



# Full wwPDB X-ray Structure Validation Report

Oct 3, 2014 – 01:31 AM EDT

PDB ID : 4H2E  
Title : Crystal structure of an MMP twin inhibitor complexing two MMP-9 catalytic domains  
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Deposited on : 2012-09-12  
Resolution : 2.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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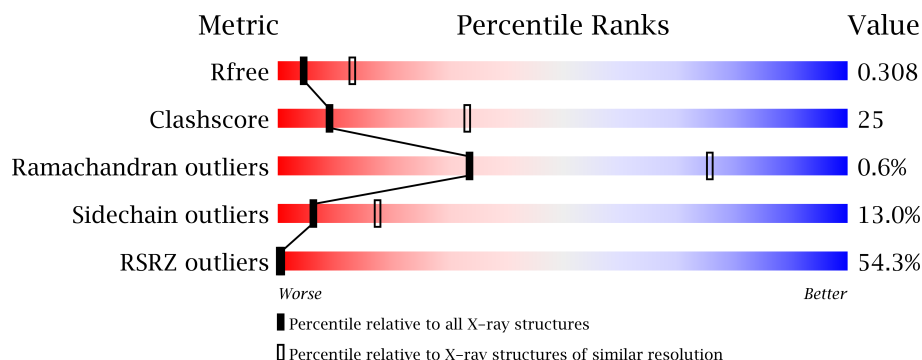
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23828  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23828

# 1 Overall quality at a glance

The reported resolution of this entry is 2.90 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))
$R_{free}$	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	164	
1	B	164	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	CA	B	305	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 2977 atoms, of which 0 are hydrogen and 0 are deuterium.

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 human MMP-9 catalytic domain wild-type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	1	0
			1315	850	223	240	2			
1	B	164	Total	C	N	O	S	0	1	0
			1315	850	223	240	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	GLY	-	EXPRESSION TAG	UNP P14780
A	227	GLU	GLN	ENGINEERED MUTATION	UNP P14780
B	106	GLY	-	EXPRESSION TAG	UNP P14780
B	227	GLU	GLN	ENGINEERED MUTATION	UNP P14780

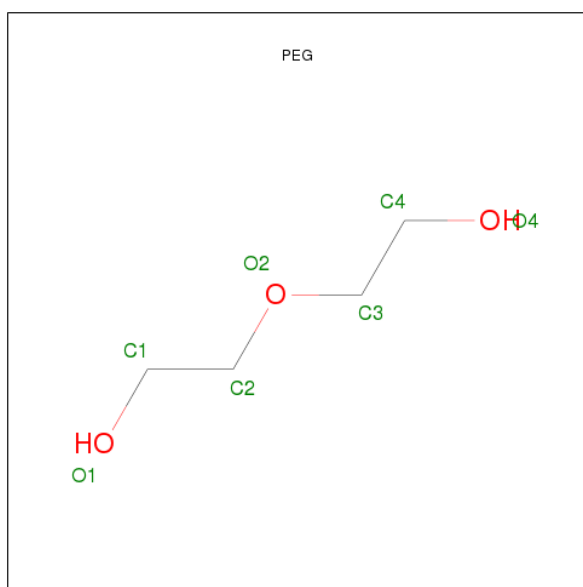
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

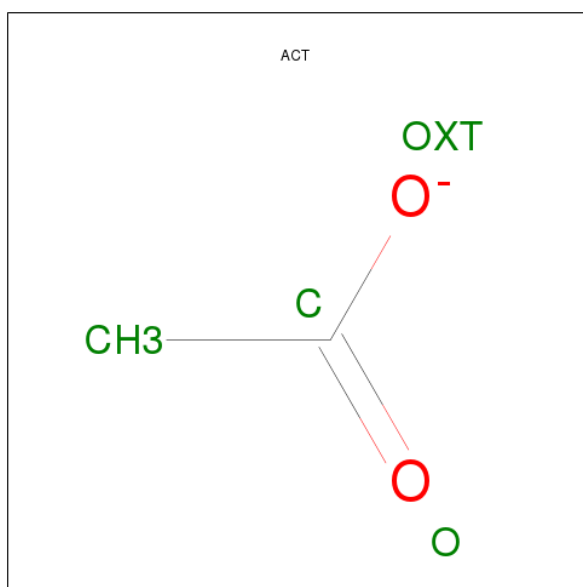
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Ca	0	0
			3	3		
3	A	2	Total	Ca	0	0
			2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



