



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2021 – 05:13 PM EDT

PDB ID : 3M62
Title : Crystal structure of Ufd2 in complex with the ubiquitin-like (UBL) domain of Rad23
Authors : Haenzelmann, P.; Schindelin, H.
Deposited on : 2010-03-15
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
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) : 2.23.2

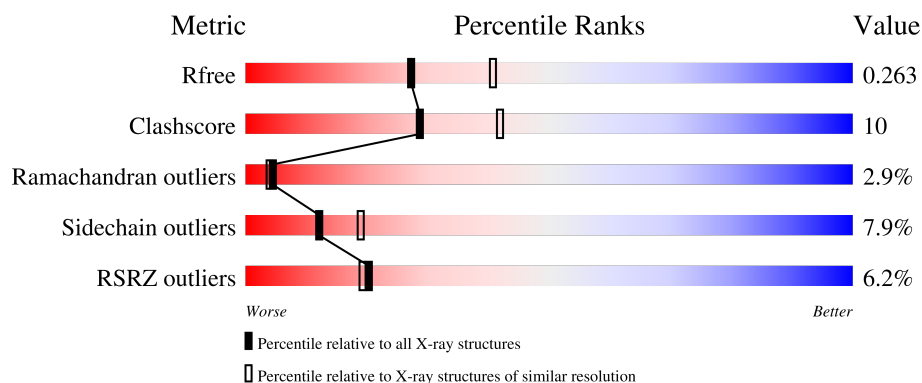
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	968	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• •</div> </div> </div>
2	B	106	<div> <div>9%</div> <div> <div></div> <div>45%</div> <div>16%</div> <div>7%</div> <div>32%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8618 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 conjugation factor E4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	955	7743	4976	1279	1459	29	0	8	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP P54860
A	-5	SER	-	expression tag	UNP P54860
A	-4	PRO	-	expression tag	UNP P54860
A	-3	GLU	-	expression tag	UNP P54860
A	-2	PHE	-	expression tag	UNP P54860
A	-1	ARG	-	expression tag	UNP P54860
A	0	SER	-	expression tag	UNP P54860
A	102	LEU	SER	engineered mutation	UNP P54860
A	677	VAL	ASP	engineered mutation	UNP P54860

- Molecule 2 is a protein called UV excision repair protein RAD23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	72	560	354	89	114	3	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

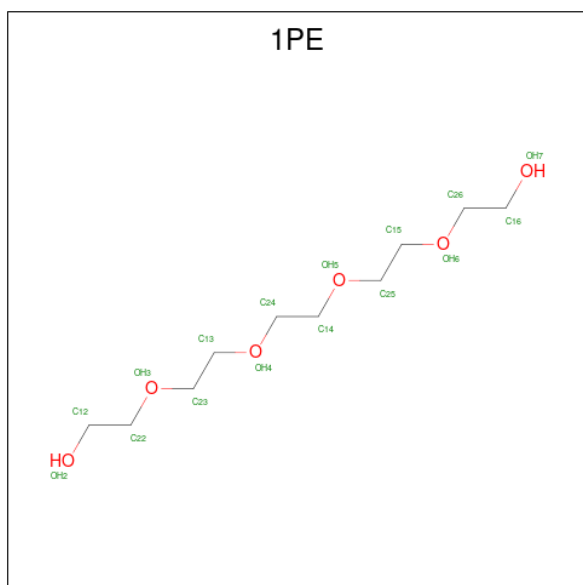
Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ARG	-	expression tag	UNP P32628
B	86	ASP	-	expression tag	UNP P32628
B	87	PRO	-	expression tag	UNP P32628
B	88	ASN	-	expression tag	UNP P32628
B	89	SER	-	expression tag	UNP P32628
B	90	SER	-	expression tag	UNP P32628
B	91	SER	-	expression tag	UNP P32628

