



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2021 – 05:03 pm BST

PDB ID : 6Z49
Title : Crystal structure of deubiquitinase Mindy2
Authors : Abdul Rehman, S.A.; Kulathu, Y.
Deposited on : 2020-05-23
Resolution : 2.00 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)
Xtrriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

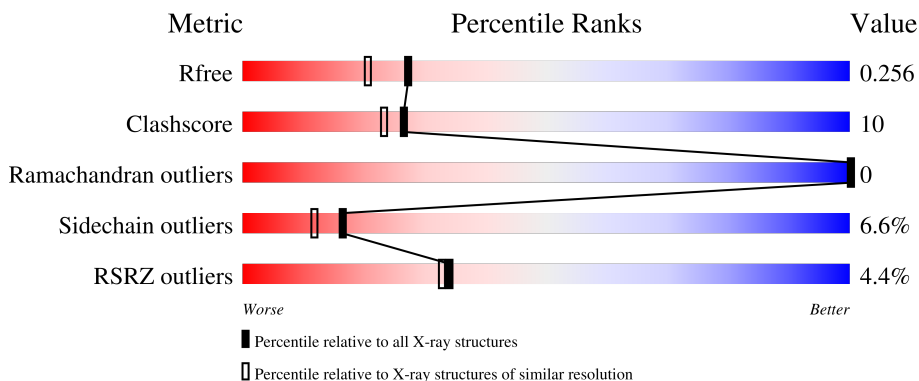
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	273	 8% 74% 16% • 8%
1	B	273	 0% 78% 14% • 7%
1	C	273	 8% 74% 17% • 5%
1	D	273	 6% 73% 16% • 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PEG	D	603	-	-	X	-
4	PG4	B	605	-	-	X	-

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 7949 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ubiquitin carboxyl-terminal hydrolase MINDY-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	252	1955	1256	316	370	13	0	0	0
1	B	254	1993	1284	319	377	13	0	0	0
1	C	258	1990	1279	325	372	14	0	0	0
1	D	243	1856	1197	305	342	12	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	GLY	-	expression tag	UNP Q8NBR6
A	233	PRO	-	expression tag	UNP Q8NBR6
A	234	LEU	-	expression tag	UNP Q8NBR6
A	235	GLY	-	expression tag	UNP Q8NBR6
A	236	SER	-	expression tag	UNP Q8NBR6
A	237	PRO	-	expression tag	UNP Q8NBR6
A	238	GLU	-	expression tag	UNP Q8NBR6
A	239	PHE	-	expression tag	UNP Q8NBR6
A	240	MET	-	expression tag	UNP Q8NBR6
B	232	GLY	-	expression tag	UNP Q8NBR6
B	233	PRO	-	expression tag	UNP Q8NBR6
B	234	LEU	-	expression tag	UNP Q8NBR6
B	235	GLY	-	expression tag	UNP Q8NBR6
B	236	SER	-	expression tag	UNP Q8NBR6
B	237	PRO	-	expression tag	UNP Q8NBR6
B	238	GLU	-	expression tag	UNP Q8NBR6
B	239	PHE	-	expression tag	UNP Q8NBR6
B	240	MET	-	expression tag	UNP Q8NBR6
C	232	GLY	-	expression tag	UNP Q8NBR6
C	233	PRO	-	expression tag	UNP Q8NBR6
C	234	LEU	-	expression tag	UNP Q8NBR6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	235	GLY	-	expression tag	UNP Q8NBR6
C	236	SER	-	expression tag	UNP Q8NBR6
C	237	PRO	-	expression tag	UNP Q8NBR6
C	238	GLU	-	expression tag	UNP Q8NBR6
C	239	PHE	-	expression tag	UNP Q8NBR6
C	240	MET	-	expression tag	UNP Q8NBR6
D	232	GLY	-	expression tag	UNP Q8NBR6
D	233	PRO	-	expression tag	UNP Q8NBR6
D	234	LEU	-	expression tag	UNP Q8NBR6
D	235	GLY	-	expression tag	UNP Q8NBR6
D	236	SER	-	expression tag	UNP Q8NBR6
D	237	PRO	-	expression tag	UNP Q8NBR6
D	238	GLU	-	expression tag	UNP Q8NBR6
D	239	PHE	-	expression tag	UNP Q8NBR6
D	240	MET	-	expression tag	UNP Q8NBR6

