



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:50 PM GMT

PDB ID : 5EDV
Title : Structure of the HOIP-RBR/UbcH5B ubiquitin transfer complex
Authors : Lechtenberg, B.C.; Mace, P.D.; Sanishvili, R.; Riedl, S.J.
Deposited on : 2015-10-22
Resolution : 3.48 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

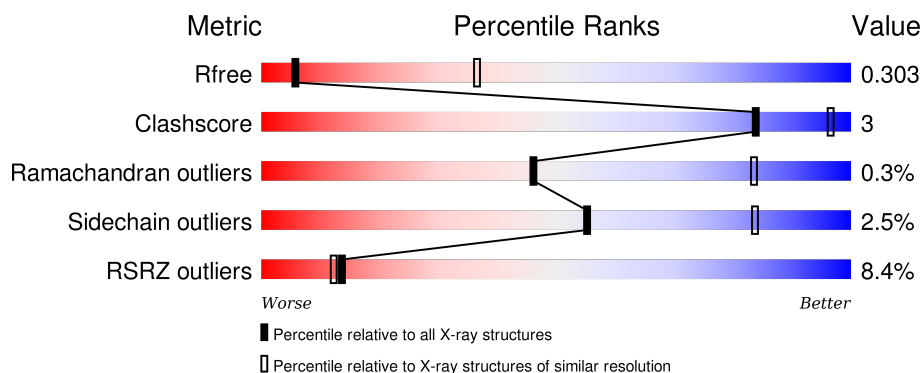
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.48 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}	91344	1173 (3.60-3.36)
Clashscore	102246	1010 (3.58-3.38)
Ramachandran outliers	100387	1245 (3.60-3.36)
Sidechain outliers	100360	1246 (3.60-3.36)
RSRZ outliers	91569	1180 (3.60-3.36)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	380	<div> <div>6%</div> <div>63% 11% 25%</div> </div>
1	B	380	<div> <div>5%</div> <div>79% 8% 12%</div> </div>
2	C	149	<div> <div>26%</div> <div>83% 14% ..</div> </div>
2	D	149	<div> <div>5%</div> <div>87% 12% ..</div> </div>
2	I	149	<div> <div>12%</div> <div>88% 11% .</div> </div>

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Mol	Chain	Length	Quality of chain
3	E	76	<div><div>%</div><div><div></div><div>95%</div><div>5%</div></div></div>
3	F	76	<div><div>4%</div><div><div></div><div>95%</div><div>5%</div></div></div>
3	G	76	<div><div>4%</div><div><div></div><div>95%</div><div>5%</div></div></div>
3	H	76	<div><div></div><div><div></div><div>95%</div><div><div></div><div>• •</div></div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10969 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 E3 ubiquitin-protein ligase RNF31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2317	1453	414	416	34			
1	B	333	Total	C	N	O	S	0	0	0
			2689	1684	479	491	35			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	693	GLY	-	expression tag	UNP Q96EP0
A	694	PRO	-	expression tag	UNP Q96EP0
A	695	GLY	-	expression tag	UNP Q96EP0
B	693	GLY	-	expression tag	UNP Q96EP0
B	694	PRO	-	expression tag	UNP Q96EP0
B	695	GLY	-	expression tag	UNP Q96EP0

- Molecule 2 is a protein called Ubiquitin-conjugating enzyme E2 D2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	145	Total	C	N	O	S	0	0	0
			1173	753	204	210	6			
2	D	148	Total	C	N	O	S	0	0	0
			1189	763	207	213	6			
2	I	147	Total	C	N	O	S	0	0	0
			1180	758	206	211	5			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP P62837
C	0	PRO	-	expression tag	UNP P62837
C	1	GLY	-	expression tag	UNP P62837
C	22	ARG	SER	engineered mutation	UNP P62837