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Chain	Residue	Modelled	Actual	Comment	Reference
B	92	VAL	-	expression tag	UNP P32628
B	93	ASP	-	expression tag	UNP P32628
B	94	LYS	-	expression tag	UNP P32628
B	95	LEU	-	expression tag	UNP P32628
B	96	ALA	-	expression tag	UNP P32628
B	97	ALA	-	expression tag	UNP P32628
B	98	ALA	-	expression tag	UNP P32628
B	99	LEU	-	expression tag	UNP P32628
B	100	GLU	-	expression tag	UNP P32628
B	101	HIS	-	expression tag	UNP P32628
B	102	HIS	-	expression tag	UNP P32628
B	103	HIS	-	expression tag	UNP P32628
B	104	HIS	-	expression tag	UNP P32628
B	105	HIS	-	expression tag	UNP P32628
B	106	HIS	-	expression tag	UNP P32628

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total K 1 1	0	0

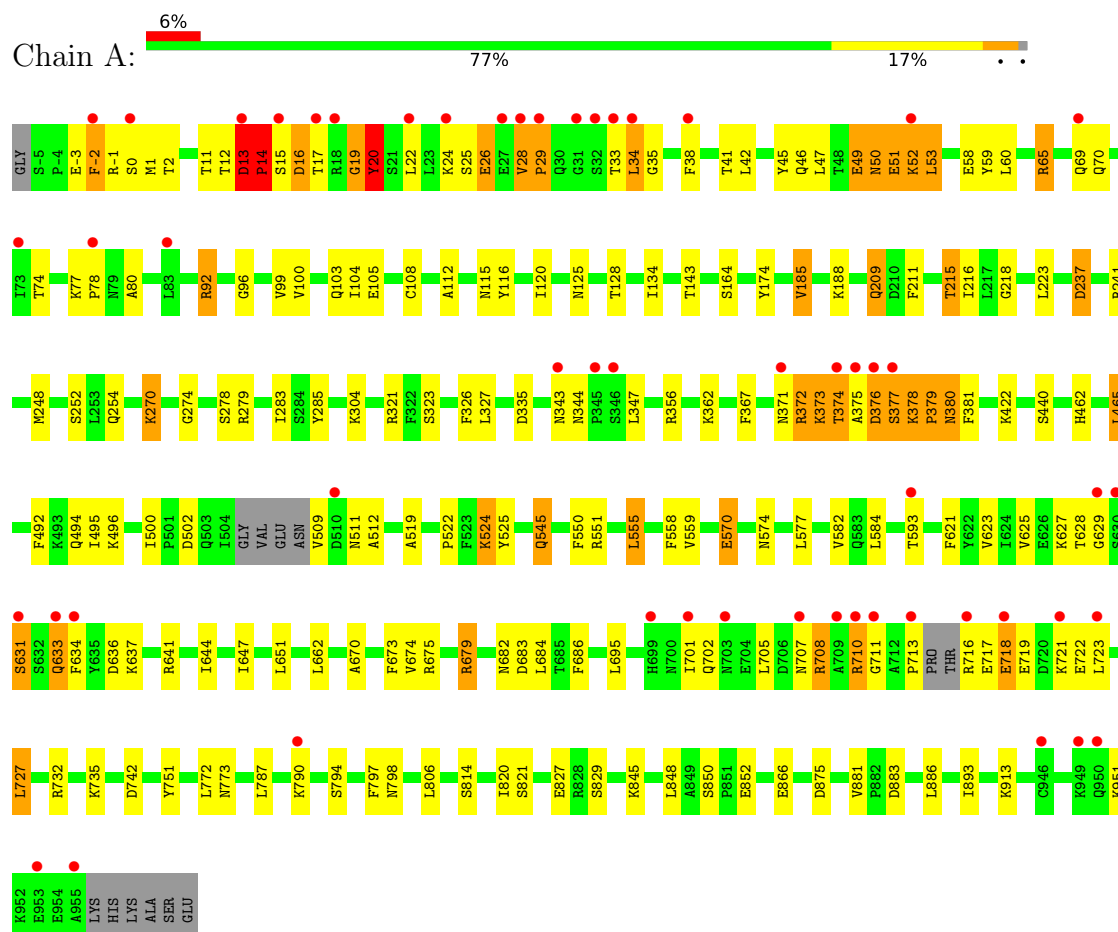
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	295	Total O 295 295	0	0
5	B	3	Total O 3 3	0	0

