



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:31 PM UTC

PDB ID : 6Z49 / pdb_00006z49
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 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
Mogul : 2022.3.0, CSD as543be (2022)
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

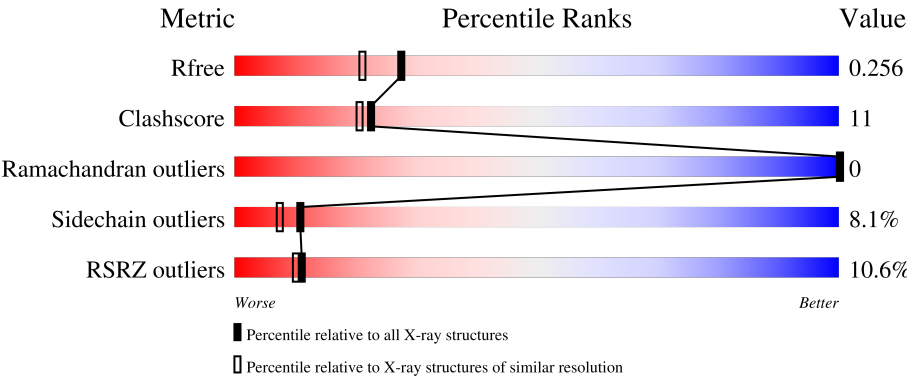
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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% 72% 16% • • 8%
1	B	273	5% 75% 17% • 7%
1	C	273	11% 73% 18% • 5%
1	D	273	14% 72% 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
1	A	252	Total	C	N	O	S	0	0	0
			1955	1256	316	370	13			
1	B	254	Total	C	N	O	S	0	0	0
			1993	1284	319	377	13			
1	C	258	Total	C	N	O	S	0	0	0
			1990	1279	325	372	14			
1	D	243	Total	C	N	O	S	0	0	0
			1856	1197	305	342	12			

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 (CCD ID: CL) (formula: Cl).

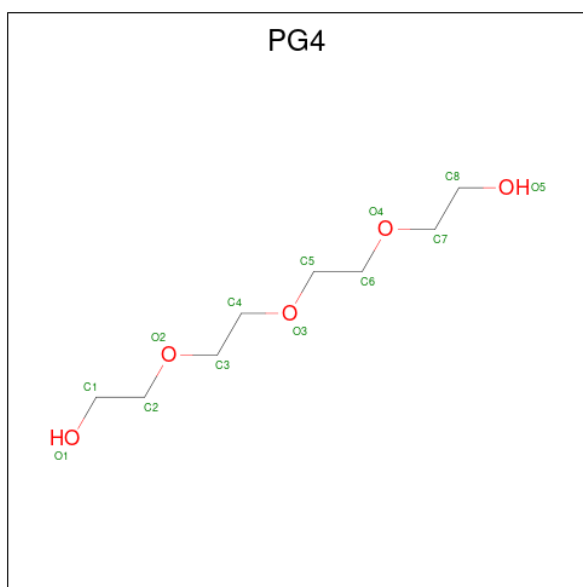
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	3	Total Cl 3 3	0	0
2	C	1	Total Cl 1 1	0	0
2	D	2	Total Cl 2 2	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: 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 (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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

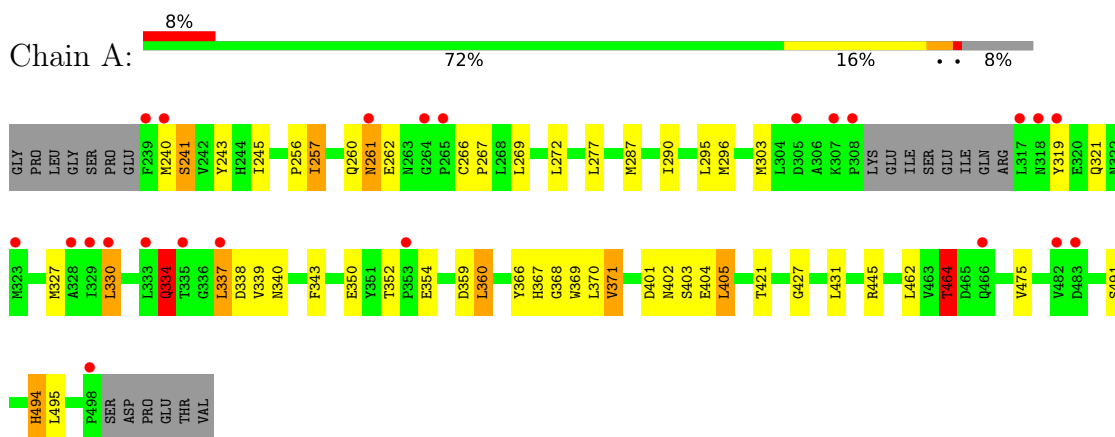
- Molecule 5 is water.