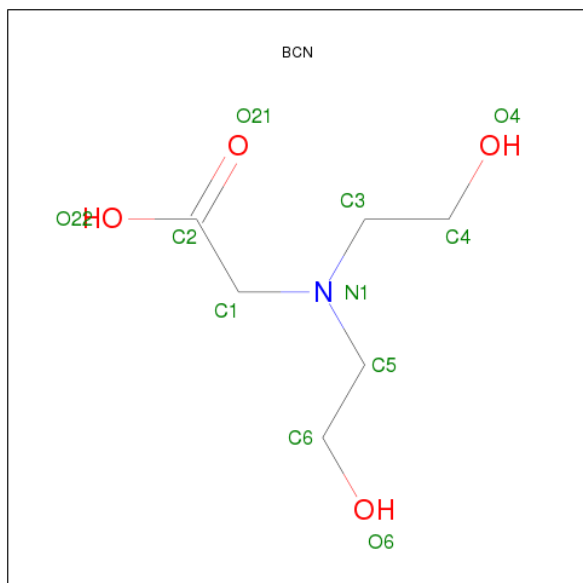
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



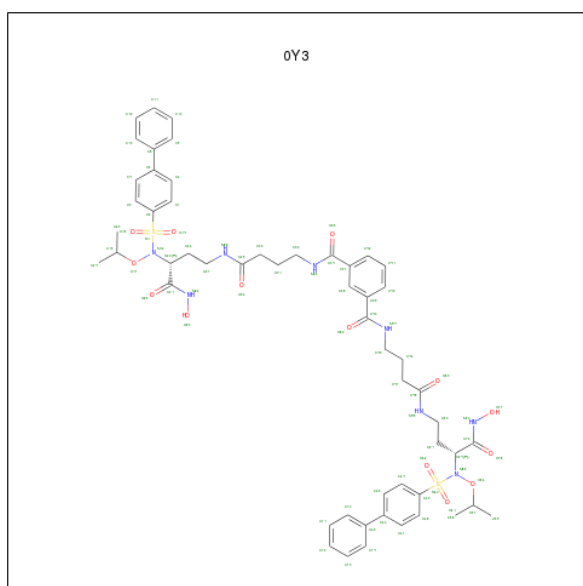
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is BICINE (three-letter code: BCN) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			11	6	1	4		
6	A	1	Total	C	N	O	0	0
			11	6	1	4		
6	B	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 7 is N,N'-BIS(4-{[(3R)-3-[(BIPHENYL-4-YLSULFONYL)(PROPAN-2-YLOXY)AMINO]-4-(HYDROXYAMINO)-4-OXOBUTYL]AMINO}-4-OXOBUTYL)BENZENE-1,3-DICARBOXAMIDE (three-letter code: 0Y3) (formula: C<sub>54</sub>H<sub>66</sub>N<sub>8</sub>O<sub>14</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			78	54	8	14	2		

