



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:29 AM GMT

PDB ID : 3M63
Title : Crystal structure of Ufd2 in complex with the ubiquitin-like (UBL) domain of Dsk2
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
<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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

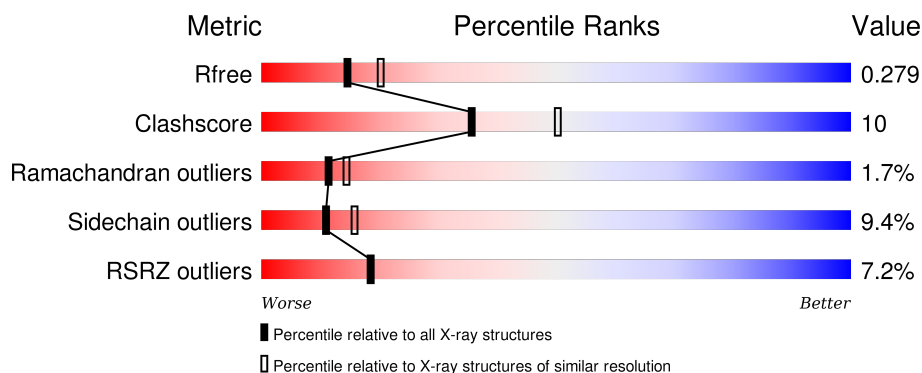
1 Overall quality at a glance

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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 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	968	<div> <div>4%</div> <div>76%</div> <div>18%</div> <div>• • •</div> </div>
2	B	101	<div> <div>37%</div> <div>43%</div> <div>21%</div> <div>8%</div> <div>29%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8488 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
1	A	953	Total	C	N	O	S	0	4	0
			7718	4959	1277	1453	29			

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	UNP P54860
A	677	VAL	ASP	ENGINEERED	UNP P54860

- Molecule 2 is a protein called Ubiquitin domain-containing protein DSK2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	72	Total	C	N	O	0	0	0
			570	359	102	109			

There are 26 discrepancies between the modelled and reference sequences:

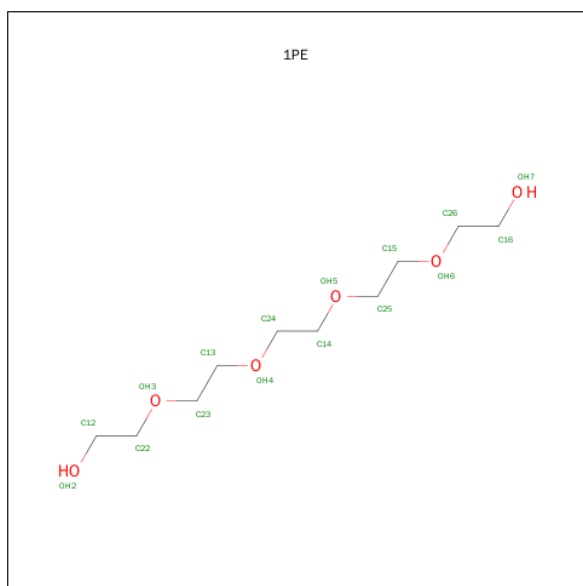
Chain	Residue	Modelled	Actual	Comment	Reference
B	-25	MET	-	EXPRESSION TAG	UNP P48510
B	-24	LYS	-	EXPRESSION TAG	UNP P48510
B	-23	HIS	-	EXPRESSION TAG	UNP P48510
B	-22	HIS	-	EXPRESSION TAG	UNP P48510
B	-21	HIS	-	EXPRESSION TAG	UNP P48510
B	-20	HIS	-	EXPRESSION TAG	UNP P48510
B	-19	HIS	-	EXPRESSION TAG	UNP P48510