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

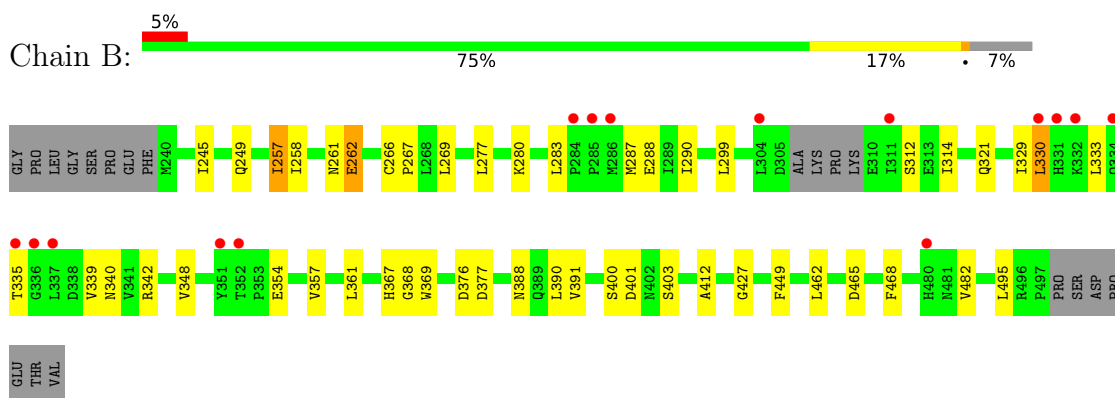
3 Residue-property plots [i](#)

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.

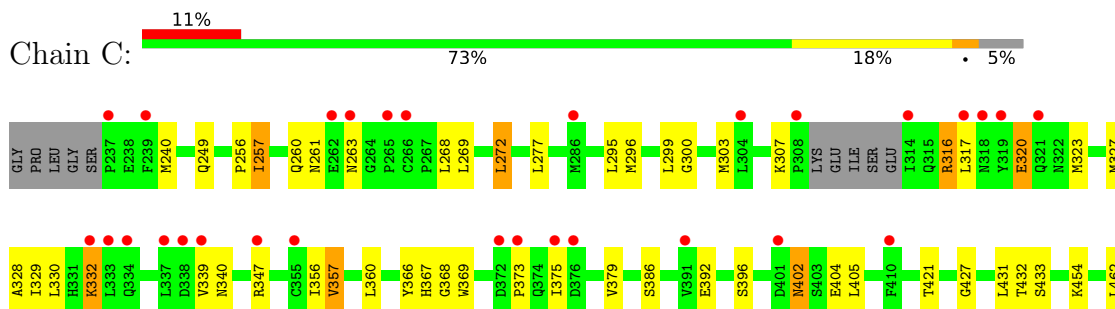
- Molecule 1: Ubiquitin carboxyl-terminal hydrolase MINDY-2