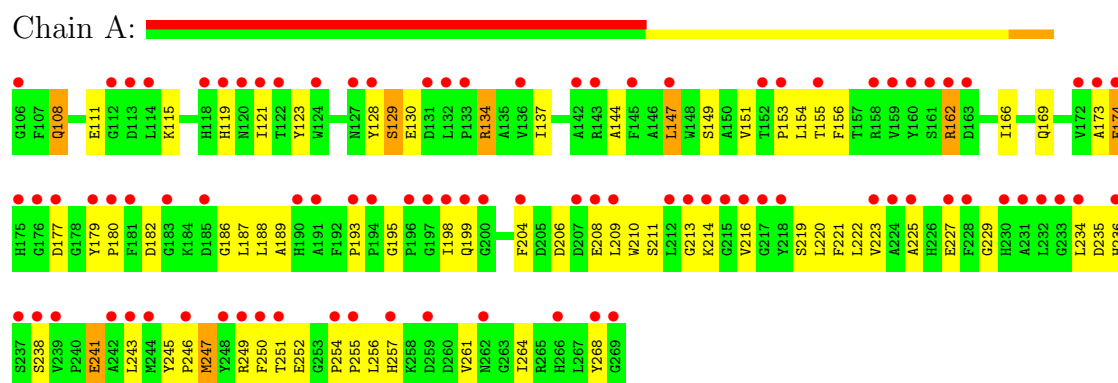
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	84	Total	O	0	0
			84	84		
8	B	64	Total	O	0	0
			64	64		

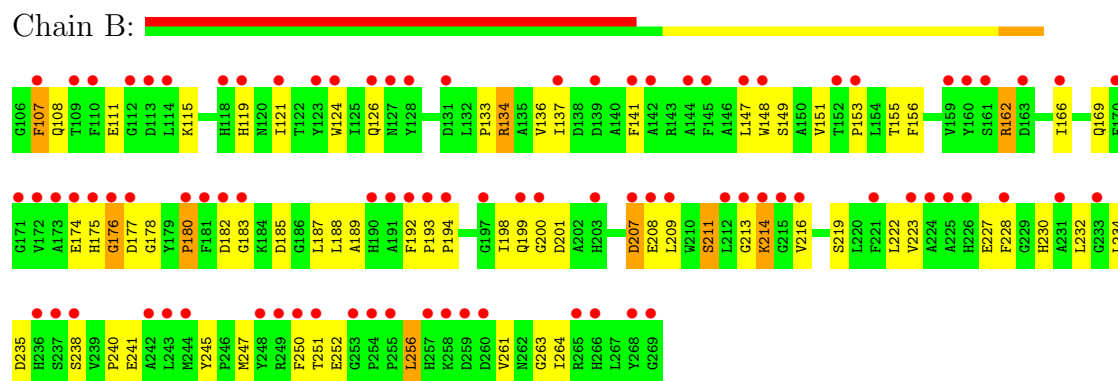
### 3 Residue-property plots

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.

- Molecule 1: human MMP-9 catalytic domain wild-type



- Molecule 1: human MMP-9 catalytic domain wild-type



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	40.18Å 97.40Å 45.69Å 90.00° 111.99° 90.00°	Depositor
Resolution (Å)	38.85 – 2.90 38.85 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.0 (38.85-2.90) 98.4 (38.85-2.90)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1069)/REFMAC	Depositor
R, $R_{free}$	0.277 , 0.311 0.279 , 0.308	Depositor DCC
$R_{free}$ test set	357 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	4 of 7156 reflections (0.056%)	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	2977	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	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 47.35 % 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 1.0045e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.



## 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: ZN, CA, OY3, BCN, ACT, 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	0.31	0/1363	0.52	0/1856
1	B	0.33	0/1363	0.57	1/1856 (0.1%)
All	All	0.32	0/2726	0.54	1/3712 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	176	GLY	N-CA-C	5.46	126.75	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1315	0	1211	57	0
1	B	1315	0	1211	74	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	42	0	60	3	0
4	B	21	0	30	2	0
5	A	12	0	9	0	0
5	B	4	0	3	0	0
6	A	22	0	24	3	0
6	B	11	0	12	7	0
7	B	78	0	64	12	0
8	A	84	0	0	1	0
8	B	64	0	0	0	0
All	All	2977	0	2624	137	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 25.

