



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 01:44 AM UTC

PDB ID : 5EDV / pdb_00005edv
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

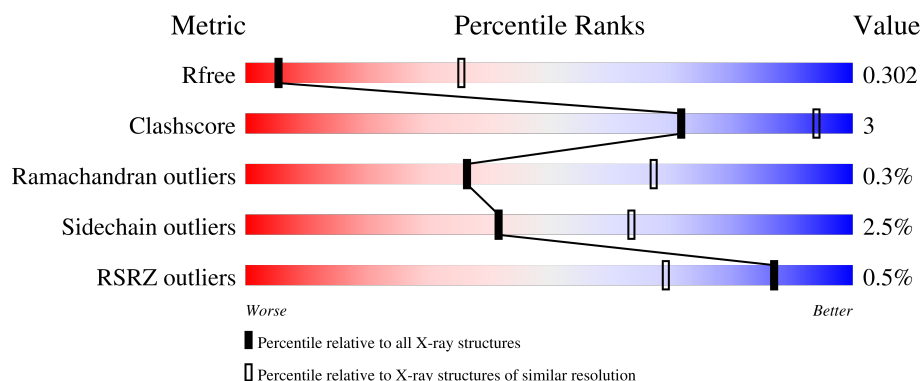
1 Overall quality at a glance

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}	180053	1083 (3.52-3.44)
Clashscore	190562	1139 (3.52-3.44)
Ramachandran outliers	187476	1111 (3.52-3.44)
Sidechain outliers	187428	1112 (3.52-3.44)
RSRZ outliers	180081	1082 (3.52-3.44)

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	380	% 63% 12% • 25%
1	B	380	78% 9% 12%
2	C	149	79% 17% ••
2	D	149	83% 15% ••
2	I	149	% 86% 12% ••

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Mol	Chain	Length	Quality of chain
3	E	76	% 93% 7%
3	F	76	% 93% 7%
3	G	76	% 93% 7%
3	H	76	% 93% 7%

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			

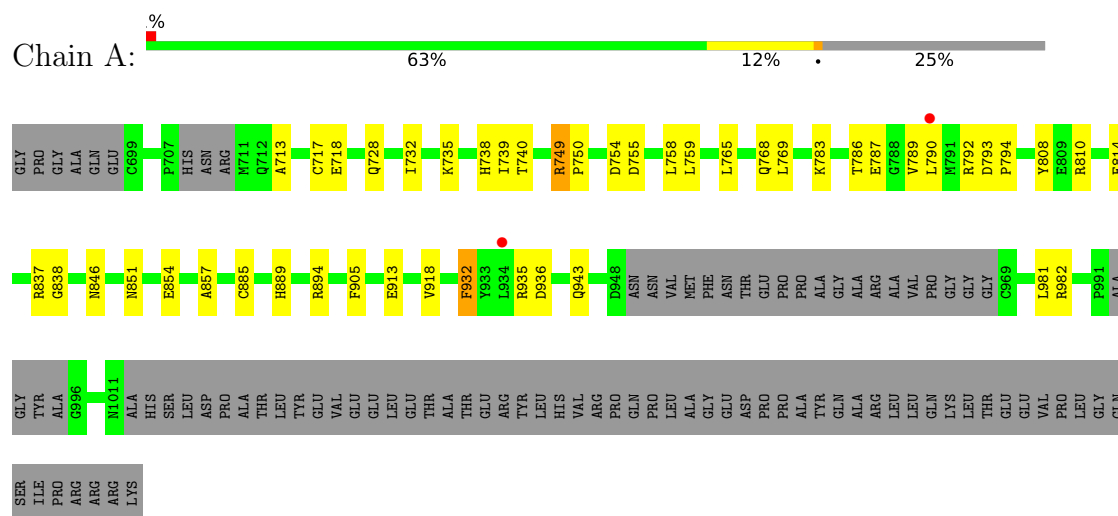
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