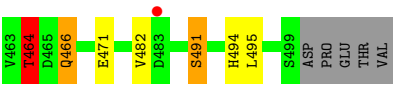


- Molecule 1: Ubiquitin carboxyl-terminal hydrolase MINDY-2

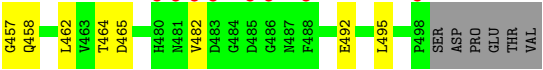
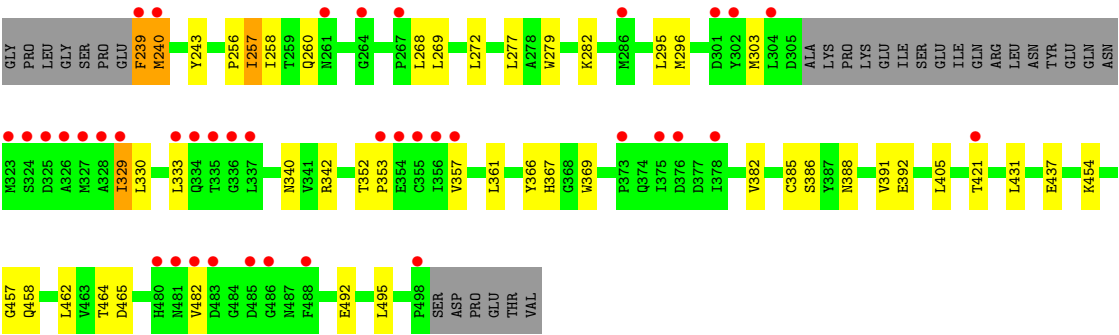


- Molecule 1: Ubiquitin carboxyl-terminal hydrolase MINDY-2





● 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)	Xtriage
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 (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.574	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
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

Xtriage'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

5.1 Standard geometry

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

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	1.05	1/1999 (0.1%)	1.42	9/2725 (0.3%)
1	B	1.06	0/2038	1.42	6/2776 (0.2%)
1	C	1.10	0/2035	1.43	2/2774 (0.1%)
1	D	1.08	0/1899	1.44	3/2589 (0.1%)
All	All	1.07	1/7971 (0.0%)	1.43	20/10864 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	494	HIS	CE1-NE2	5.54	1.38	1.32

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	437	GLU	CB-CA-C	8.10	119.77	109.80
1	A	464	THR	CB-CA-C	6.85	120.89	109.38
1	A	261	ASN	CA-C-N	6.59	130.00	120.38
1	A	261	ASN	C-N-CA	6.59	130.00	120.38
1	A	464	THR	N-CA-CB	-5.91	102.72	110.88
1	C	464	THR	CB-CA-C	5.89	119.28	109.38
1	A	352	THR	CB-CA-C	5.78	118.00	109.22
1	A	321	GLN	O-C-N	5.59	127.83	122.07
1	A	334	GLN	N-CA-C	-5.46	107.62	114.56
1	B	376	ASP	CA-C-N	5.46	127.91	120.54
1	B	376	ASP	C-N-CA	5.46	127.91	120.54
1	B	288	GLU	N-CA-C	-5.27	107.51	114.04
1	B	377	ASP	CB-CA-C	-5.19	102.51	110.81
1	B	261	ASN	N-CA-C	-5.16	99.81	110.80
1	B	401	ASP	N-CA-C	-5.13	105.49	112.26
1	C	464	THR	N-CA-CB	-5.11	103.83	110.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	TYR	CA-C-N	5.07	127.03	120.44
1	A	319	TYR	C-N-CA	5.07	127.03	120.44
1	D	465	ASP	CA-C-N	5.05	127.30	120.38
1	D	465	ASP	C-N-CA	5.05	127.30	120.38

There are no chirality outliers.

There are no planarity outliers.

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	1955	0	1828	35	0
1	B	1993	0	1893	53	0
1	C	1990	0	1870	43	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
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	160	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 11.