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

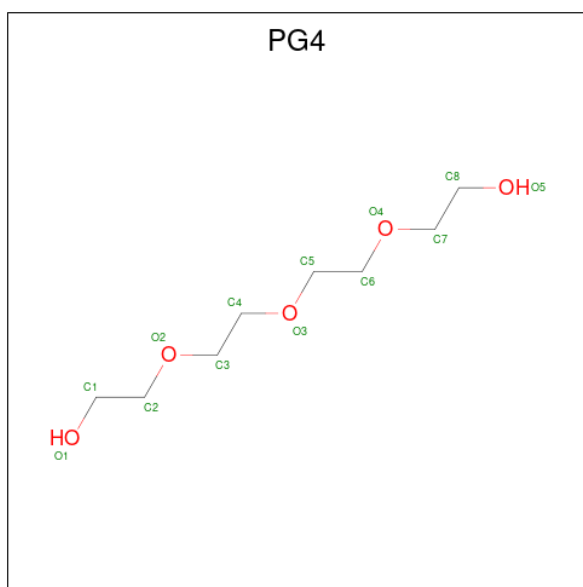
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	3	Total Cl 3 3	0	0
2	C	1	Total Cl 1 1	0	0
2	D	2	Total Cl 2 2	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	8	5		

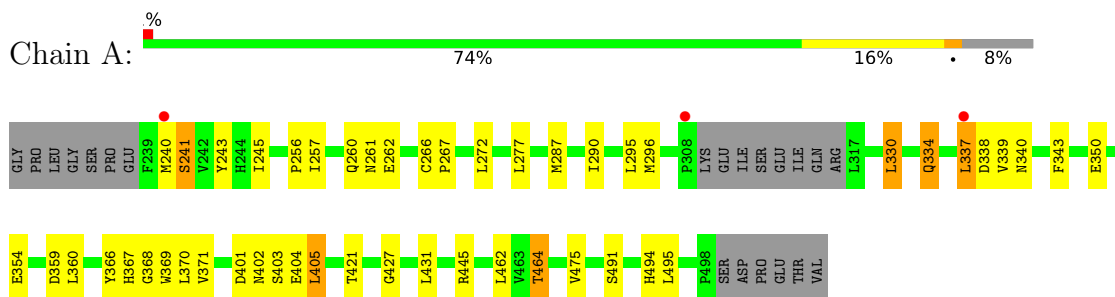
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	35	Total O 35 35	0	0
5	B	42	Total O 42 42	0	0
5	C	20	Total O 20 20	0	0
5	D	17	Total O 17 17	0	0

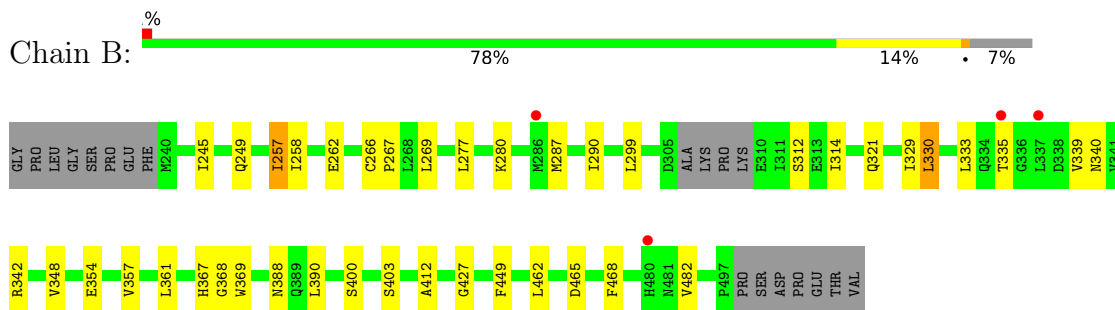
3 Residue-property plots [i](#)

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.