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	HIS	-	EXPRESSION TAG	UNP P48510
B	-17	PRO	-	EXPRESSION TAG	UNP P48510
B	-16	MET	-	EXPRESSION TAG	UNP P48510
B	-15	SER	-	EXPRESSION TAG	UNP P48510
B	-14	ASP	-	EXPRESSION TAG	UNP P48510
B	-13	TYR	-	EXPRESSION TAG	UNP P48510
B	-12	ASP	-	EXPRESSION TAG	UNP P48510
B	-11	ILE	-	EXPRESSION TAG	UNP P48510
B	-10	PRO	-	EXPRESSION TAG	UNP P48510
B	-9	THR	-	EXPRESSION TAG	UNP P48510
B	-8	THR	-	EXPRESSION TAG	UNP P48510
B	-7	GLU	-	EXPRESSION TAG	UNP P48510
B	-6	ASN	-	EXPRESSION TAG	UNP P48510
B	-5	LEU	-	EXPRESSION TAG	UNP P48510
B	-4	TYR	-	EXPRESSION TAG	UNP P48510
B	-3	PHE	-	EXPRESSION TAG	UNP P48510
B	-2	GLN	-	EXPRESSION TAG	UNP P48510
B	-1	GLY	-	EXPRESSION TAG	UNP P48510
B	0	ALA	-	EXPRESSION TAG	UNP P48510

- 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	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	183	Total	O	0	0
			183	183		

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

Chain A:

Chain B:

37%

43%

21%

8%

29%

MET LYS HIS HIS HIS HIS HIS PRO MET SER ASP TYR ASP ASP ILE PRO THR THR GLU ASN LEU TVR PRE GLN GLY ALA MET SER L3 H4 I5 H6 I7 K8 S9 G10 Q11 D12 K13 W14 F15 V16 M17 V18 A19 P20 F21 S22 T23 V24 L25 Q26 F27 H28 E29 A30 I31 N32 K33 L34