All (160) 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:287:MET:HE1	1:B:290:ILE:HD12	1.30	1.07
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: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:HE3	1:B:290:ILE:HB	1.57	0.86
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:B:245:ILE:HD11	1:B:287:MET:HE3	1.67	0.76
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:287:MET:HE1	1:B:290:ILE:CD1	2.17	0.67
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
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:A:296:MET:HE1	1:A:330:LEU:O	2.00	0.61
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ASN:HD22	1:A:350:GLU:CD	2.11	0.59
1:B:280:LYS:CE	4:B:605:PG4:H72	2.32	0.59
1:B:245:ILE:HD11	1:B:287:MET:CE	2.31	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:B:280:LYS:HZ3	4:B:605:PG4:C1	2.17	0.57
1:D:260:GLN:HG2	1:D:464:THR:O	2.03	0.57
1:C:402:ASN:C	1:C:402:ASN:HD22	2.13	0.57
1:D:367:HIS:HD2	1:D:369:TRP:H	1.52	0.57
1:A:337:LEU:HD11	1:A:354:GLU:HG2	1.86	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:B:257:ILE:CG1	1:B:462:LEU:HD21	2.36	0.54
1:B:245:ILE:CD1	1:B:287:MET:CE	2.86	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:C:261:ASN:OD1	1:C:261:ASN:C	2.52	0.53
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
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:268:LEU:HD22	1:C:296:MET:HE2	1.92	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:A:303:MET:HE2	1:A:360:LEU:HD13	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:LEU:HD11	1:B:412:ALA:HB1	1.94	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:B:245:ILE:CD1	1:B:287:MET:HE3	2.37	0.49
1:A:260:GLN:OE1	1:A:464:THR:HG22	2.12	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:C:432:THR:O	1:C:454:LYS:NZ	2.40	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:D:352:THR:O	1:D:353:PRO:C	2.57	0.47
1:A:337:LEU:HD21	1:A:354:GLU:HG2	1.96	0.47
1:B:280:LYS:HZ3	4:B:605:PG4:H11	1.65	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:283:LEU:HD13	1:B:287:MET:HE2	1.99	0.45
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
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:B:262:GLU:CD	1:B:262:GLU:H	2.25	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:245:ILE:CD1	1:B:287:MET:HE2	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: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: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:C:300:GLY:HA2	1:C:327:MET:HE1	2.02	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: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:B:245:ILE:HD13	1:B:287:MET:HE2	2.03	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%)	189 (91%)	18 (9%)	9	6
1	B	214/249 (86%)	202 (94%)	12 (6%)	19	16
1	C	208/249 (84%)	186 (89%)	22 (11%)	6	4
1	D	190/249 (76%)	176 (93%)	14 (7%)	13	9
All	All	819/996 (82%)	753 (92%)	66 (8%)	11	7

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	240	MET
1	A	241	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	257	ILE
1	A	269	LEU
1	A	272	LEU
1	A	327	MET
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	371	VAL
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	391	VAL
1	B	400	SER
1	B	403	SER
1	B	482	VAL
1	B	495	LEU
1	C	240	MET
1	C	257	ILE
1	C	269	LEU
1	C	272	LEU
1	C	316	ARG
1	C	320	GLU
1	C	332	LYS
1	C	339	VAL
1	C	347	ARG
1	C	357	VAL
1	C	392	GLU
1	C	396	SER
1	C	402	ASN
1	C	405	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	257	ILE
1	D	269	LEU
1	D	296	MET
1	D	303	MET
1	D	329	ILE
1	D	342	ARG
1	D	405	LEU
1	D	421	THR
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 (26) 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	260	GLN
1	B	294	GLN
1	B	322	ASN
1	B	331	HIS
1	B	340	ASN
1	B	367	HIS
1	B	417	ASN
1	C	321	GLN
1	C	367	HIS
1	C	402	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	414	GLN
1	C	417	ASN
1	C	448	HIS
1	C	480	HIS
1	C	494	HIS
1	D	249	GLN
1	D	367	HIS
1	D	414	GLN
1	D	448	HIS
1	D	458	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
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
4	PG4	B	605	-	12,12,12	0.13	0	11,11,11	0.11	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	-
3	PEG	B	604	-	-	1/4/4/4	-
3	PEG	A	602	-	-	1/4/4/4	-
4	PG4	B	605	-	-	8/10/10/10	-