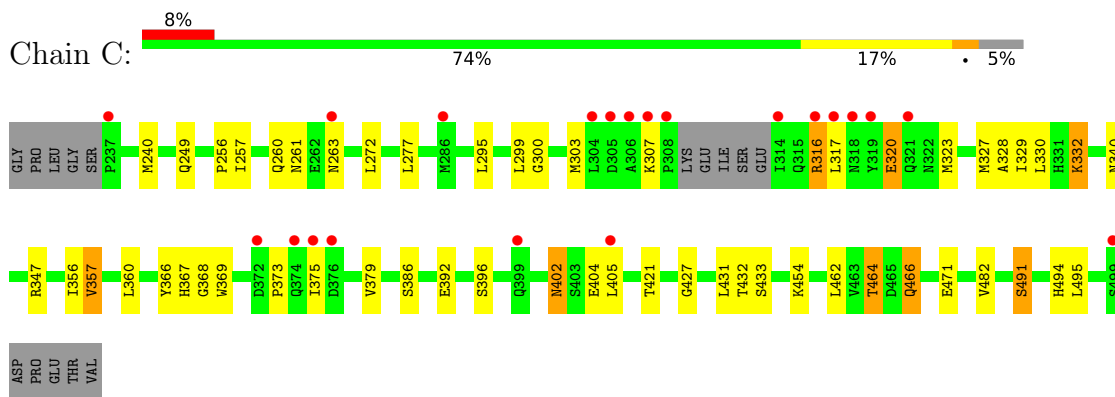
- Molecule 1: Ubiquitin carboxyl-terminal hydrolase MINDY-2



- Molecule 1: Ubiquitin carboxyl-terminal hydrolase MINDY-2

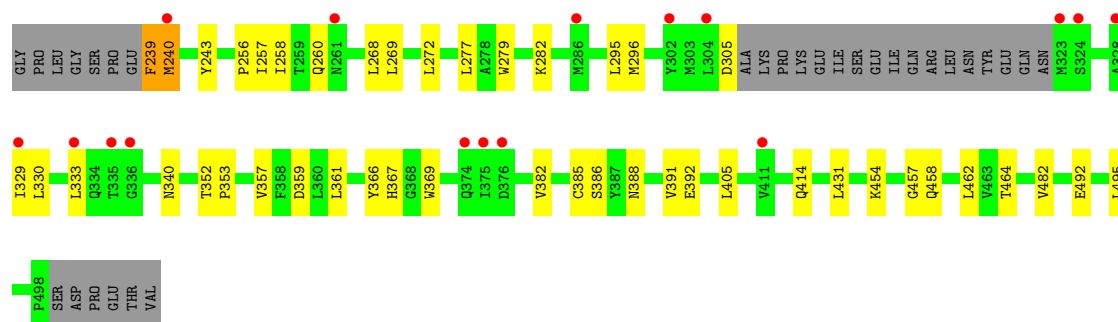


- Molecule 1: Ubiquitin carboxyl-terminal hydrolase MINDY-2



- Molecule 1: Ubiquitin carboxyl-terminal hydrolase MINDY-2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.11Å 120.42Å 78.38Å 90.00° 92.94° 90.00°	Depositor
Resolution (Å)	47.72 – 2.00 47.72 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.72-2.00) 99.6 (47.72-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.215 , 0.251 0.227 , 0.256	Depositor DCC
R_{free} test set	4169 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtrriage
Anisotropy	0.574	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7949	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.4502e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, CL, PG4

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	0.71	0/1999	0.83	0/2725
1	B	0.71	0/2038	0.83	0/2776
1	C	0.73	0/2035	0.82	0/2774
1	D	0.72	0/1899	0.81	0/2589
All	All	0.72	0/7971	0.82	0/10864