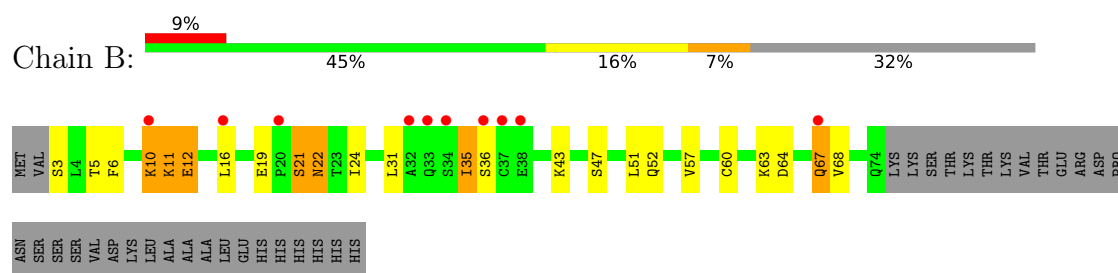
3 Residue-property plots [i](#)

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 conjugation factor E4



• Molecule 2: UV excision repair protein RAD23



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.04Å 126.55Å 180.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.22 – 2.40 44.22 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.22-2.40) 100.0 (44.22-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.200 , 0.257 0.209 , 0.263	Depositor DCC
R_{free} test set	2973 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8618	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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: K, 1PE

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	0.80	0/7938	0.82	4/10729 (0.0%)
2	B	0.61	0/565	0.65	0/757
All	All	0.79	0/8503	0.81	4/11486 (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	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	ASP	C-N-CD	-14.36	89.01	120.60
1	A	92	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	A	13	ASP	C-N-CA	7.13	151.96	122.00
1	A	92	ARG	NE-CZ-NH1	6.28	123.44	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	ASP	Peptide
1	A	14	PRO	Peptide
1	A	16	ASP	Peptide
1	A	52	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	7743	0	7740	145	0
2	B	560	0	582	17	0
3	A	16	0	21	1	0
4	A	1	0	0	0	0
5	A	295	0	0	6	0
5	B	3	0	0	1	0
All	All	8618	0	8343	161	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 10.