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
4	B	605	PG4	C3-C4-O3-C5
3	D	603	PEG	C4-C3-O2-C2
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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.50	23 (9%)	15	13	25, 38, 76, 106	0
1	B	254/273 (93%)	0.48	15 (5%)	28	27	27, 40, 67, 110	0
1	C	258/273 (94%)	0.83	30 (11%)	9	8	28, 49, 89, 123	0
1	D	243/273 (89%)	0.99	39 (16%)	5	4	30, 50, 90, 109	0
All	All	1007/1092 (92%)	0.70	107 (10%)	11	10	25, 44, 82, 123	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	318	ASN	8.6
1	C	319	TYR	7.0
1	D	375	ILE	6.4
1	D	326	ALA	5.7
1	D	333	LEU	5.6
1	B	337	LEU	5.3
1	B	335	THR	4.9
1	D	334	GLN	4.9
1	D	336	GLY	4.7
1	C	334	GLN	4.7
1	D	335	THR	4.7
1	D	355	CYS	4.6
1	C	317	LEU	4.5
1	D	239	PHE	4.2
1	C	373	PRO	4.1
1	A	337	LEU	4.1
1	C	375	ILE	4.1
1	C	237	PRO	3.9
1	B	336	GLY	3.9
1	A	329	ILE	3.9
1	A	318	ASN	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	376	ASP	3.7
1	B	304	LEU	3.6
1	D	327	MET	3.6
1	A	317	LEU	3.6
1	D	267	PRO	3.6
1	C	263	ASN	3.6
1	A	319	TYR	3.4
1	D	485	ASP	3.4
1	C	314	ILE	3.3
1	D	323	MET	3.3
1	D	337	LEU	3.3
1	A	240	MET	3.2
1	C	376	ASP	3.2
1	D	286	MET	3.2
1	B	330	LEU	3.1
1	D	240	MET	3.1
1	C	239	PHE	3.1
1	C	308	PRO	3.1
1	C	262	GLU	3.1
1	C	338	ASP	3.0
1	C	286	MET	3.0
1	B	351	TYR	3.0
1	D	486	GLY	3.0
1	A	265	PRO	2.9
1	A	239	PHE	2.9
1	D	324	SER	2.9
1	D	498	PRO	2.9
1	D	421	THR	2.9
1	A	335	THR	2.8
1	A	308	PRO	2.8
1	D	354	GLU	2.8
1	D	261	ASN	2.8
1	D	329	ILE	2.8
1	C	337	LEU	2.8
1	D	325	ASP	2.7
1	D	488	PHE	2.7
1	C	265	PRO	2.7
1	D	356	ILE	2.7
1	C	410	PHE	2.7
1	C	332	LYS	2.7
1	B	352	THR	2.6
1	C	333	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	311	ILE	2.6
1	D	357	VAL	2.6
1	A	483	ASP	2.5
1	A	498	PRO	2.5
1	B	286	MET	2.4
1	B	334	GLN	2.4
1	D	482	VAL	2.4
1	C	391	VAL	2.4
1	B	285	PRO	2.4
1	D	328	ALA	2.4
1	A	307	LYS	2.4
1	B	332	LYS	2.4
1	A	261	ASN	2.3
1	A	330	LEU	2.3
1	C	483	ASP	2.3
1	D	301	ASP	2.3
1	D	483	ASP	2.3
1	C	266	CYS	2.3
1	A	323	MET	2.3
1	A	482	VAL	2.3
1	C	355	CYS	2.3
1	B	480	HIS	2.2
1	A	466	GLN	2.2
1	C	339	VAL	2.2
1	D	373	PRO	2.2
1	D	481	ASN	2.2
1	C	347	ARG	2.2
1	B	284	PRO	2.2
1	A	305	ASP	2.2
1	C	372	ASP	2.2
1	D	378	ILE	2.2
1	A	353	PRO	2.1
1	D	353	PRO	2.1
1	B	331	HIS	2.1
1	A	328	ALA	2.1
1	D	304	LEU	2.1
1	D	264	GLY	2.1
1	C	304	LEU	2.1
1	C	401	ASP	2.1
1	C	321	GLN	2.1
1	D	302	TYR	2.1
1	D	480	HIS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	333	LEU	2.0
1	A	264	GLY	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 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(Å ²)	Q<0.9
3	PEG	D	603	7/7	0.86	0.17	73,73,76,76	0
4	PG4	B	605	13/13	0.87	0.13	55,65,76,77	0
3	PEG	B	604	7/7	0.88	0.13	53,54,61,67	0
2	CL	B	602	1/1	0.88	0.12	69,69,69,69	0
2	CL	B	603	1/1	0.88	0.11	77,77,77,77	0
3	PEG	A	602	7/7	0.89	0.11	50,54,61,61	0
2	CL	C	601	1/1	0.92	0.09	69,69,69,69	0
2	CL	A	601	1/1	0.93	0.12	72,72,72,72	0
2	CL	D	601	1/1	0.94	0.16	56,56,56,56	0
2	CL	D	602	1/1	0.95	0.11	82,82,82,82	0
2	CL	B	601	1/1	0.96	0.13	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.