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1955	0	1828	35	0
1	B	1993	0	1893	51	0
1	C	1990	0	1870	42	0
1	D	1856	0	1728	30	0
2	A	1	0	0	0	0
2	B	3	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
3	A	7	0	10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	7	0	10	0	0
3	D	7	0	10	5	0
4	B	13	0	18	10	0
5	A	35	0	0	0	0
5	B	42	0	0	1	0
5	C	20	0	0	0	0
5	D	17	0	0	0	0
All	All	7949	0	7367	157	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 (157) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:LYS:NZ	4:B:605:PG4:H11	1.71	1.05
1:D:282:LYS:HE2	3:D:603:PEG:H22	1.38	1.01
1:A:421:THR:HG22	1:A:445:ARG:HH21	1.25	0.99
1:A:421:THR:CG2	1:A:445:ARG:HH21	1.75	0.99
1:B:287:MET:HE3	1:B:290:ILE:HB	1.45	0.98
1:B:333:LEU:HD11	1:B:357:VAL:HG21	1.51	0.92
1:D:282:LYS:CE	3:D:603:PEG:H22	2.01	0.90
1:B:287:MET:HE1	1:B:290:ILE:HD12	1.53	0.89
1:B:299:LEU:HB3	1:B:330:LEU:HD21	1.58	0.84
1:B:340:ASN:HD21	1:B:388:ASN:H	1.21	0.83
1:B:367:HIS:HD2	1:B:369:TRP:H	1.26	0.83
1:B:287:MET:CE	1:B:290:ILE:HD12	2.12	0.78
1:B:257:ILE:HG12	1:B:462:LEU:HD21	1.67	0.77
1:B:280:LYS:HE3	4:B:605:PG4:H72	1.67	0.77
1:C:272:LEU:CD2	1:C:295:LEU:HD22	2.17	0.75
1:A:421:THR:CG2	1:A:445:ARG:NH2	2.49	0.74
1:B:280:LYS:HZ1	4:B:605:PG4:H11	1.52	0.73
1:B:314:ILE:H	1:B:314:ILE:HD12	1.54	0.73
1:B:280:LYS:NZ	4:B:605:PG4:C1	2.53	0.70
1:C:260:GLN:OE1	1:C:464:THR:HG22	1.92	0.70
1:B:340:ASN:ND2	1:B:388:ASN:H	1.90	0.69
1:C:307:LYS:HE2	1:C:317:LEU:O	1.93	0.69
1:C:367:HIS:HD2	1:C:369:TRP:H	1.42	0.68
1:B:245:ILE:CD1	1:B:287:MET:HE2	2.24	0.68
1:A:257:ILE:HD11	1:A:277:LEU:HD21	1.78	0.66
1:B:340:ASN:HD21	1:B:388:ASN:N	1.94	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:PRO:O	1:C:257:ILE:HD12	1.97	0.64
1:C:257:ILE:HD11	1:C:277:LEU:HD21	1.80	0.64
1:B:465:ASP:HB3	1:B:468:PHE:HD2	1.63	0.64
1:D:279:TRP:CD2	3:D:603:PEG:H32	2.33	0.64
1:A:337:LEU:HD12	1:A:339:VAL:HG23	1.81	0.63
1:B:367:HIS:CD2	1:B:369:TRP:H	2.11	0.63
1:A:367:HIS:HD2	1:A:369:TRP:H	1.47	0.62
1:C:272:LEU:HD22	1:C:295:LEU:HD22	1.81	0.62
1:C:320:GLU:HB3	1:C:323:MET:HB3	1.80	0.62
1:C:257:ILE:HD11	1:C:277:LEU:CD2	2.30	0.61
1:D:282:LYS:HE2	3:D:603:PEG:C2	2.23	0.61
1:B:245:ILE:HD13	1:B:287:MET:HE2	1.84	0.60
1:B:245:ILE:HD11	1:B:287:MET:CE	2.31	0.60
1:B:257:ILE:HD11	1:B:277:LEU:HD21	1.82	0.60
1:C:316:ARG:NH2	1:C:316:ARG:HG2	2.16	0.59
1:C:329:ILE:HG21	1:C:357:VAL:CG2	2.32	0.59
1:B:280:LYS:CE	4:B:605:PG4:H72	2.32	0.59
1:B:465:ASP:HB3	1:B:468:PHE:CD2	2.38	0.58
1:A:245:ILE:HD12	1:A:287:MET:HG2	1.86	0.58
1:C:261:ASN:O	1:C:263:ASN:O	2.21	0.57
1:D:260:GLN:HG2	1:D:464:THR:O	2.03	0.57
1:D:367:HIS:HD2	1:D:369:TRP:H	1.52	0.57
1:B:280:LYS:HZ3	4:B:605:PG4:C1	2.19	0.56