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.13Å 125.70Å 181.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.50 – 2.40 73.50 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.3 (73.50-2.40) 98.3 (73.50-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.206 , 0.270 0.215 , 0.279	Depositor DCC
R_{free} test set	2951 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	51.6	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 58038 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8488	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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: 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	0.77	1/7895 (0.0%)	0.78	8/10668 (0.1%)
2	B	0.42	0/580	0.59	0/784
All	All	0.75	1/8475 (0.0%)	0.77	8/11452 (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	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	385	CYS	CB-SG	-5.41	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	ASP	C-N-CD	-11.02	96.37	120.60
1	A	662	LEU	CA-CB-CG	-6.50	100.35	115.30
1	A	13	ASP	C-N-CA	5.79	146.32	122.00
1	A	414	LEU	CA-CB-CG	5.45	127.84	115.30
1	A	397	LEU	CB-CG-CD1	-5.36	101.90	111.00
1	A	684	LEU	CB-CG-CD1	5.33	120.06	111.00
1	A	237	ASP	N-CA-CB	-5.17	101.29	110.60
1	A	210	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	ASP	Peptide
1	A	14	PRO	Peptide
1	A	378	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	7718	0	7708	148	0
2	B	570	0	571	17	0
3	A	16	0	22	0	0
4	A	1	0	0	0	0
5	A	183	0	0	5	0
All	All	8488	0	8301	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:344:ASN:HB3	1:A:372:ARG:O	1.44	1.14
1:A:494:GLN:HE21	1:A:495:ILE:H	1.09	0.92
1:A:50:ASN:O	1:A:51:GLU:HG2	1.68	0.92
1:A:209:GLN:H	1:A:209:GLN:NE2	1.70	0.90
2:B:23:THR:HA	2:B:56:THR:HA	1.58	0.84
1:A:209:GLN:HG2	1:A:304:LYS:O	1.78	0.84
1:A:-5:SER:HB2	1:A:-2:PHE:HB2	1.61	0.82
1:A:382:ILE:HD12	1:A:382:ILE:H	1.47	0.79
1:A:209:GLN:H	1:A:209:GLN:HE21	1.29	0.79
1:A:494:GLN:HE21	1:A:495:ILE:N	1.82	0.78
1:A:117:ILE:HD13	1:A:155:LEU:HD13	1.66	0.78
1:A:104:ILE:HD11	2:B:71:VAL:HG11	1.66	0.76
1:A:429:ASP:OD1	1:A:433:ARG:NH1	2.20	0.75
2:B:20:PRO:HB2	2:B:58:GLU:HG3	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:GLY:HA3	1:A:713:PRO:HD3	1.69	0.74
1:A:112:ALA:H	1:A:115:ASN:HD22	1.32	0.73
1:A:26:GLU:HB3	1:A:29:PRO:HD2	1.71	0.73
1:A:347:LEU:CD1	1:A:378:LYS:HB3	2.19	0.72
1:A:372:ARG:O	1:A:373:LYS:HB2	1.88	0.72
1:A:11:THR:HB	1:A:14:PRO:HB2	1.71	0.71
1:A:46:GLN:O	1:A:53:LEU:HD22	1.90	0.71
1:A:378:LYS:HE3	1:A:379:PRO:HD3	1.72	0.71
1:A:695:LEU:HD13	1:A:787:LEU:HD21	1.72	0.70
1:A:33:THR:O	1:A:34:LEU:HB2	1.92	0.67
1:A:954:GLU:HG2	1:A:955:ALA:H	1.59	0.67
1:A:375:ALA:O	1:A:376:ASP:HB2	1.96	0.66
1:A:46:GLN:HA	1:A:46:GLN:NE2	2.12	0.65
1:A:704:GLU:OE2	1:A:713:PRO:HD2	1.97	0.64
1:A:46:GLN:NE2	1:A:51:GLU:OE2	2.29	0.64
1:A:344:ASN:N	1:A:344:ASN:OD1	2.30	0.64