All (161) 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:209:GLN:NE2	1:A:209:GLN:H	1.51	1.08
1:A:209:GLN:H	1:A:209:GLN:HE21	1.05	0.99
1:A:20:TYR:H	1:A:20:TYR:HD1	1.12	0.96
1:A:494:GLN:HE21	1:A:495:ILE:H	1.16	0.92
1:A:633:GLN:H	1:A:633:GLN:HE21	1.22	0.85
1:A:662[A]:LEU:HD11	1:A:751:TYR:CZ	2.12	0.84
1:A:26:GLU:HB3	1:A:29:PRO:HD2	1.62	0.81
1:A:209:GLN:HG2	1:A:304:LYS:O	1.81	0.80
1:A:662[A]:LEU:HD11	1:A:751:TYR:CE1	2.19	0.76
1:A:24:LYS:O	1:A:45:TYR:CE1	2.41	0.74
1:A:558:PHE:HE2	1:A:584:LEU:CD2	2.01	0.74
1:A:711:GLY:HA3	1:A:713:PRO:HD3	1.70	0.74
1:A:112:ALA:H	1:A:115:ASN:HD22	1.37	0.73
2:B:11:LYS:O	2:B:12:GLU:CB	2.38	0.72
2:B:24:ILE:HD11	2:B:60:CYS:SG	2.30	0.71
1:A:46:GLN:HE21	1:A:46:GLN:HA	1.55	0.71
1:A:494:GLN:HE21	1:A:495:ILE:N	1.88	0.70
1:A:-2:PHE:O	1:A:0:SER:N	2.24	0.69
2:B:3:SER:HA	2:B:64:ASP:HB3	1.73	0.69
1:A:550:PHE:O	1:A:551:ARG:HG2	1.91	0.68
2:B:67:GLN:O	2:B:67:GLN:NE2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ASN:ND2	1:A:378:LYS:HG2	2.09	0.68
1:A:670:ALA:O	1:A:674[B]:VAL:HG13	1.94	0.67
1:A:46:GLN:HA	1:A:46:GLN:NE2	2.10	0.66
2:B:11:LYS:O	2:B:12:GLU:HB2	1.96	0.65
1:A:14:PRO:HD2	1:A:15:SER:OG	1.95	0.65
1:A:-3:GLU:HA	1:A:-3:GLU:OE1	1.96	0.65
1:A:850[A]:SER:OG	1:A:852:GLU:OE2	2.14	0.65
1:A:550:PHE:HD2	1:A:551:ARG:HH11	1.43	0.64
1:A:26:GLU:HB3	1:A:29:PRO:CD	2.27	0.64
1:A:209:GLN:NE2	1:A:209:GLN:N	2.36	0.63
1:A:662[A]:LEU:CD1	1:A:751:TYR:CE1	2.83	0.61
1:A:47:LEU:O	1:A:108:CYS:HA	2.01	0.61
1:A:881:VAL:HG21	1:A:886:LEU:HD21	1.83	0.61
1:A:51:GLU:HG2	1:A:53:LEU:H	1.66	0.60
1:A:92:ARG:NH2	2:B:47:SER:OG	2.33	0.60
1:A:379:PRO:O	1:A:380:ASN:HB3	2.01	0.60
1:A:49:GLU:O	1:A:50:ASN:HB2	2.02	0.60
2:B:35:ILE:HG22	2:B:36:SER:H	1.67	0.59
1:A:679:ARG:HH22	1:A:682[B]:ASN:HD22	1.50	0.58
1:A:209:GLN:HE21	1:A:209:GLN:N	1.88	0.58
1:A:20:TYR:HD1	1:A:20:TYR:N	1.93	0.58
2:B:24:ILE:CD1	2:B:60:CYS:SG	2.91	0.57
1:A:209:GLN:CG	1:A:304:LYS:O	2.50	0.57
1:A:679:ARG:NH2	1:A:682[B]:ASN:HD22	2.03	0.56
1:A:787:LEU:HD23	1:A:797:PHE:CE2	2.40	0.56
1:A:11:THR:HG22	1:A:12:THR:H	1.70	0.56
1:A:519:ALA:HB3	1:A:524:LYS:HE2	1.89	0.55
1:A:11:THR:CG2	1:A:14:PRO:HB2	2.37	0.55
1:A:50:ASN:O	1:A:51:GLU:OE2	2.25	0.55
1:A:14:PRO:CD	1:A:15:SER:N	2.66	0.55
1:A:633:GLN:HE21	1:A:633:GLN:N	1.99	0.54
1:A:695:LEU:HD13	1:A:787:LEU:HD21	1.89	0.54
1:A:283:ILE:HD11	1:A:381:PHE:CE1	2.43	0.54