1:A:337:LEU:HD11	1:A:354:GLU:HG2	1.86	0.55
1:B:245:ILE:HD11	1:B:287:MET:HE3	1.88	0.55
1:C:332:LYS:HE3	1:D:392:GLU:HG2	1.89	0.55
1:C:366:TYR:HB3	1:C:431:LEU:HD11	1.87	0.55
1:B:329:ILE:CG2	1:B:357:VAL:HG22	2.36	0.55
1:A:402:ASN:HD22	1:A:405:LEU:H	1.55	0.55
1:A:494:HIS:CE1	1:C:494:HIS:CE1	2.95	0.55
1:D:240:MET:O	1:D:240:MET:HG2	2.06	0.55
1:C:299:LEU:HD23	1:C:330:LEU:HD13	1.89	0.55
1:C:316:ARG:HG2	1:C:316:ARG:HH21	1.70	0.55
1:A:340:ASN:HD22	1:A:350:GLU:CD	2.11	0.54
1:B:257:ILE:CG1	1:B:462:LEU:HD21	2.36	0.54
1:B:257:ILE:HD11	1:B:277:LEU:CD2	2.38	0.54
1:D:243:TYR:HB3	1:D:258:ILE:HG23	1.89	0.54
1:B:245:ILE:CD1	1:B:287:MET:CE	2.86	0.54
1:D:330:LEU:HA	1:D:333:LEU:HD12	1.90	0.53
1:D:279:TRP:CE3	3:D:603:PEG:H32	2.44	0.53
1:C:320:GLU:HB3	1:C:323:MET:CB	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:SER:OG	1:A:262:GLU:OE2	2.26	0.52
1:D:257:ILE:CG1	1:D:462:LEU:HD21	2.39	0.52
1:B:280:LYS:CD	4:B:605:PG4:H32	2.40	0.52
1:C:402:ASN:C	1:C:402:ASN:HD22	2.13	0.52
1:D:256:PRO:O	1:D:257:ILE:HD12	2.10	0.51
1:C:260:GLN:O	1:C:466:GLN:HG3	2.11	0.51
1:A:257:ILE:HD11	1:A:277:LEU:CD2	2.40	0.51
1:A:337:LEU:CD1	1:A:354:GLU:HG2	2.40	0.51
1:A:266:CYS:HB2	1:A:267:PRO:HD2	1.92	0.50
1:D:366:TYR:HB3	1:D:431:LEU:HD11	1.93	0.50
1:B:342:ARG:HD3	5:B:701:HOH:O	2.12	0.50
1:C:299:LEU:O	1:C:303:MET:HG3	2.11	0.50
1:B:314:ILE:HD12	1:B:314:ILE:N	2.23	0.49
1:B:390:LEU:HD11	1:B:412:ALA:HB1	1.94	0.49
1:C:300:GLY:HA2	1:C:327:MET:HE1	1.95	0.49
1:A:256:PRO:O	1:A:257:ILE:HD12	2.12	0.49
1:D:257:ILE:HG13	1:D:462:LEU:HD21	1.94	0.49
1:A:260:GLN:OE1	1:A:464:THR:HG22	2.12	0.49
1:C:261:ASN:OD1	1:C:261:ASN:C	2.52	0.49
1:D:272:LEU:HD13	1:D:295:LEU:HD13	1.94	0.49
1:B:342:ARG:HB2	1:B:348:VAL:HG12	1.94	0.49
1:A:260:GLN:OE1	1:A:464:THR:CG2	2.61	0.48
1:C:316:ARG:HH21	1:C:316:ARG:CG	2.25	0.48
1:B:340:ASN:HD21	1:B:388:ASN:HB2	1.78	0.47
1:A:337:LEU:HD21	1:A:354:GLU:HG2	1.96	0.47
1:D:257:ILE:HD11	1:D:277:LEU:CD2	2.44	0.47
1:A:243:TYR:CE1	1:A:261:ASN:OD1	2.68	0.47
1:B:354:GLU:O	1:B:357:VAL:HG23	2.14	0.47
1:C:299:LEU:CD2	1:C:330:LEU:HD13	2.43	0.47
4:B:605:PG4:H21	4:B:605:PG4:H41	1.34	0.46
1:D:333:LEU:HD11	1:D:357:VAL:HG21	1.96	0.46
1:B:357:VAL:HG12	1:B:361:LEU:HD12	1.97	0.46
1:D:268:LEU:HG	1:D:272:LEU:HD12	1.97	0.46
1:D:388:ASN:O	1:D:391:VAL:HG22	2.16	0.46
1:B:280:LYS:NZ	4:B:605:PG4:H32	2.31	0.46
1:C:367:HIS:CD2	1:C:369:TRP:H	2.28	0.46
1:B:258:ILE:HG22	1:B:269:LEU:HD11	1.98	0.45
1:D:382:VAL:O	1:D:385:CYS:HB2	2.16	0.45
1:D:340:ASN:ND2	1:D:386:SER:HB2	2.31	0.45
1:A:370:LEU:HD22	1:A:427:GLY:HA2	1.99	0.45
1:B:266:CYS:HB2	1:B:267:PRO:HD2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ASN:ND2	1:B:388:ASN:HB2	2.32	0.44