All (137) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:214:LYS:HA	1:B:214:LYS:HE2	1.21	1.11
1:B:174:GLU:HB3	6:B:311:BCN:H12	1.04	1.04
1:B:177:ASP:HB3	1:B:198:ILE:HD11	1.42	1.02
1:B:216:VAL:HG12	1:B:216:VAL:O	1.60	1.01
1:B:174:GLU:HB3	6:B:311:BCN:C1	1.91	0.99
1:B:174:GLU:CB	6:B:311:BCN:H12	1.96	0.96
1:B:214:LYS:CA	1:B:214:LYS:HE2	1.93	0.95
1:B:177:ASP:HB3	1:B:198:ILE:CD1	1.99	0.92
1:B:137:ILE:HG22	1:B:141:PHE:CE2	2.09	0.88
1:A:257:HIS:O	1:A:261:VAL:HG23	1.79	0.82
1:A:213:GLY:HA3	1:A:250:PHE:CE2	2.15	0.82
1:B:214:LYS:HA	1:B:214:LYS:CE	2.08	0.81
1:A:119:HIS:NE2	1:A:153:PRO:HB2	1.96	0.81
1:A:219:SER:HB3	1:A:222:LEU:HB2	1.66	0.76
1:A:222:LEU:HD11	1:A:251:THR:HG22	1.68	0.76
1:B:107:PHE:O	7:B:306:OY3:H42	1.88	0.74
4:A:306:PEG:H31	4:B:308:PEG:H22	1.71	0.73
1:B:175:HIS:CD2	1:B:176:GLY:H	2.05	0.73
6:B:311:BCN:H31	6:B:311:BCN:O21	1.87	0.72
1:B:216:VAL:O	1:B:216:VAL:CG1	2.35	0.70
1:B:209:LEU:HD23	1:B:216:VAL:O	1.92	0.69
1:B:227:GLU:HA	1:B:227:GLU:OE1	1.92	0.69
1:B:137:ILE:HG22	1:B:141:PHE:HE2	1.57	0.68
1:A:189:ALA:O	7:B:306:OY3:H56	1.95	0.67
1:A:119:HIS:CD2	1:A:153:PRO:HB2	2.30	0.66
1:A:108:GLN:OE1	1:B:107:PHE:CD2	2.49	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:A:315:BCN:O21	6:A:315:BCN:H31	1.96	0.65
1:A:245:TYR:CD2	1:A:247:MET:HB3	2.33	0.64
1:A:129:SER:HB3	1:A:206:ASP:OD1	1.99	0.63
1:B:134[A]:ARG:HB3	1:B:134[A]:ARG:CZ	2.28	0.63
1:B:148:TRP:CZ3	1:B:264:ILE:HG21	2.34	0.62
1:B:192:PHE:HB3	1:B:199:GLN:HA	1.82	0.61
1:B:198:ILE:O	1:B:201:ASP:HB2	2.01	0.60
1:B:177:ASP:CB	1:B:198:ILE:HD11	2.24	0.60
1:A:119:HIS:HD2	1:A:154:LEU:HD23	1.67	0.60
1:A:241:GLU:OE2	4:A:306:PEG:H22	2.03	0.59
1:B:119:HIS:CD2	1:B:153:PRO:HB2	2.37	0.59
1:A:123:TYR:HA	1:A:166:ILE:O	2.03	0.59
1:B:189:ALA:O	7:B:306:OY3:H11	2.03	0.59
1:B:230:HIS:CD2	7:B:306:OY3:O77	2.56	0.58
1:A:162:ARG:NH1	1:A:162:ARG:HB3	2.19	0.58
1:B:209:LEU:CD2	1:B:216:VAL:O	2.52	0.57
1:B:175:HIS:CG	1:B:176:GLY:H	2.20	0.57
1:B:247:MET:HB2	7:B:306:OY3:H63	1.85	0.57
1:B:245:TYR:CE2	1:B:247:MET:HB3	2.39	0.57
1:B:183:GLY:HA2	1:B:207:ASP:CB	2.35	0.56
1:B:134[A]:ARG:HB2	1:B:134[A]:ARG:NH2	2.19	0.56
1:A:252:GLU:HA	1:A:252:GLU:OE1	2.05	0.56