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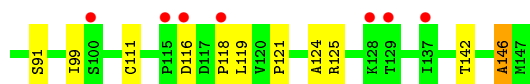
Chain	Residue	Modelled	Actual	Comment	Reference
C	85	LYS	CYS	engineered mutation	UNP P62837
D	-1	GLY	-	expression tag	UNP P62837
D	0	PRO	-	expression tag	UNP P62837
D	1	GLY	-	expression tag	UNP P62837
D	22	ARG	SER	engineered mutation	UNP P62837
D	85	LYS	CYS	engineered mutation	UNP P62837
I	-1	GLY	-	expression tag	UNP P62837
I	0	PRO	-	expression tag	UNP P62837
I	1	GLY	-	expression tag	UNP P62837
I	22	ARG	SER	engineered mutation	UNP P62837
I	85	LYS	CYS	engineered mutation	UNP P62837

- Molecule 3 is a protein called Polyubiquitin-B.

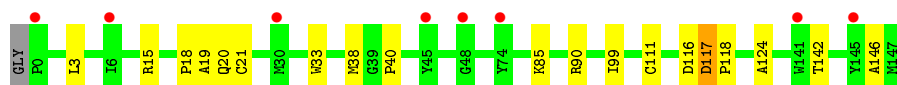
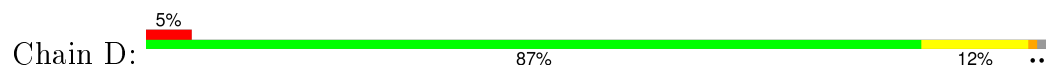
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			
3	F	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			
3	G	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			
3	H	76	Total	C	N	O	S	0	0	0
			602	378	105	118	1			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

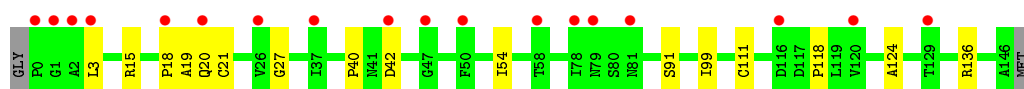
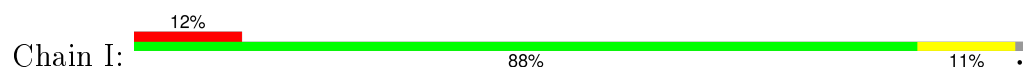
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	8	Total	Zn	0	0
			8	8		
4	A	8	Total	Zn	0	0
			8	8		



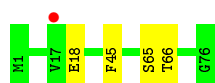
- Molecule 2: Ubiquitin-conjugating enzyme E2 D2



- Molecule 2: Ubiquitin-conjugating enzyme E2 D2



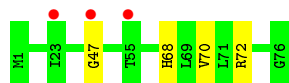
- Molecule 3: Polyubiquitin-B



- Molecule 3: Polyubiquitin-B



- Molecule 3: Polyubiquitin-B



- Molecule 3: Polyubiquitin-B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	104.82Å 75.74Å 120.96Å 90.00° 95.56° 90.00°	Depositor
Resolution (Å)	29.69 – 3.48 29.69 – 3.48	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.69-3.48) 98.8 (29.69-3.48)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.47Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.249 , 0.303 0.253 , 0.303	Depositor DCC
R_{free} test set	1213 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	162.2	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 125.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 24143 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10969	wwPDB-VP
Average B, all atoms (Å ²)	185.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.47	0/2374	0.77	4/3199 (0.1%)
1	B	0.47	0/2754	0.70	0/3714
2	C	0.51	0/1209	0.74	0/1646
2	D	0.51	0/1226	0.81	3/1669 (0.2%)
2	I	0.50	0/1217	0.77	0/1659
3	E	0.46	0/607	0.70	0/816
3	F	0.46	0/607	0.71	0/816
3	G	0.47	0/607	0.74	1/816 (0.1%)
3	H	0.45	0/608	0.82	2/816 (0.2%)
All	All	0.48	0/11209	0.75	10/15151 (0.1%)