1:A:337:LEU:HA	1:A:337:LEU:HD22	1.79	0.44
1:C:272:LEU:HD23	1:C:295:LEU:HD22	1.97	0.44
1:D:257:ILE:HD11	1:D:277:LEU:HD21	1.99	0.44
1:A:296:MET:SD	1:A:334:GLN:OE1	2.75	0.44
1:B:339:VAL:HG21	1:B:449:PHE:CZ	2.52	0.43
1:A:343:PHE:O	1:A:371:VAL:HG12	2.18	0.43
1:A:296:MET:HE3	1:A:330:LEU:HB3	2.01	0.43
1:B:280:LYS:HZ3	4:B:605:PG4:H32	1.83	0.43
1:A:368:GLY:O	1:A:427:GLY:HA3	2.19	0.43
1:C:329:ILE:CG2	1:C:357:VAL:HG21	2.49	0.43
1:A:337:LEU:HD11	1:A:354:GLU:CG	2.48	0.43
1:C:329:ILE:HG21	1:C:357:VAL:HG22	2.00	0.43
1:D:352:THR:O	1:D:353:PRO:C	2.57	0.43
1:B:329:ILE:HG21	1:B:357:VAL:HG22	2.00	0.43
1:C:249:GLN:O	1:C:491:SER:HB3	2.19	0.43
1:D:239:PHE:CD1	1:D:239:PHE:N	2.87	0.43
1:B:329:ILE:HG22	1:B:357:VAL:HG22	2.01	0.42
1:C:261:ASN:OD1	1:C:263:ASN:N	2.52	0.42
1:A:402:ASN:HD21	1:A:404:GLU:HB3	1.84	0.42
1:B:340:ASN:HD21	1:B:388:ASN:CB	2.32	0.42
1:B:339:VAL:HG21	1:B:449:PHE:HZ	1.83	0.42
1:C:375:ILE:HD12	1:C:375:ILE:H	1.85	0.42
1:A:287:MET:SD	1:A:290:ILE:HD12	2.58	0.42
1:D:329:ILE:O	1:D:333:LEU:HG	2.19	0.42
1:A:337:LEU:CD2	1:A:354:GLU:HG2	2.49	0.42
1:C:368:GLY:O	1:C:427:GLY:HA3	2.19	0.42
1:A:475:VAL:HG21	1:A:491:SER:HB3	2.02	0.42
1:A:257:ILE:HG13	1:A:462:LEU:HD21	2.02	0.42
1:A:296:MET:HE1	1:A:330:LEU:O	2.19	0.42
1:B:258:ILE:CG2	1:B:269:LEU:HD11	2.50	0.42
1:C:328:ALA:O	1:C:332:LYS:HD3	2.20	0.41
1:C:432:THR:O	1:C:454:LYS:NZ	2.40	0.41
1:D:357:VAL:HG12	1:D:361:LEU:HD12	2.02	0.41
1:A:366:TYR:HB3	1:A:431:LEU:HD11	2.02	0.41
1:C:356:ILE:O	1:C:360:LEU:HG	2.21	0.41
1:B:287:MET:HE1	1:B:290:ILE:CD1	2.39	0.41
1:B:368:GLY:O	1:B:427:GLY:HA3	2.21	0.41
1:C:329:ILE:HG21	1:C:357:VAL:HG21	2.02	0.41
1:C:367:HIS:HD2	1:C:369:TRP:N	2.13	0.41
1:B:287:MET:HE3	1:B:290:ILE:CB	2.32	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:454:LYS:HE3	1:D:457:GLY:HA2	2.03	0.41
1:C:257:ILE:CG1	1:C:462:LEU:HD21	2.50	0.40
1:D:257:ILE:HD11	1:D:277:LEU:HG	2.03	0.40
1:C:373:PRO:HA	1:C:379:VAL:CG2	2.51	0.40
1:C:340:ASN:ND2	1:C:386:SER:HB2	2.37	0.40
1:C:402:ASN:HD21	1:C:404:GLU:HB2	1.87	0.40
1:A:295:LEU:HD23	1:A:295:LEU:HA	1.86	0.40
1:D:257:ILE:HG12	1:D:462:LEU:HD21	2.03	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	248/273 (91%)	243 (98%)	5 (2%)	0	100	100
1	B	250/273 (92%)	242 (97%)	8 (3%)	0	100	100
1	C	254/273 (93%)	244 (96%)	10 (4%)	0	100	100
1	D	239/273 (88%)	231 (97%)	8 (3%)	0	100	100
All	All	991/1092 (91%)	960 (97%)	31 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	207/249 (83%)	193 (93%)	14 (7%)	16	11
1	B	214/249 (86%)	204 (95%)	10 (5%)	26	22
1	C	208/249 (84%)	190 (91%)	18 (9%)	10	6
1	D	190/249 (76%)	178 (94%)	12 (6%)	18	13
All	All	819/996 (82%)	765 (93%)	54 (7%)	16	12