1:A:344:ASN:CB	1:A:372:ARG:O	2.36	0.64
1:A:550:PHE:O	1:A:551:ARG:HG2	1.98	0.64
1:A:494:GLN:NE2	1:A:495:ILE:H	1.91	0.63
1:A:50:ASN:C	1:A:51:GLU:CG	2.66	0.63
1:A:46:GLN:HA	1:A:46:GLN:HE21	1.64	0.62
1:A:207:LYS:HB3	1:A:209:GLN:HE22	1.64	0.62
1:A:39:ILE:HA	1:A:42:LEU:HD12	1.82	0.62
1:A:378:LYS:HB2	1:A:379:PRO:HD3	1.82	0.62
1:A:347:LEU:HD13	1:A:378:LYS:HB3	1.81	0.61
1:A:215:THR:HG21	1:A:285:TYR:OH	2.01	0.61
1:A:938:GLU:OE1	1:A:938:GLU:HA	1.99	0.61
1:A:705:LEU:O	1:A:708:ARG:NH2	2.33	0.61
1:A:343:ASN:HD21	1:A:522:PRO:HB3	1.65	0.60
1:A:92:ARG:NH2	2:B:47:SER:OG	2.34	0.60
1:A:716:ARG:HG2	1:A:718:GLU:H	1.66	0.60
1:A:211:PHE:O	1:A:215:THR:HB	2.02	0.59
1:A:185:VAL:O	1:A:270:LYS:HG2	2.02	0.59
1:A:22:LEU:H	1:A:22:LEU:HD12	1.67	0.59
1:A:637:LYS:O	1:A:641:ARG:HG3	2.03	0.59
1:A:380:ASN:HD22	1:A:383:SER:H	1.51	0.59
1:A:50:ASN:C	1:A:51:GLU:HG2	2.23	0.58
1:A:380:ASN:ND2	1:A:383:SER:H	2.01	0.58
1:A:50:ASN:O	1:A:51:GLU:CG	2.47	0.58
1:A:881:VAL:HG11	1:A:893:ILE:HD13	1.86	0.58
1:A:489:GLU:HG2	1:A:493:LYS:HD2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:SER:O	1:A:820:ILE:HD11	2.05	0.57
1:A:117:ILE:HG12	1:A:154:THR:HG22	1.87	0.57
1:A:679:ARG:HG2	1:A:679:ARG:HH11	1.69	0.57
1:A:344:ASN:ND2	5:A:1088:HOH:O	2.38	0.55
1:A:215:THR:CG2	1:A:285:TYR:OH	2.54	0.55
1:A:382:ILE:CD1	1:A:382:ILE:H	2.19	0.55
1:A:378:LYS:HB2	1:A:379:PRO:CD	2.35	0.55
1:A:707:ASN:OD1	1:A:708:ARG:N	2.40	0.54
1:A:344:ASN:ND2	1:A:373:LYS:HD2	2.23	0.53
1:A:379:PRO:O	1:A:380:ASN:HB3	2.07	0.53
1:A:107:PHE:CD2	2:B:45:ILE:HD13	2.43	0.53
1:A:494:GLN:HA	1:A:494:GLN:NE2	2.23	0.53
1:A:371:ASN:C	1:A:372:ARG:HG3	2.29	0.53
1:A:12:THR:HG22	1:A:13:ASP:CG	2.29	0.53
1:A:12:THR:HG22	1:A:13:ASP:OD1	2.09	0.53
1:A:14:PRO:HD2	1:A:15:SER:OG	2.10	0.52
1:A:719:GLU:HG3	1:A:721:LYS:H	1.75	0.52
2:B:3:LEU:N	2:B:18:VAL:O	2.42	0.52
2:B:22:SER:OG	2:B:26:GLN:HG3	2.10	0.52
1:A:99:VAL:HG12	1:A:103:GLN:NE2	2.25	0.52
1:A:117:ILE:C	1:A:117:ILE:HD12	2.31	0.51
1:A:787:LEU:HD23	1:A:797:PHE:CE2	2.44	0.51
1:A:946:CYS:O	1:A:950:GLN:HG2	2.10	0.51
1:A:711:GLY:CA	1:A:713:PRO:HD3	2.37	0.51
1:A:898:VAL:HB	1:A:934:VAL:HG13	1.92	0.50
1:A:394:HIS:O	1:A:398:GLY:HA3	2.11	0.50
1:A:374:THR:O	1:A:377:SER:HB3	2.11	0.50
1:A:11:THR:HB	1:A:14:PRO:CB	2.40	0.50
1:A:376:ASP:O	1:A:378:LYS:HE2	2.11	0.50
1:A:605:GLU:HB2	1:A:655:ILE:HD13	1.93	0.50
1:A:105:GLU:OE2	1:A:112:ALA:HB1	2.12	0.49
1:A:378:LYS:CE	1:A:379:PRO:HD3	2.41	0.49
1:A:679:ARG:HG2	1:A:679:ARG:NH1	2.28	0.49
1:A:711:GLY:HA3	1:A:713:PRO:CD	2.42	0.49
1:A:334:ILE:HD11	1:A:479:PHE:HA	1.94	0.48
1:A:379:PRO:O	1:A:380:ASN:CB	2.60	0.48
2:B:20:PRO:O	2:B:58:GLU:HB2	2.13	0.48
2:B:32:ASN:HD22	2:B:32:ASN:C	2.17	0.48
2:B:24:VAL:HB	2:B:52:LYS:O	2.13	0.48
1:A:28:VAL:HB	1:A:29:PRO:HD3	1.96	0.48
1:A:519:ALA:HB3	1:A:524:LYS:HE2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ARG:O	1:A:20:TYR:N	2.44	0.47
1:A:14:PRO:HD3	5:A:1111:HOH:O	2.13	0.47