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	B	0	1
2	C	0	1
All	All	0	4

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	90	ARG	NE-CZ-NH1	6.90	123.75	120.30
2	D	90	ARG	NE-CZ-NH2	-6.25	117.18	120.30
2	D	117	ASP	CB-CA-C	5.52	121.45	110.40
1	A	852	ASP	CB-CG-OD1	5.52	123.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	4	PHE	CB-CG-CD2	-5.33	117.07	120.80
1	A	917	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	749	ARG	NE-CZ-NH1	5.28	122.94	120.30
3	G	72	ARG	N-CA-C	-5.12	97.18	111.00
3	H	4	PHE	CB-CG-CD1	5.11	124.38	120.80
1	A	982	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	749	ARG	Peptide
1	A	754	ASP	Peptide
1	B	749	ARG	Peptide
2	C	146	ALA	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	2317	0	2198	26	1
1	B	2689	0	2544	19	0
2	C	1173	0	1162	18	1
2	D	1189	0	1180	9	0
2	I	1180	0	1171	4	2
3	E	601	0	629	2	0
3	F	601	0	629	4	0
3	G	601	0	629	3	0
3	H	602	0	629	3	0
4	A	8	0	0	0	0
4	B	8	0	0	0	0
All	All	10969	0	10771	66	3

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 3.

All (66) 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:A:932:PHE:CZ	2:C:116:ASP:O	2.36	0.78
1:B:974:GLN:OE1	3:F:72:ARG:NH1	2.23	0.71
1:A:935:ARG:HE	2:C:121:PRO:HB3	1.58	0.69
1:A:936:ASP:HB3	2:C:125:ARG:HD3	1.74	0.69
1:A:789:VAL:HG11	3:G:47:GLY:O	1.95	0.67
1:A:786:THR:HG21	3:G:68:HIS:CD2	2.32	0.63
1:B:714:LEU:HD22	1:B:744:CYS:HB2	1.81	0.63
1:B:783:LYS:O	1:B:787:GLU:HB2	2.00	0.61
1:A:717:CYS:SG	1:A:718:GLU:N	2.73	0.61
1:A:932:PHE:CE2	2:C:116:ASP:O	2.53	0.61
1:B:885:CYS:SG	2:D:85:LYS:NZ	2.65	0.61
1:A:783:LYS:O	1:A:787:GLU:HB2	2.01	0.60
1:A:932:PHE:HZ	2:C:116:ASP:O	1.81	0.60
2:C:33:TRP:CZ3	2:C:99:ILE:CD1	2.86	0.59
2:D:33:TRP:CZ3	2:D:99:ILE:CD1	2.85	0.59
1:A:885:CYS:SG	2:C:85:LYS:HD3	2.44	0.57
1:B:876:PHE:CE2	3:F:71:LEU:HD12	2.40	0.57
1:A:755:ASP:O	1:A:759:LEU:HD13	2.08	0.53
2:C:142:THR:O	2:C:146:ALA:HB3	2.08	0.53
2:D:142:THR:O	2:D:146:ALA:HB3	2.07	0.53
1:B:922:LEU:O	2:D:116:ASP:HB2	2.10	0.52
1:A:889:HIS:CG	2:C:91:SER:CB	2.93	0.52
2:D:40:PRO:HB3	2:D:111:CYS:SG	2.51	0.51
1:A:854:GLU:HA	1:A:857:ALA:HB3	1.93	0.51
2:I:40:PRO:HB3	2:I:111:CYS:SG	2.51	0.50
2:D:33:TRP:CZ3	2:D:99:ILE:HD11	2.47	0.50
2:C:40:PRO:HB3	2:C:111:CYS:SG	2.51	0.50
1:A:894:ARG:HD2	1:B:740:THR:HG21	1.92	0.50
2:D:20:GLN:HE21	2:D:38:MET:HB2	1.78	0.49
1:A:814:GLU:OE1	1:A:837:ARG:NH2	2.46	0.48
2:D:118:PRO:HB3	2:D:124:ALA:HB2	1.95	0.48
2:C:33:TRP:CZ3	2:C:99:ILE:HD11	2.47	0.48
2:I:118:PRO:HB3	2:I:124:ALA:HB2	1.94	0.48
2:C:118:PRO:HB3	2:C:124:ALA:HB2	1.95	0.47
1:A:889:HIS:CE1	2:C:91:SER:HB2	2.50	0.47
1:A:740:THR:HG21	1:B:894:ARG:HD2	1.96	0.46
1:B:765:LEU:HD22	1:B:769:LEU:HD11	1.98	0.46
1:A:765:LEU:HD22	1:A:769:LEU:HD11	1.97	0.45
1:B:790:LEU:HD21	3:H:70:VAL:HG21	1.98	0.44
1:B:804:PHE:HB2	1:B:819:GLN:OE1	2.18	0.44
2:C:18:PRO:O	2:C:19:ALA:HB3	2.18	0.44
1:A:935:ARG:NE	2:C:121:PRO:HB3	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:LEU:HD21	3:G:70:VAL:HG21	1.99	0.44
3:E:45:PHE:HE2	3:E:65:SER:HB3	1.82	0.44
2:I:18:PRO:O	2:I:19:ALA:HB3	2.17	0.44
1:B:915:ASN:HD21	1:B:1035:HIS:HB2	1.83	0.43
1:B:876:PHE:CZ	3:F:71:LEU:HD12	2.53	0.43
2:D:18:PRO:O	2:D:19:ALA:HB3	2.17	0.43
2:I:54:ILE:HG21	2:I:99:ILE:HD11	1.99	0.43
1:A:808:TYR:CE2	1:A:810:ARG:HB2	2.53	0.43
2:C:11:ASN:O	2:C:15:ARG:HG3	2.19	0.42
2:C:85:LYS:HG2	2:C:119:LEU:HD22	2.01	0.42
1:A:713:ALA:HA	1:A:718:GLU:HG2	2.01	0.42
1:B:808:TYR:CE2	1:B:810:ARG:HB2	2.55	0.41
1:A:735:LYS:O	3:F:31:GLN:NE2	2.39	0.41
1:B:743:VAL:HG12	1:B:744:CYS:N	2.35	0.41
1:B:792:ARG:C	1:B:794:PRO:HD3	2.40	0.41
1:B:793:ASP:N	1:B:794:PRO:CD	2.83	0.41
1:B:819:GLN:CD	3:H:9:THR:HG22	2.41	0.41
1:B:918:VAL:O	1:B:918:VAL:HG13	2.20	0.41
3:H:4:PHE:HB2	3:H:66:THR:HG23	2.03	0.41
1:A:918:VAL:O	1:A:918:VAL:HG13	2.21	0.41
1:A:728:GLN:O	1:A:732:ILE:HG12	2.21	0.41
2:C:60:TYR:CG	2:C:61:PRO:HA	2.55	0.41
1:A:905:PHE:C	1:A:905:PHE:CD1	2.94	0.40
3:E:18:GLU:N	3:E:18:GLU:OE1	2.54	0.40