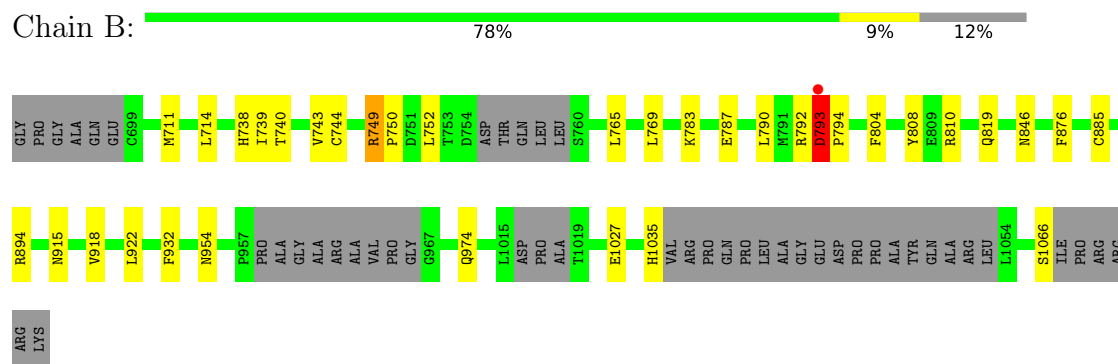
3 Residue-property plots

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.

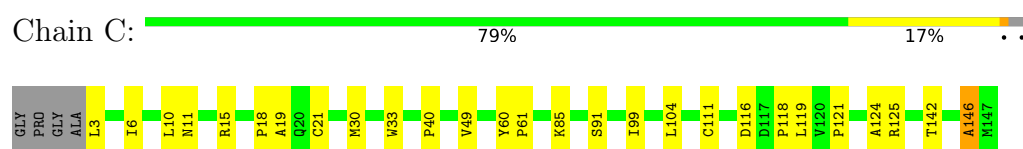
- Molecule 1: E3 ubiquitin-protein ligase RNF31



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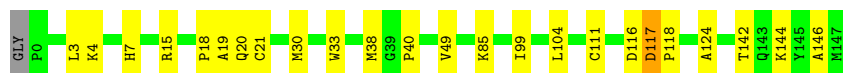


- Molecule 2: Ubiquitin-conjugating enzyme E2 D2



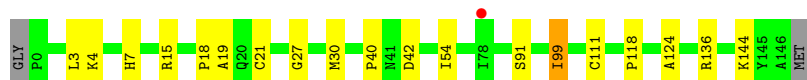
- Molecule 2: Ubiquitin-conjugating enzyme E2 D2

Chain D:  83% 15% ..

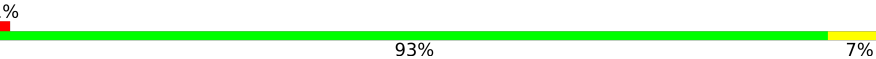


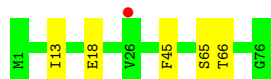
- Molecule 2: Ubiquitin-conjugating enzyme E2 D2

Chain I:  86% 12% ..