1:A:773:ASN:HB3	1:A:829:SER:HB2	1.90	0.54
2:B:35:ILE:HG22	2:B:36:SER:N	2.22	0.54
1:A:164:SER:HB2	5:A:1043:HOH:O	2.08	0.54
1:A:99:VAL:O	1:A:103:GLN:HG3	2.07	0.53
1:A:215:THR:HG21	1:A:285:TYR:OH	2.08	0.53
1:A:356:ARG:NH1	1:A:525:TYR:O	2.41	0.53
2:B:24:ILE:HD13	2:B:51:LEU:HB3	1.90	0.53
1:A:14:PRO:HD2	1:A:15:SER:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ILE:HD12	1:A:105:GLU:H	1.74	0.52
1:A:637:LYS:O	1:A:641:ARG:HG3	2.10	0.52
2:B:52:GLN:HA	5:B:283:HOH:O	2.09	0.52
2:B:19:GLU:HG3	2:B:21:SER:HB3	1.92	0.51
1:A:188:LYS:HE3	1:A:274:GLY:HA2	1.91	0.51
1:A:628:THR:O	1:A:628:THR:HG23	2.10	0.51
1:A:215:THR:HG22	1:A:218:GLY:H	1.76	0.51
2:B:19:GLU:O	2:B:22:ASN:ND2	2.44	0.51
1:A:20:TYR:N	1:A:20:TYR:CD1	2.65	0.51
1:A:211:PHE:O	1:A:215:THR:HB	2.11	0.50
1:A:344:ASN:HB2	1:A:378:LYS:HZ3	1.77	0.50
1:A:344:ASN:HD22	1:A:378:LYS:NZ	2.09	0.50
1:A:701:ILE:HG21	1:A:727:LEU:HB2	1.92	0.50
1:A:254:GLN:HB3	1:A:462:HIS:CE1	2.47	0.50
1:A:719:GLU:CG	1:A:721:LYS:HG2	2.41	0.50
1:A:717:GLU:HG3	1:A:723:LEU:HD11	1.94	0.50
1:A:376:ASP:O	1:A:378:LYS:N	2.37	0.49
1:A:502:ASP:OD1	5:A:1044:HOH:O	2.19	0.49
1:A:707:ASN:OD1	1:A:710:ARG:HA	2.12	0.49
1:A:13:ASP:H	1:A:14:PRO:HB3	1.78	0.49
1:A:323:SER:HA	1:A:326:PHE:CZ	2.48	0.49
1:A:716:ARG:HB3	1:A:716:ARG:NH1	2.27	0.49
1:A:46:GLN:HG3	1:A:59:TYR:OH	2.12	0.48
1:A:58:GLU:N	5:A:1125:HOH:O	2.35	0.48
1:A:702:GLN:HG2	1:A:727:LEU:HD11	1.95	0.48
1:A:13:ASP:N	1:A:14:PRO:HB3	2.29	0.48
1:A:51:GLU:HG2	1:A:53:LEU:N	2.28	0.48
1:A:125:ASN:HB2	5:A:1255:HOH:O	2.13	0.48
2:B:64:ASP:OD1	2:B:64:ASP:N	2.42	0.47
1:A:343:ASN:HD21	1:A:522:PRO:HB3	1.78	0.47
1:A:574:ASN:OD1	1:A:574:ASN:C	2.52	0.47
1:A:647:ILE:O	1:A:651:LEU:HG	2.15	0.47
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.85	0.47
1:A:707:ASN:OD1	1:A:708:ARG:N	2.48	0.47
1:A:372:ARG:HB3	1:A:372:ARG:CZ	2.46	0.46
1:A:881:VAL:HG23	1:A:886:LEU:HD11	1.96	0.46
1:A:11:THR:HG22	1:A:14:PRO:HB3	1.97	0.46
1:A:550:PHE:HD2	1:A:551:ARG:NH1	2.13	0.46
1:A:24:LYS:O	1:A:45:TYR:HE1	1.96	0.46
1:A:69:GLN:NE2	1:A:69:GLN:HA	2.31	0.46
1:A:347:LEU:CD1	1:A:378:LYS:HB2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ALA:O	1:A:377:SER:N	2.47	0.46
1:A:50:ASN:HB3	1:A:51:GLU:H	1.42	0.46
1:A:662[B]:LEU:HD22	1:A:751:TYR:CE1	2.51	0.46
1:A:628:THR:HG1	1:A:631:SER:HG	1.52	0.45
1:A:623:VAL:HG11	1:A:675:ARG:NE	2.31	0.45
1:A:65:ARG:CB	1:A:65:ARG:HH11	2.29	0.45