All (3) 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:838:GLY:O	2:C:15:ARG:O[2_11511]	1.94	0.26
2:I:27:GLY:O	2:I:136:ARG:NE[2_12511]	2.01	0.19
2:I:27:GLY:O	2:I:136:ARG:CD[2_12511]	2.05	0.15

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	278/380 (73%)	253 (91%)	23 (8%)	2 (1%)	26	72
1	B	323/380 (85%)	292 (90%)	29 (9%)	2 (1%)	30	74
2	C	143/149 (96%)	139 (97%)	4 (3%)	0	100	100
2	D	146/149 (98%)	141 (97%)	5 (3%)	0	100	100
2	I	145/149 (97%)	141 (97%)	4 (3%)	0	100	100
3	E	74/76 (97%)	74 (100%)	0	0	100	100
3	F	74/76 (97%)	74 (100%)	0	0	100	100
3	G	74/76 (97%)	74 (100%)	0	0	100	100
3	H	74/76 (97%)	74 (100%)	0	0	100	100
All	All	1331/1511 (88%)	1262 (95%)	65 (5%)	4 (0%)	46	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	793	ASP
1	B	793	ASP
1	A	750	PRO
1	B	750	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	254/327 (78%)	245 (96%)	9 (4%)	43	78
1	B	293/327 (90%)	286 (98%)	7 (2%)	57	85
2	C	130/131 (99%)	128 (98%)	2 (2%)	72	90
2	D	131/131 (100%)	127 (97%)	4 (3%)	47	81
2	I	130/131 (99%)	124 (95%)	6 (5%)	33	72
3	E	68/68 (100%)	67 (98%)	1 (2%)	72	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	68/68 (100%)	67 (98%)	1 (2%)	72	90
3	G	68/68 (100%)	68 (100%)	0	100	100
3	H	68/68 (100%)	68 (100%)	0	100	100
All	All	1210/1319 (92%)	1180 (98%)	30 (2%)	55	84