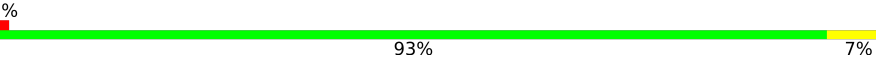


- Molecule 3: Polyubiquitin-B

Chain E:  93% 7%

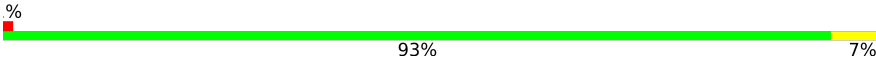


- Molecule 3: Polyubiquitin-B

Chain F:  93% 7%

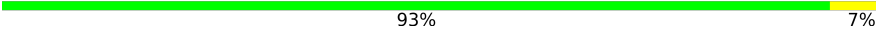


- Molecule 3: Polyubiquitin-B

Chain G:  93% 7%



- Molecule 3: Polyubiquitin-B

Chain H:  93% 7%



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) 98.5 (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 , 0.302	Depositor DCC
R_{free} test set	1213 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	162.2	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 143.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.64	0/2374	0.93	3/3199 (0.1%)
1	B	0.65	0/2754	0.94	5/3714 (0.1%)
2	C	0.74	1/1209 (0.1%)	0.89	0/1646
2	D	0.74	2/1226 (0.2%)	0.94	3/1669 (0.2%)
2	I	0.73	1/1217 (0.1%)	0.92	2/1659 (0.1%)
3	E	0.66	0/607	0.90	1/816 (0.1%)
3	F	0.65	0/607	0.90	1/816 (0.1%)
3	G	0.69	0/607	0.96	2/816 (0.2%)
3	H	0.67	0/608	0.97	1/816 (0.1%)
All	All	0.68	4/11209 (0.0%)	0.93	18/15151 (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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	49	VAL	C-O	-6.21	1.17	1.24
2	D	49	VAL	C-O	-5.78	1.17	1.24
2	I	4	LYS	C-O	-5.35	1.17	1.24
2	D	4	LYS	C-O	-5.25	1.18	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	72	ARG	N-CA-C	-7.39	97.18	109.07
1	B	752	LEU	N-CA-C	6.76	120.99	111.52
1	A	749	ARG	CB-CA-C	-6.72	101.74	111.01
2	D	117	ASP	CB-CA-C	6.61	121.45	111.14
3	H	13	ILE	CB-CA-C	-6.58	101.79	111.19
3	G	13	ILE	CB-CA-C	-6.55	101.83	111.19
3	E	13	ILE	CB-CA-C	-6.49	101.92	111.19
3	F	13	ILE	CB-CA-C	-6.46	101.96	111.19
1	A	749	ARG	N-CA-C	6.00	121.71	108.64
1	B	711	MET	N-CA-C	5.84	119.59	112.23
2	I	144	LYS	N-CA-CB	5.74	118.65	110.16
2	D	144	LYS	N-CA-CB	5.68	118.56	110.16
1	A	739	ILE	N-CA-C	5.53	116.93	110.62
1	B	749	ARG	N-CA-C	5.51	120.65	108.64
1	B	954	ASN	N-CA-C	5.35	118.04	110.50
1	B	739	ILE	N-CA-C	5.25	116.61	110.62
2	D	144	LYS	N-CA-C	5.22	117.05	111.36
2	I	144	LYS	N-CA-C	5.08	116.90	111.36

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	28	1
1	B	2689	0	2544	19	0
2	C	1173	0	1162	20	1
2	D	1189	0	1180	10	0
2	I	1180	0	1171	5	2
3	E	601	0	629	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	72	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 (72) 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
2:C:10:LEU:HD22	2:C:30:MET:HE1	1.72	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:C:40:PRO:HB3	2:C:111:CYS:SG	2.51	0.50
2:D:33:TRP:CZ3	2:D:99:ILE:HD11	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:792:ARG:C	1:B:794:PRO:HD3	2.40	0.46
1:B:819:GLN:CD	3:H:9:THR:HG22	2.41	0.45
1:A:905:PHE:CD1	1:A:905:PHE:C	2.94	0.45
1:A:765:LEU:HD22	1:A:769:LEU:HD11	1.97	0.45
2:I:7:HIS:CE1	2:I:30:MET:HE3	2.52	0.45
2:D:7:HIS:CE1	2:D:30:MET:HE3	2.51	0.44
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
1:A:935:ARG:NE	2:C:121:PRO:HB3	2.28	0.44
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
1:A:808:TYR:CE2	1:A:810:ARG:HB2	2.53	0.43
1:A:981:LEU:C	1:A:982:ARG:HG2	2.43	0.43
2:I:54:ILE:HG21	2:I:99:ILE:HD11	1.99	0.43
2:C:18:PRO:O	2:C:19:ALA:HB3	2.18	0.43
2:C:6:ILE:HG22	2:C:30:MET:HE3	2.01	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:A:735:LYS:O	3:F:31:GLN:NE2	2.39	0.41
1:B:808:TYR:CE2	1:B:810:ARG:HB2	2.55	0.41
1:B:743:VAL:HG12	1:B:744:CYS:N	2.35	0.41
1:A:792:ARG:C	1:A:794:PRO:HD3	2.44	0.41
1:B:793:ASP:N	1:B:794:PRO:CD	2.83	0.41
1:A:918:VAL:HG13	1:A:918:VAL:O	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:E:18:GLU:OE1	3:E:18:GLU:N	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	278/380 (73%)	253 (91%)	23 (8%)	2 (1%)	18	51
1	B	323/380 (85%)	292 (90%)	29 (9%)	2 (1%)	21	53
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%)	36	67