1:B:134[A]:ARG:CB	1:B:134[A]:ARG:CZ	2.83	0.56
1:B:107:PHE:CE2	1:B:235:ASP:OD2	2.58	0.56
1:A:137:ILE:HG23	1:A:220:LEU:HD21	1.87	0.56
1:A:147:LEU:HD13	1:A:256:LEU:HG	1.88	0.56
1:A:173:ALA:HB1	4:A:309:PEG:H41	1.87	0.55
1:B:214:LYS:HE3	1:B:250:PHE:CE1	2.42	0.55
1:B:166:ILE:HG12	1:B:200:GLY:O	2.07	0.55
1:A:144:ALA:HA	1:A:221:PHE:HE1	1.71	0.54
1:B:178:GLY:O	4:B:309:PEG:H22	2.08	0.54
1:A:193:PRO:O	1:A:199:GLN:HB3	2.08	0.54
1:A:222:LEU:O	7:B:306:OY3:H66	2.08	0.54
1:B:235:ASP:OD2	7:B:306:OY3:H41	2.08	0.52
1:A:210:TRP:HZ3	1:A:223:VAL:HG21	1.75	0.52
1:A:162:ARG:HH11	1:A:162:ARG:HB3	1.74	0.51
1:B:211:SER:O	1:B:219:SER:HA	2.09	0.51
1:B:245:TYR:CD2	1:B:247:MET:HB3	2.45	0.51
1:A:151:VAL:CG2	1:A:264:ILE:HD12	2.41	0.50
1:A:245:TYR:HD2	1:A:247:MET:HB3	1.74	0.50
1:B:175:HIS:CG	1:B:176:GLY:N	2.79	0.50
1:B:213:GLY:HA3	1:B:219:SER:HB2	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:235:ASP:CG	1:A:236:HIS:H	2.15	0.50
1:B:227:GLU:OE2	7:B:306:OY3:N76	2.45	0.49
1:B:174:GLU:CG	1:B:174:GLU:O	2.60	0.49
1:A:245:TYR:CE2	1:A:247:MET:HB3	2.47	0.49
6:B:311:BCN:O21	6:B:311:BCN:C3	2.57	0.49
1:A:115:LYS:HB2	1:A:268:TYR:CE1	2.48	0.49
1:B:137:ILE:CG2	1:B:141:PHE:CE2	2.92	0.48
1:A:204:PHE:HB3	1:A:210:TRP:CZ2	2.49	0.48
1:B:134[A]:ARG:CB	1:B:134[A]:ARG:NH2	2.77	0.48
1:A:151:VAL:HG21	1:A:264:ILE:CD1	2.44	0.48
1:A:261:VAL:HA	1:A:264:ILE:HG12	1.96	0.48
1:B:252:GLU:OE1	1:B:252:GLU:HA	2.14	0.47
1:B:174:GLU:HA	1:B:180:PRO:HB3	1.96	0.47
1:B:162:ARG:NH1	1:B:162:ARG:HB3	2.29	0.47
1:A:225:ALA:HB1	1:A:243:LEU:HD21	1.97	0.46
1:B:192:PHE:CB	1:B:199:GLN:HA	2.46	0.46
1:A:227:GLU:HA	1:A:227:GLU:OE1	2.15	0.46
1:B:240:PRO:HA	1:B:245:TYR:CD1	2.51	0.46
1:A:211:SER:O	1:A:219:SER:HA	2.16	0.46
1:B:234:LEU:HD21	1:B:263:GLY:HA3	1.98	0.46
6:B:311:BCN:H51	6:B:311:BCN:H42	1.57	0.46
1:B:174:GLU:HB3	6:B:311:BCN:C2	2.43	0.45
1:A:134[A]:ARG:HB2	1:A:134[A]:ARG:HE	1.53	0.45
1:A:182:ASP:OD1	1:A:186:GLY:HA3	2.15	0.45
1:A:213:GLY:HA3	1:A:250:PHE:HE2	1.77	0.45
1:B:182:ASP:OD2	1:B:182:ASP:N	2.47	0.45
1:A:216:VAL:O	1:A:216:VAL:HG12	2.15	0.45
1:B:175:HIS:CD2	1:B:176:GLY:N	2.81	0.45
1:A:151:VAL:CG2	1:A:264:ILE:CD1	2.95	0.45
1:B:134[A]:ARG:HB2	1:B:134[A]:ARG:HH21	1.82	0.45