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	717	CYS
1	A	725	CYS
1	A	738	HIS
1	A	758	LEU
1	A	846	ASN
1	A	851	ASN
1	A	913	GLU
1	A	932	PHE
1	A	943	GLN
1	B	708	HIS
1	B	725	CYS
1	B	738	HIS
1	B	793	ASP
1	B	846	ASN
1	B	932	PHE
1	B	1066	SER
2	C	3	LEU
2	C	21	CYS
2	D	3	LEU
2	D	15	ARG
2	D	21	CYS
2	D	117	ASP
3	E	66	THR
3	F	66	THR
2	I	3	LEU
2	I	15	ARG
2	I	20	GLN
2	I	21	CYS
2	I	42	ASP
2	I	91	SER

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

Mol	Chain	Res	Type
2	D	20	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 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 ⓘ

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	286/380 (75%)	0.36	23 (8%) 15 13	104, 183, 272, 316	0
1	B	333/380 (87%)	0.13	19 (5%) 27 23	92, 179, 254, 308	0
2	C	145/149 (97%)	1.29	39 (26%) 1 1	178, 238, 287, 328	0
2	D	148/149 (99%)	0.08	8 (5%) 29 24	125, 174, 222, 246	0
2	I	147/149 (98%)	0.77	18 (12%) 5 6	145, 188, 230, 261	0
3	E	76/76 (100%)	0.28	1 (1%) 79 71	109, 162, 200, 229	0
3	F	76/76 (100%)	0.22	3 (3%) 43 36	102, 152, 184, 187	0
3	G	76/76 (100%)	0.24	3 (3%) 43 36	142, 180, 221, 236	0
3	H	76/76 (100%)	-0.06	0 100 100	113, 152, 174, 199	0
All	All	1363/1511 (90%)	0.37	114 (8%) 14 12	92, 180, 260, 328	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	0	PRO	9.1
1	A	927	PRO	7.6
2	C	19	ALA	6.4
2	I	2	ALA	6.2
1	A	928	ARG	6.2
1	A	934	LEU	6.1
2	C	47	GLY	6.0
2	I	78	ILE	5.3
2	C	6	ILE	5.1
2	C	10	LEU	5.1
2	I	1	GLY	5.1
1	B	1015	LEU	4.7
2	C	56	PHE	4.7
2	C	49	VAL	4.6
2	C	38	MET	4.5