1:A:950:GLN:HB2	1:A:951:LYS:HZ2	1.80	0.47
1:A:181:PHE:O	1:A:185:VAL:HB	2.16	0.46
1:A:434:PHE:O	1:A:438[B]:GLN:HG2	2.14	0.46
1:A:74:THR:HG23	1:A:80:ALA:HA	1.98	0.46
1:A:647:ILE:O	1:A:651:LEU:HG	2.14	0.46
1:A:716:ARG:NH2	1:A:718:GLU:HG2	2.30	0.46
1:A:704:GLU:O	1:A:707:ASN:ND2	2.49	0.46
1:A:33:THR:HB	1:A:34:LEU:H	1.57	0.45
1:A:188:LYS:HB3	1:A:189:PRO:HD3	1.99	0.45
1:A:323:SER:HA	1:A:326:PHE:CZ	2.51	0.45
1:A:357:LEU:HD22	1:A:572:VAL:HG22	1.98	0.45
1:A:683:ASP:HA	1:A:686:PHE:CE2	2.52	0.45
1:A:156:LEU:HD12	1:A:156:LEU:HA	1.65	0.45
2:B:63:GLN:HB2	2:B:66:HIS:CG	2.52	0.45
1:A:332:LYS:NZ	5:A:1112:HOH:O	2.50	0.45
1:A:24:LYS:HA	1:A:25:SER:HA	1.72	0.45
1:A:380:ASN:HD21	1:A:382:ILE:HB	1.82	0.45
1:A:462:HIS:ND1	1:A:465:LEU:HD22	2.32	0.45
1:A:173:ILE:O	1:A:177:VAL:HG23	2.17	0.44
1:A:380:ASN:HD22	1:A:383:SER:CB	2.30	0.44
1:A:954:GLU:CG	1:A:955:ALA:H	2.29	0.44
1:A:47:LEU:O	1:A:108:CYS:HA	2.17	0.44
1:A:463:ARG:O	1:A:467:LEU:HB2	2.18	0.44
1:A:279:ARG:HG3	1:A:381:PHE:CD1	2.53	0.44
1:A:49:GLU:HG3	2:B:10:GLY:HA2	1.99	0.44
1:A:89:GLU:OE2	1:A:92:ARG:NH1	2.50	0.44
2:B:20:PRO:CB	2:B:58:GLU:HG3	2.44	0.43
1:A:415:LYS:NZ	5:A:1131:HOH:O	2.49	0.43
1:A:804:LYS:HE2	1:A:848:LEU:O	2.18	0.43
1:A:931:LEU:O	1:A:934:VAL:HB	2.19	0.43
1:A:679:ARG:NH2	1:A:682[B]:ASN:HD22	2.16	0.43
1:A:-2:PHE:O	1:A:2:THR:HG23	2.19	0.43
1:A:51:GLU:HB2	1:A:52:LYS:H	1.63	0.43
2:B:43:ARG:HD2	2:B:73:SER:HB2	1.99	0.43
1:A:117:ILE:HA	1:A:120:ILE:HD12	2.00	0.43
1:A:558:PHE:HE2	1:A:584:LEU:CD2	2.32	0.42
1:A:555:LEU:HD22	1:A:559:VAL:HG23	2.01	0.42
1:A:14:PRO:CD	5:A:1111:HOH:O	2.67	0.42
1:A:881:VAL:HG21	1:A:886:LEU:HD21	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:ASN:O	1:A:372:ARG:HG3	2.20	0.42
1:A:372:ARG:O	1:A:373:LYS:CB	2.64	0.42
1:A:633:GLN:HB2	1:A:633:GLN:HE21	1.70	0.42
1:A:380:ASN:ND2	1:A:382:ILE:HB	2.35	0.41
1:A:70:GLN:O	1:A:74:THR:HB	2.20	0.41
2:B:43:ARG:O	2:B:70:LEU:HD12	2.20	0.41
1:A:701:ILE:HG21	1:A:727:LEU:HB2	2.01	0.41
1:A:250:HIS:O	1:A:254:GLN:HG3	2.19	0.41
2:B:37:ILE:HA	2:B:38:PRO:HD3	1.87	0.41
1:A:42:LEU:O	1:A:46:GLN:HG2	2.21	0.41
1:A:675:ARG:HE	1:A:675:ARG:HB3	1.75	0.41
1:A:905:MET:HG3	1:A:924:PHE:CD1	2.55	0.41
1:A:665:GLN:NE2	1:A:669:ASN:HB3	2.35	0.41
1:A:859:ASN:ND2	1:A:863:LYS:HE2	2.36	0.41
1:A:707:ASN:O	1:A:709:ALA:N	2.52	0.41
1:A:637:LYS:HE3	1:A:638:PHE:CZ	2.56	0.41
1:A:893:ILE:H	1:A:893:ILE:HG12	1.38	0.41
1:A:712:ALA:HA	1:A:713:PRO:HD3	1.88	0.41
1:A:13:ASP:N	1:A:14:PRO:HB3	2.36	0.41
1:A:8:LEU:HB2	1:A:10:ILE:HG22	2.02	0.41
1:A:117:ILE:HD13	1:A:155:LEU:CD1	2.41	0.41
1:A:755:ILE:O	1:A:756:PRO:C	2.58	0.40
1:A:74:THR:HG21	1:A:87:PHE:HE2	1.85	0.40
2:B:25:LEU:HB2	2:B:53:ASP:O	2.22	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	949/968 (98%)	884 (93%)	48 (5%)	17 (2%)	11 13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	70/101 (69%)	59 (84%)	11 (16%)	0	100	100
All	All	1019/1069 (95%)	943 (92%)	59 (6%)	17 (2%)	11	14