1:A:545:GLN:HE21	1:A:545:GLN:HA	1.81	0.45
1:A:719:GLU:HG3	1:A:721:LYS:HG2	1.99	0.45
1:A:96:GLY:O	1:A:100:VAL:HG23	2.17	0.45
1:A:46:GLN:HE21	1:A:46:GLN:CA	2.27	0.44
1:A:558:PHE:CE2	1:A:584:LEU:CD2	2.91	0.44
1:A:116:TYR:O	1:A:120:ILE:HG13	2.18	0.44
1:A:143:THR:HG21	5:A:1219:HOH:O	2.17	0.44
1:A:367:PHE:O	1:A:371:ASN:HB2	2.17	0.44
1:A:422:LYS:NZ	5:A:1022:HOH:O	2.50	0.44
1:A:462:HIS:ND1	1:A:465:LEU:HD22	2.32	0.44
1:A:24:LYS:O	1:A:45:TYR:CD1	2.70	0.44
1:A:24:LYS:HA	1:A:25:SER:HA	1.77	0.44
1:A:492:PHE:CD1	3:A:962:1PE:H121	2.53	0.44
1:A:683:ASP:HA	1:A:686:PHE:CE2	2.53	0.44
1:A:237:ASP:HB3	1:A:241:ARG:HH12	1.83	0.43
1:A:662[B]:LEU:HD11	1:A:673:PHE:HE1	1.83	0.43
1:A:19:GLY:O	1:A:20:TYR:O	2.36	0.43
1:A:105:GLU:OE2	1:A:112:ALA:HB1	2.16	0.43
1:A:628:THR:OG1	1:A:631:SER:OG	2.13	0.43
1:A:99:VAL:HG22	1:A:134:ILE:HG23	2.01	0.43
1:A:462:HIS:CE1	1:A:465:LEU:HD22	2.53	0.43
1:A:814:SER:O	1:A:820:ILE:HD11	2.19	0.43
1:A:379:PRO:O	1:A:380:ASN:CB	2.64	0.43
2:B:11:LYS:O	2:B:12:GLU:HB3	2.17	0.43
1:A:500:ILE:HG12	1:A:570:GLU:OE1	2.19	0.43
1:A:38:PHE:O	1:A:42:LEU:HG	2.19	0.43
1:A:34:LEU:HB3	1:A:35:GLY:H	1.61	0.42
1:A:47:LEU:HD11	1:A:60:LEU:HD21	2.02	0.42
1:A:881:VAL:CG2	1:A:886:LEU:HD21	2.48	0.42
1:A:215:THR:CG2	1:A:285:TYR:OH	2.66	0.42
1:A:717:GLU:O	1:A:718:GLU:C	2.56	0.42
1:A:773:ASN:CB	1:A:829:SER:HB2	2.49	0.42
1:A:496:LYS:HD3	1:A:496:LYS:HA	1.85	0.42
1:A:773:ASN:HB3	1:A:829:SER:CB	2.49	0.42
1:A:11:THR:CG2	1:A:14:PRO:CB	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ARG:HB3	1:A:373:LYS:H	1.66	0.42
1:A:28:VAL:HG12	1:A:29:PRO:HD3	2.01	0.41
2:B:10:LYS:O	2:B:10:LYS:HG2	2.20	0.41
1:A:77:LYS:HB3	1:A:78:PRO:HD2	2.02	0.41
1:A:185:VAL:O	1:A:270:LYS:HG2	2.20	0.41
1:A:74:THR:HG22	1:A:80:ALA:HA	2.03	0.41
1:A:577:LEU:HD12	1:A:577:LEU:HA	1.84	0.41
1:A:621:PHE:HD2	1:A:644:ILE:HD11	1.86	0.41
2:B:6:PHE:HE2	2:B:16:LEU:HB2	1.85	0.41
1:A:372:ARG:HB3	1:A:372:ARG:NH1	2.36	0.41
1:A:772:LEU:HD22	1:A:806:LEU:HD12	2.02	0.41
1:A:372:ARG:NH1	1:A:373:LYS:H	2.19	0.40
1:A:343:ASN:HB3	1:A:371:ASN:HD22	1.86	0.40
1:A:215:THR:O	1:A:216:ILE:C	2.60	0.40
1:A:555:LEU:HD22	1:A:559:VAL:HG23	2.03	0.40
1:A:735:LYS:HE3	1:A:794:SER:O	2.21	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	957/968 (99%)	888 (93%)	43 (4%)	26 (3%)	5	5
2	B	70/106 (66%)	62 (89%)	4 (6%)	4 (6%)	1	0
All	All	1027/1074 (96%)	950 (92%)	47 (5%)	30 (3%)	4	4