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	240	MET
1	A	241	SER
1	A	272	LEU
1	A	330	LEU
1	A	334	GLN
1	A	337	LEU
1	A	338	ASP
1	A	359	ASP
1	A	360	LEU
1	A	401	ASP
1	A	403	SER
1	A	405	LEU
1	A	464	THR
1	A	495	LEU
1	B	249	GLN
1	B	257	ILE
1	B	262	GLU
1	B	312	SER
1	B	321	GLN
1	B	330	LEU
1	B	335	THR
1	B	400	SER
1	B	403	SER
1	B	482	VAL
1	C	240	MET
1	C	316	ARG
1	C	320	GLU
1	C	332	LYS
1	C	347	ARG
1	C	357	VAL
1	C	392	GLU
1	C	396	SER
1	C	402	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	405	LEU
1	C	421	THR
1	C	433	SER
1	C	464	THR
1	C	466	GLN
1	C	471	GLU
1	C	482	VAL
1	C	491	SER
1	C	495	LEU
1	D	239	PHE
1	D	240	MET
1	D	269	LEU
1	D	296	MET
1	D	305	ASP
1	D	359	ASP
1	D	405	LEU
1	D	414	GLN
1	D	458	GLN
1	D	482	VAL
1	D	492	GLU
1	D	495	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	367	HIS
1	A	402	ASN
1	A	414	GLN
1	A	426	HIS
1	A	480	HIS
1	A	494	HIS
1	B	322	ASN
1	B	340	ASN
1	B	367	HIS
1	B	417	ASN
1	B	480	HIS
1	C	321	GLN
1	C	367	HIS
1	C	402	ASN
1	C	414	GLN
1	C	458	GLN
1	C	480	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	494	HIS
1	D	260	GLN
1	D	367	HIS
1	D	414	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 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	PEG	D	603	-	6,6,6	0.10	0	5,5,5	0.08	0
4	PG4	B	605	-	12,12,12	0.14	0	11,11,11	0.12	0
3	PEG	B	604	-	6,6,6	0.12	0	5,5,5	0.08	0
3	PEG	A	602	-	6,6,6	0.11	0	5,5,5	0.07	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	PEG	D	603	-	-	3/4/4/4	-
4	PG4	B	605	-	-	8/10/10/10	-
3	PEG	B	604	-	-	1/4/4/4	-
3	PEG	A	602	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	605	PG4	C4-C3-O2-C2
4	B	605	PG4	O3-C5-C6-O4
4	B	605	PG4	O2-C3-C4-O3
3	B	604	PEG	O1-C1-C2-O2
3	D	603	PEG	O2-C3-C4-O4
4	B	605	PG4	O4-C7-C8-O5
3	D	603	PEG	C4-C3-O2-C2
4	B	605	PG4	C3-C4-O3-C5
3	D	603	PEG	C1-C2-O2-C3
4	B	605	PG4	O1-C1-C2-O2
4	B	605	PG4	C6-C5-O3-C4
3	A	602	PEG	C1-C2-O2-C3
4	B	605	PG4	C1-C2-O2-C3