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	PRO
1	A	17	THR
1	A	34	LEU
1	A	51	GLU
1	A	373	LYS
1	A	378	LYS
1	A	379	PRO
1	A	636	ASP
1	A	19	GLY
1	A	710	ARG
1	A	50	ASN
1	A	708	ARG
1	A	16	ASP
1	A	78	PRO
1	A	372	ARG
1	A	380	ASN
1	A	-4	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	864/873 (99%)	790 (91%)	74 (9%)	13	19
2	B	64/91 (70%)	51 (80%)	13 (20%)	1	1
All	All	928/964 (96%)	841 (91%)	87 (9%)	11	16

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	PHE
1	A	2	THR
1	A	9	GLN
1	A	22	LEU
1	A	26	GLU
1	A	32	SER
1	A	33	THR
1	A	34	LEU
1	A	49	GLU
1	A	51	GLU
1	A	52	LYS
1	A	65	ARG
1	A	70	GLN
1	A	73	ILE
1	A	74	THR
1	A	75	LYS
1	A	77	LYS
1	A	104	ILE
1	A	109	MET
1	A	117	ILE
1	A	163	VAL
1	A	174	TYR
1	A	185	VAL
1	A	209	GLN
1	A	215	THR
1	A	223	LEU
1	A	252	SER
1	A	258	LYS
1	A	270	LYS
1	A	279	ARG
1	A	327	LEU
1	A	344	ASN
1	A	346	SER
1	A	361	PHE
1	A	372	ARG
1	A	378	LYS
1	A	419	GLU
1	A	440	SER
1	A	465	LEU
1	A	494	GLN
1	A	511	ASN
1	A	555	LEU
1	A	570	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	595	ASN
1	A	602	ASP
1	A	633	GLN
1	A	636	ASP
1	A	662	LEU
1	A	679	ARG
1	A	684	LEU
1	A	705	LEU
1	A	708	ARG
1	A	722	GLU
1	A	726	ARG
1	A	732	ARG
1	A	742	ASP
1	A	750	ILE
1	A	770	SER
1	A	790	LYS
1	A	798	ASN
1	A	827	GLU
1	A	845	LYS
1	A	848	LEU
1	A	859	ASN
1	A	881	VAL
1	A	883	ASP
1	A	884	GLU
1	A	893	ILE
1	A	918	SER
1	A	932	GLU
1	A	934	VAL
1	A	950	GLN
1	A	951	LYS
1	A	953	GLU
2	B	9	SER
2	B	17	ASN
2	B	22	SER
2	B	26	GLN
2	B	29	GLU
2	B	32	ASN
2	B	33	LYS
2	B	35	ASN
2	B	43	ARG
2	B	47	SER
2	B	58	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	66	HIS
2	B	73	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	70	GLN
1	A	103	GLN
1	A	115	ASN
1	A	209	GLN
1	A	343	ASN
1	A	380	ASN
1	A	488	HIS
1	A	494	GLN
1	A	511	ASN
1	A	633	GLN
1	A	665	GLN
1	A	667	GLN
1	A	669	ASN
1	A	700	ASN
1	A	831	ASN
1	A	859	ASN
2	B	4	ASN
2	B	6	HIS
2	B	32	ASN
2	B	42	GLN
2	B	74	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	0.63	0	14,14,14	0.31	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	-	0/13/13/13	0/0/0/0