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Mol	Chain	Res	Type	RSRZ
2	I	3	LEU	4.5
2	C	18	PRO	4.2
1	A	933	TYR	4.1
2	I	116	ASP	4.1
2	C	20	GLN	4.0
2	C	74	TYR	4.0
1	A	937	TRP	3.8
2	C	37	ILE	3.8
2	C	35	ALA	3.8
2	C	40	PRO	3.7
2	I	58	THR	3.5
2	C	46	GLN	3.5
2	C	52	LEU	3.5
1	B	716	SER	3.4
1	A	970	ARG	3.4
2	C	42	ASP	3.4
1	A	917	ARG	3.3
2	D	30	MET	3.3
1	B	708	HIS	3.3
2	I	79	ASN	3.2
2	C	23	ALA	3.1
2	I	42	ASP	3.1
1	B	957	PRO	3.0
1	B	970	ARG	3.0
2	C	129	THR	3.0
3	F	46	ALA	3.0
2	C	45	TYR	3.0
2	I	47	GLY	2.9
2	C	75	HIS	2.9
2	I	37	ILE	2.9
1	B	1013	HIS	2.9
1	A	942	LEU	2.9
1	A	981	LEU	2.9
2	C	77	ASN	2.8
2	C	116	ASP	2.8
2	D	48	GLY	2.8
1	A	946	LEU	2.8
1	B	709	ASN	2.8
1	A	985	ALA	2.8
1	A	1010	ILE	2.8
1	A	751	ASP	2.8
2	C	33	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	48	GLY	2.7
3	G	47	GLY	2.7
1	A	915	ASN	2.7
2	C	118	PRO	2.7
2	I	129	THR	2.6
1	B	994	TYR	2.6
1	B	711	MET	2.6
2	D	45	TYR	2.5
2	I	20	GLN	2.5
2	C	21	CYS	2.5
1	B	715	THR	2.5
1	A	906	TYR	2.5
1	A	1006	LEU	2.5
2	C	17	PRO	2.5
2	I	50	PHE	2.5
2	I	81	ASN	2.5
1	B	991	PRO	2.4
1	B	992	ALA	2.4
2	C	3	LEU	2.4
3	E	17	VAL	2.4
1	B	793	ASP	2.4
1	B	1021	TYR	2.4
2	C	50	PHE	2.4
2	C	137	ILE	2.4
1	B	902	TYR	2.3
1	A	996	GLY	2.3
2	D	74	TYR	2.3
1	B	897	PHE	2.3
3	F	9	THR	2.3
2	C	128	LYS	2.3
2	I	26	VAL	2.3
2	C	72	ARG	2.3
2	C	31	PHE	2.3
1	A	897	PHE	2.3
1	A	887	HIS	2.3
1	A	750	PRO	2.2
3	G	23	ILE	2.2
2	C	30	MET	2.2
1	B	1023	VAL	2.2
2	I	120	VAL	2.2
1	A	904	ALA	2.2
3	F	45	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	930	CYS	2.2
1	B	707	PRO	2.2
2	I	18	PRO	2.2
2	C	69	PHE	2.1
2	C	60	TYR	2.1
2	D	0	PRO	2.1
2	C	100	SER	2.1
2	C	115	PRO	2.1
2	C	68	ALA	2.1
2	D	6	ILE	2.1
1	A	929	ASP	2.1
3	G	55	THR	2.0
2	D	141	TRP	2.0
1	B	710	ARG	2.0
2	D	145	TYR	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
4	ZN	A	2006	1/1	0.93	0.14	-1.00	188,188,188,188	0
4	ZN	A	2007	1/1	0.80	0.17	-1.11	195,195,195,195	0
4	ZN	B	2008	1/1	0.98	0.10	-1.27	169,169,169,169	0
4	ZN	B	2003	1/1	0.99	0.07	-1.34	105,105,105,105	0
4	ZN	B	2005	1/1	0.98	0.04	-1.40	126,126,126,126	0
4	ZN	B	2002	1/1	0.66	0.10	-1.53	187,187,187,187	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	ZN	A	2005	1/1	0.98	0.03	-1.71	146,146,146,146	0
4	ZN	A	2001	1/1	0.98	0.02	-1.77	149,149,149,149	0
4	ZN	A	2003	1/1	0.97	0.07	-1.84	114,114,114,114	0
4	ZN	B	2001	1/1	0.73	0.10	-1.90	200,200,200,200	0
4	ZN	B	2006	1/1	0.87	0.07	-1.90	140,140,140,140	0
4	ZN	A	2002	1/1	0.95	0.04	-1.94	176,176,176,176	0
4	ZN	A	2008	1/1	0.94	0.05	-2.33	185,185,185,185	0
4	ZN	B	2004	1/1	0.98	0.06	-	120,120,120,120	0
4	ZN	B	2007	1/1	0.95	0.05	-	169,169,169,169	0
4	ZN	A	2004	1/1	0.94	0.04	-	127,127,127,127	0

6.5 Other polymers [i](#)

There are no such residues in this entry.