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	603	PEG	5	0
4	B	605	PG4	10	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	252/273 (92%)	-0.03	3 (1%) 79 78	25, 38, 76, 106	0
1	B	254/273 (93%)	-0.08	4 (1%) 72 70	27, 40, 67, 110	0
1	C	258/273 (94%)	0.37	21 (8%) 12 11	28, 49, 89, 123	0
1	D	243/273 (89%)	0.31	16 (6%) 18 17	30, 50, 90, 109	0
All	All	1007/1092 (92%)	0.14	44 (4%) 34 33	25, 44, 82, 123	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	319	TYR	10.7
1	C	318	ASN	9.7
1	C	317	LEU	6.5
1	D	336	GLY	5.8
1	B	337	LEU	5.4
1	C	308	PRO	4.9
1	D	333	LEU	4.1
1	D	323	MET	4.0
1	D	375	ILE	4.0
1	B	480	HIS	3.4
1	C	304	LEU	3.3
1	C	263	ASN	3.2
1	C	307	LYS	3.2
1	D	328	ALA	3.1
1	D	240	MET	3.1
1	C	376	ASP	3.1
1	D	335	THR	2.9
1	B	335	THR	2.8
1	D	304	LEU	2.8
1	C	372	ASP	2.8
1	C	286	MET	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	286	MET	2.7
1	D	302	TYR	2.7
1	D	374	GLN	2.7
1	D	376	ASP	2.6
1	D	329	ILE	2.6
1	A	337	LEU	2.5
1	A	308	PRO	2.5
1	C	237	PRO	2.4
1	D	324	SER	2.4
1	C	316	ARG	2.3
1	C	321	GLN	2.3
1	C	499	SER	2.3
1	C	374	GLN	2.3
1	A	240	MET	2.2
1	C	399	GLN	2.1
1	D	261	ASN	2.1
1	C	306	ALA	2.1
1	C	405	LEU	2.1
1	C	305	ASP	2.1
1	C	375	ILE	2.1
1	B	286	MET	2.1
1	D	411	VAL	2.0
1	C	314	ILE	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.

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CL	B	603	1/1	0.70	0.12	77,77,77,77	0
2	CL	A	601	1/1	0.82	0.17	72,72,72,72	0
4	PG4	B	605	13/13	0.85	0.14	55,65,76,77	0
3	PEG	A	602	7/7	0.89	0.14	50,54,61,61	0
3	PEG	B	604	7/7	0.90	0.16	53,54,61,67	0
2	CL	C	601	1/1	0.90	0.07	69,69,69,69	0
2	CL	D	602	1/1	0.91	0.06	82,82,82,82	0
2	CL	B	602	1/1	0.93	0.11	69,69,69,69	0
2	CL	D	601	1/1	0.93	0.09	56,56,56,56	0
3	PEG	D	603	7/7	0.94	0.09	73,73,76,76	0
2	CL	B	601	1/1	0.97	0.13	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.