1:A:222:LEU:HA	1:A:222:LEU:HD23	1.85	0.45
1:B:261:VAL:HA	1:B:264:ILE:HG12	1.98	0.45
1:B:222:LEU:HA	1:B:222:LEU:HD23	1.83	0.45
1:A:174:GLU:O	1:A:174:GLU:HG2	2.16	0.44
1:B:121:ILE:HB	1:B:156:PHE:CD1	2.52	0.44
1:A:209:LEU:HD23	1:A:216:VAL:O	2.17	0.44
1:B:185:ASP:N	1:B:208:GLU:OE2	2.50	0.44
1:B:121:ILE:O	1:B:156:PHE:HA	2.18	0.44
1:A:261:VAL:HA	1:A:264:ILE:CG1	2.48	0.44
1:B:183:GLY:HA2	1:B:207:ASP:CG	2.37	0.44
1:B:223:VAL:HA	7:B:306:OY3:H14	2.00	0.44
1:B:115:LYS:HA	1:B:194:PRO:HG2	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:210:TRP:CZ3	1:A:223:VAL:HG21	2.53	0.43
1:A:195:GLY:C	1:A:199:GLN:HB2	2.39	0.43
1:A:254:PRO:HA	1:A:255:PRO:HD3	1.67	0.43
1:B:124:TRP:CH2	1:B:126:GLN:HG3	2.54	0.43
1:B:147:LEU:HG	1:B:256:LEU:HD13	2.00	0.43
1:B:148:TRP:CE3	1:B:264:ILE:HG21	2.54	0.43
1:A:177:ASP:HB3	1:A:198:ILE:HD11	2.01	0.42
1:B:133:PRO:O	1:B:136:VAL:N	2.53	0.42
6:A:315:BCN:O21	6:A:315:BCN:C3	2.65	0.42
1:A:179:TYR:HA	1:A:180:PRO:HD3	1.84	0.42
1:A:238:SER:HB3	8:A:476:HOH:O	2.20	0.42
1:A:182:ASP:HA	6:A:314:BCN:H31	2.01	0.42
1:A:245:TYR:HA	1:A:246:PRO:HD2	1.79	0.42
1:B:193:PRO:O	1:B:199:GLN:HB3	2.20	0.42
1:B:250:PHE:CG	1:B:251:THR:N	2.88	0.42
1:A:219:SER:O	1:A:223:VAL:HG23	2.20	0.41
1:A:229:GLY:O	1:A:234:LEU:HB2	2.19	0.41
1:B:250:PHE:CE2	1:B:251:THR:HG23	2.55	0.41
1:B:183:GLY:HA2	1:B:207:ASP:OD1	2.21	0.41
1:A:121:ILE:O	1:A:156:PHE:HA	2.20	0.41
1:B:222:LEU:O	7:B:306:OY3:H15	2.21	0.41
1:A:128:TYR:HD2	1:A:137:ILE:HD12	1.86	0.41
1:A:223:VAL:HA	7:B:306:OY3:H5	2.02	0.41
1:B:192:PHE:HA	1:B:193:PRO:HD3	1.94	0.40
1:B:228:PHE:O	1:B:232:LEU:HG	2.21	0.40
7:B:306:OY3:H59	7:B:306:OY3:O15	2.22	0.40
1:A:252:GLU:CA	1:A:252:GLU:OE1	2.67	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	163/164 (99%)	160 (98%)	3 (2%)	0	100	100
1	B	163/164 (99%)	154 (94%)	6 (4%)	3 (2%)	13	44
All	All	326/328 (99%)	314 (96%)	9 (3%)	3 (1%)	33	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	134[A]	ARG
1	B	134[B]	ARG
1	B	180	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	132/131 (101%)	113 (86%)	19 (14%)	5	13
1	B	132/131 (101%)	116 (88%)	16 (12%)	7	20
All	All	264/262 (101%)	229 (87%)	35 (13%)	6	16