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%)	246 (97%)	8 (3%)	35	60
1	B	293/327 (90%)	287 (98%)	6 (2%)	48	66
2	C	130/131 (99%)	127 (98%)	3 (2%)	44	64
2	D	131/131 (100%)	126 (96%)	5 (4%)	29	56
2	I	130/131 (99%)	124 (95%)	6 (5%)	24	50
3	E	68/68 (100%)	67 (98%)	1 (2%)	57	71
3	F	68/68 (100%)	67 (98%)	1 (2%)	57	71
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%)	42	63

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

Mol	Chain	Res	Type
1	A	738	HIS
1	A	758	LEU
1	A	768	GLN
1	A	846	ASN
1	A	851	ASN
1	A	913	GLU
1	A	932	PHE
1	A	943	GLN
1	B	738	HIS
1	B	793	ASP
1	B	846	ASN

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Mol	Chain	Res	Type
1	B	932	PHE
1	B	1027	GLU
1	B	1066	SER
2	C	3	LEU
2	C	21	CYS
2	C	104	LEU
2	D	3	LEU
2	D	15	ARG
2	D	21	CYS
2	D	104	LEU
2	D	117	ASP
3	E	66	THR
3	F	66	THR
2	I	3	LEU
2	I	15	ARG
2	I	21	CYS
2	I	42	ASP
2	I	91	SER
2	I	99	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	768	GLN
1	A	895	HIS
1	A	943	GLN
1	A	1011	ASN
1	B	845	GLN
1	B	896	GLN
1	B	915	ASN
2	C	7	HIS
2	C	143	GLN
2	D	7	HIS
2	D	20	GLN
3	H	68	HIS
2	I	7	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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%)	-0.67	2 (0%) 84 63	104, 183, 272, 316	0
1	B	333/380 (87%)	-0.71	1 (0%) 90 77	92, 179, 254, 308	0
2	C	145/149 (97%)	-0.20	0 100 100	178, 238, 287, 328	0
2	D	148/149 (99%)	-0.82	0 100 100	125, 174, 222, 246	0
2	I	147/149 (98%)	-0.53	1 (0%) 84 63	145, 188, 230, 261	0
3	E	76/76 (100%)	-0.48	1 (1%) 75 51	109, 162, 200, 229	0
3	F	76/76 (100%)	-0.55	1 (1%) 75 51	102, 152, 184, 187	0
3	G	76/76 (100%)	-0.57	1 (1%) 75 51	142, 180, 221, 236	0
3	H	76/76 (100%)	-0.54	0 100 100	113, 152, 174, 199	0
All	All	1363/1511 (90%)	-0.60	7 (0%) 87 69	92, 180, 260, 328	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	790	LEU	3.0
3	G	44	ILE	2.8
1	A	934	LEU	2.6
2	I	78	ILE	2.4
1	B	793	ASP	2.1
3	E	26	VAL	2.0
3	F	46	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
4	ZN	B	2001	1/1	0.87	0.06	200,200,200,200	0
4	ZN	A	2006	1/1	0.90	0.07	188,188,188,188	0
4	ZN	B	2002	1/1	0.91	0.07	187,187,187,187	0
4	ZN	A	2007	1/1	0.94	0.05	195,195,195,195	0
4	ZN	A	2002	1/1	0.97	0.03	176,176,176,176	0
4	ZN	A	2008	1/1	0.97	0.03	185,185,185,185	0
4	ZN	B	2006	1/1	0.97	0.04	140,140,140,140	0
4	ZN	B	2007	1/1	0.97	0.03	169,169,169,169	0
4	ZN	B	2008	1/1	0.97	0.06	169,169,169,169	0
4	ZN	B	2004	1/1	0.99	0.02	120,120,120,120	0
4	ZN	B	2005	1/1	0.99	0.04	126,126,126,126	0
4	ZN	A	2004	1/1	0.99	0.02	127,127,127,127	0
4	ZN	A	2001	1/1	0.99	0.03	149,149,149,149	0
4	ZN	A	2003	1/1	0.99	0.03	114,114,114,114	0
4	ZN	B	2003	1/1	1.00	0.01	105,105,105,105	0
4	ZN	A	2005	1/1	1.00	0.03	146,146,146,146	0

6.5 Other polymers [i](#)

There are no such residues in this entry.