1.55
1:B:477:LYS:CE	1:B:477:LYS:NZ	1.79	1.43
1:A:409:ASP:OD1	1:A:457:THR:HG23	1.28	1.25
1:D:451:CYS:HB3	1:D:502:CYS:SG	1.89	1.11
1:B:297:THR:OG1	4:B:801:HOH:O	1.87	0.93

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	341/360 (95%)	332 (97%)	8 (2%)	1 (0%)	41	61
1	B	325/360 (90%)	319 (98%)	6 (2%)	0	100	100
1	C	327/360 (91%)	320 (98%)	7 (2%)	0	100	100
1	D	337/360 (94%)	326 (97%)	10 (3%)	1 (0%)	41	61
2	E	72/81 (89%)	70 (97%)	2 (3%)	0	100	100
2	F	72/81 (89%)	70 (97%)	2 (3%)	0	100	100
2	G	70/81 (86%)	68 (97%)	2 (3%)	0	100	100
2	H	63/81 (78%)	61 (97%)	1 (2%)	1 (2%)	9	17
All	All	1607/1764 (91%)	1566 (97%)	38 (2%)	3 (0%)	47	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	505	HIS
1	D	503	LYS
2	H	33	LYS

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	303/315 (96%)	292 (96%)	11 (4%)	35 61
1	B	295/315 (94%)	290 (98%)	5 (2%)	60 82
1	C	295/315 (94%)	290 (98%)	5 (2%)	60 82
1	D	300/315 (95%)	291 (97%)	9 (3%)	41 68
2	E	65/71 (92%)	64 (98%)	1 (2%)	65 85
2	F	65/71 (92%)	64 (98%)	1 (2%)	65 85
2	G	64/71 (90%)	62 (97%)	2 (3%)	40 67
2	H	58/71 (82%)	57 (98%)	1 (2%)	60 82
All	All	1445/1544 (94%)	1410 (98%)	35 (2%)	49 74

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	577	MET
1	D	625	SER
2	G	18	GLU
1	B	299	PHE
1	B	298	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	372	GLN
1	C	283	ASN

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Mol	Chain	Res	Type
1	C	581	HIS
2	H	2	GLN
2	H	25	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	343/360 (95%)	-0.05	8 (2%) 60 63	22, 44, 92, 132	0
1	B	332/360 (92%)	-0.13	4 (1%) 79 80	19, 40, 76, 89	0
1	C	334/360 (92%)	-0.06	5 (1%) 73 75	23, 43, 80, 109	0
1	D	343/360 (95%)	0.01	6 (1%) 70 72	22, 45, 98, 198	0
2	E	74/81 (91%)	0.16	2 (2%) 54 58	41, 60, 90, 98	0
2	F	74/81 (91%)	0.00	1 (1%) 75 77	33, 61, 86, 92	0
2	G	72/81 (88%)	0.82	9 (12%) 3 3	55, 88, 129, 144	0
2	H	69/81 (85%)	1.20	18 (26%) 0 0	56, 93, 113, 120	0
All	All	1641/1764 (93%)	0.05	53 (3%) 47 51	19, 48, 97, 198	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	30	ILE	6.6
2	H	36	ILE	5.7
1	A	409	ASP	5.0
1	B	559	ASN	4.9
2	H	69	LEU	4.9

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ZN	A	700	1/1	0.59	0.14	117,117,117,117	0
3	ZN	D	701	1/1	0.85	0.21	185,185,185,185	0
3	ZN	B	701	1/1	0.92	0.13	57,57,57,57	0
3	ZN	C	701	1/1	0.93	0.15	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.