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	953/968 (98%)	0.21	37 (3%) 43 44	25, 38, 68, 104	0
2	B	72/101 (71%)	2.24	37 (51%) 0 0	24, 51, 66, 106	0
All	All	1025/1069 (95%)	0.36	74 (7%) 18 18	24, 38, 68, 106	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	40	ALA	6.8
2	B	14	TRP	6.7
1	A	28	VAL	6.5
2	B	29	GLU	6.0
1	A	25	SER	5.8
2	B	5	ILE	5.6
1	A	34	LEU	5.6
1	A	376	ASP	5.4
2	B	27	PHE	4.8
2	B	37	ILE	4.7
1	A	13	ASP	4.5
2	B	33	LYS	4.5
2	B	30	ALA	4.3
2	B	6	HIS	4.2
2	B	7	ILE	4.2
2	B	32	ASN	3.8
1	A	84	HIS	3.8
1	A	78	PRO	3.7
2	B	45	ILE	3.7
2	B	36	GLY	3.6
1	A	12	THR	3.5
1	A	346	SER	3.5
2	B	61	HIS	3.5
2	B	20	PRO	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	10	ILE	3.5
2	B	51	LEU	3.5
1	A	29	PRO	3.4
2	B	31	ILE	3.4
1	A	24	LYS	3.4
1	A	32	SER	3.4
1	A	716	ARG	3.4
2	B	16	VAL	3.3
2	B	72	LYS	3.3
2	B	8	LYS	3.3
2	B	28	LYS	3.2
1	A	374	THR	3.2
2	B	4	ASN	3.2
1	A	83	LEU	3.1
2	B	38	PRO	3.1
1	A	18	ARG	3.0
2	B	44	LEU	3.0
1	A	27	GLU	2.9
1	A	377	SER	2.9
2	B	3	LEU	2.8
2	B	62	ILE	2.8
1	A	22	LEU	2.8
2	B	35	ASN	2.8
1	A	955	ALA	2.8
2	B	39	VAL	2.7
2	B	24	VAL	2.7
2	B	73	SER	2.6
2	B	12	ASP	2.6
2	B	9	SER	2.5
1	A	713	PRO	2.5
2	B	70	LEU	2.5
1	A	718	GLU	2.5
1	A	11	THR	2.5
1	A	107	PHE	2.4
1	A	23	LEU	2.4
2	B	66	HIS	2.4
1	A	-1	ARG	2.3
2	B	17	ASN	2.3
1	A	632	SER	2.3
1	A	38	PHE	2.3
1	A	345	PRO	2.3
2	B	63	GLN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	36	VAL	2.3
1	A	-2	PHE	2.2
1	A	33	THR	2.1
2	B	64	ASP	2.1
1	A	945	LEU	2.1
1	A	-4	PRO	2.1
1	A	326	PHE	2.1
1	A	86	THR	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(Å ²)	Q<0.9
3	1PE	A	962	16/16	0.90	0.16	0.51	73,77,82,84	0
4	K	A	963	1/1	0.97	0.12	-	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.