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-2	PHE
1	A	-1	ARG

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Mol	Chain	Res	Type
1	A	14	PRO
1	A	17	THR
1	A	20	TYR
1	A	34	LEU
1	A	51	GLU
1	A	377	SER
1	A	379	PRO
1	A	636	ASP
1	A	718	GLU
2	B	12	GLU
1	A	19	GLY
1	A	50	ASN
1	A	629	GLY
1	A	631	SER
2	B	21	SER
1	A	237	ASP
1	A	372	ARG
1	A	373	LYS
1	A	374	THR
1	A	380	ASN
2	B	35	ILE
1	A	29	PRO
1	A	362	LYS
1	A	376	ASP
1	A	512	ALA
1	A	627	LYS
1	A	710	ARG
2	B	11	LYS

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	871/873 (100%)	805 (92%)	66 (8%)	13	20
2	B	68/99 (69%)	59 (87%)	9 (13%)	4	4
All	All	939/972 (97%)	864 (92%)	75 (8%)	12	18

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	THR
1	A	13	ASP
1	A	14	PRO
1	A	16	ASP
1	A	20	TYR
1	A	22	LEU
1	A	26	GLU
1	A	28	VAL
1	A	33	THR
1	A	41	THR
1	A	49	GLU
1	A	52	LYS
1	A	53	LEU
1	A	65	ARG
1	A	70	GLN
1	A	128	THR
1	A	174	TYR
1	A	185	VAL
1	A	209	GLN
1	A	215	THR
1	A	223	LEU
1	A	248[A]	MET
1	A	248[B]	MET
1	A	252	SER
1	A	270	LYS
1	A	278	SER
1	A	279	ARG
1	A	321	ARG
1	A	327	LEU
1	A	335	ASP
1	A	374	THR
1	A	378	LYS
1	A	440	SER
1	A	465	LEU
1	A	509	VAL
1	A	511	ASN
1	A	524	LYS
1	A	545	GLN
1	A	555	LEU
1	A	570	GLU
1	A	582	VAL

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Mol	Chain	Res	Type
1	A	593	THR
1	A	625	VAL
1	A	633	GLN
1	A	634	PHE
1	A	679	ARG
1	A	684	LEU
1	A	705	LEU
1	A	708	ARG
1	A	722	GLU
1	A	727	LEU
1	A	732	ARG
1	A	742	ASP
1	A	790	LYS
1	A	798	ASN
1	A	821	SER
1	A	827	GLU
1	A	845	LYS
1	A	848	LEU
1	A	866	GLU
1	A	875	ASP
1	A	883	ASP
1	A	893	ILE
1	A	913	LYS
1	A	951	LYS
2	B	5	THR
2	B	10	LYS
2	B	22	ASN
2	B	31	LEU
2	B	43	LYS
2	B	57	VAL
2	B	63	LYS
2	B	67	GLN
2	B	68	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	69	GLN
1	A	115	ASN
1	A	209	GLN
1	A	343	ASN

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Mol	Chain	Res	Type
1	A	344	ASN
1	A	371	ASN
1	A	380	ASN
1	A	494	GLN
1	A	511	ASN
1	A	545	GLN
1	A	576	HIS
1	A	595	ASN
1	A	633	GLN
1	A	639	ASN
1	A	665	GLN
1	A	667	GLN
1	A	669	ASN
1	A	793	GLN
2	B	22	ASN

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 ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	1PE	A	962	4	15,15,15	0.86	0	14,14,14	0.75	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1PE	A	962	4	-	4/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	962	1PE	OH4-C13-C23-OH3
3	A	962	1PE	C12-C22-OH3-C23
3	A	962	1PE	C24-C14-OH5-C25
3	A	962	1PE	C23-C13-OH4-C24

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	962	1PE	1	0

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	955/968 (98%)	0.01	54 (5%)	23 22	11, 23, 43, 79	0
2	B	72/106 (67%)	0.77	10 (13%)	2 2	14, 27, 38, 76	0
All	All	1027/1074 (95%)	0.06	64 (6%)	20 19	11, 23, 43, 79	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	375	ALA	7.3
1	A	376	ASP	6.9
2	B	36	SER	6.5
1	A	630	SER	6.4
1	A	34	LEU	5.8
1	A	24	LYS	5.0
2	B	33	GLN	4.5
1	A	955	ALA	4.4
1	A	711	GLY	4.3
1	A	28	VAL	4.2
1	A	716	ARG	4.0
2	B	37	CYS	3.9
1	A	377	SER	3.9
1	A	346	SER	3.8
1	A	710	ARG	3.7
2	B	20	PRO	3.6
1	A	634	PHE	3.6
1	A	345	PRO	3.5
1	A	32	SER	3.5
1	A	13	ASP	3.4
1	A	713	PRO	3.4
1	A	703	ASN	3.3
1	A	18	ARG	3.2
1	A	593	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	701	ILE	3.2
2	B	34	SER	3.2
1	A	629	GLY	3.1
1	A	-2	PHE	3.0
1	A	17	THR	3.0
1	A	949	LYS	2.7
2	B	32	ALA	2.6
1	A	718	GLU	2.6
1	A	73	ILE	2.6
1	A	33	THR	2.5
1	A	723	LEU	2.4
1	A	31	GLY	2.4
1	A	52	LYS	2.4
2	B	38	GLU	2.4
1	A	946	CYS	2.4
1	A	709	ALA	2.4
1	A	38	PHE	2.3
1	A	27	GLU	2.3
1	A	0	SER	2.3
1	A	69	GLN	2.3
1	A	343	ASN	2.2
1	A	22	LEU	2.2
1	A	721	LYS	2.2
1	A	631	SER	2.2
1	A	950	GLN	2.2
1	A	953	GLU	2.2
1	A	633	GLN	2.2
1	A	29	PRO	2.2
1	A	15	SER	2.1
1	A	78	PRO	2.1
1	A	510	ASP	2.1
2	B	67	GLN	2.1
1	A	790	LYS	2.1
1	A	699	HIS	2.1
1	A	374	THR	2.0
1	A	83	LEU	2.0
1	A	707	ASN	2.0
2	B	16	LEU	2.0
1	A	371	ASN	2.0
2	B	10	LYS	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](#)

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(\AA^2)	Q<0.9
3	1PE	A	962	16/16	0.90	0.13	51,55,66,67	0
4	K	A	963	1/1	0.97	0.05	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.