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	111	GLU
1	A	129	SER
1	A	130	GLU
1	A	134[A]	ARG
1	A	134[B]	ARG
1	A	147	LEU
1	A	149	SER
1	A	155	THR
1	A	162	ARG
1	A	169	GLN
1	A	174	GLU
1	A	187	LEU
1	A	188	LEU

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Mol	Chain	Res	Type
1	A	208	GLU
1	A	214	LYS
1	A	241	GLU
1	A	247	MET
1	A	249	ARG
1	B	107	PHE
1	B	108	GLN
1	B	111	GLU
1	B	149	SER
1	B	151	VAL
1	B	155	THR
1	B	162	ARG
1	B	169	GLN
1	B	187	LEU
1	B	188	LEU
1	B	207	ASP
1	B	211	SER
1	B	214	LYS
1	B	238	SER
1	B	241	GLU
1	B	256	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	119	HIS
1	A	199	GLN
1	B	119	HIS
1	B	175	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 26 ligands modelled in this entry, 9 are monoatomic - leaving 17 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	$\# Z  > 2$
4	PEG	A	305	-	6,6,6	0.48	0	5,5,5	0.24	0
4	PEG	A	306	-	6,6,6	0.54	0	5,5,5	0.34	0
4	PEG	A	307	-	6,6,6	0.49	0	5,5,5	0.17	0
4	PEG	A	308	-	6,6,6	0.51	0	5,5,5	0.35	0
4	PEG	A	309	-	6,6,6	0.45	0	5,5,5	0.34	0
4	PEG	A	310	-	6,6,6	0.40	0	5,5,5	0.20	0
5	ACT	A	311	-	1,3,3	1.24	0	0,3,3	0.00	-
5	ACT	A	312	-	1,3,3	1.24	0	0,3,3	0.00	-
5	ACT	A	313	-	1,3,3	1.17	0	0,3,3	0.00	-
6	BCN	A	314	-	10,10,10	0.64	0	11,11,11	1.85	3 (27%)
6	BCN	A	315	-	10,10,10	0.63	0	11,11,11	1.89	3 (27%)
7	0Y3	B	306	2	82,82,82	2.09	7 (8%)	112,112,112	407.49	14 (12%)
4	PEG	B	307	-	6,6,6	0.56	0	5,5,5	0.26	0
4	PEG	B	308	-	6,6,6	0.35	0	5,5,5	0.21	0
4	PEG	B	309	-	6,6,6	0.42	0	5,5,5	0.36	0
5	ACT	B	310	-	1,3,3	1.12	0	0,3,3	0.00	-
6	BCN	B	311	-	10,10,10	0.61	0	11,11,11	1.90	3 (27%)

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
4	PEG	A	305	-	-	0/4/4/4	0/0/0/0
4	PEG	A	306	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	A	307	-	-	0/4/4/4	0/0/0/0
4	PEG	A	308	-	-	0/4/4/4	0/0/0/0
4	PEG	A	309	-	-	0/4/4/4	0/0/0/0
4	PEG	A	310	-	-	0/4/4/4	0/0/0/0
5	ACT	A	311	-	-	0/0/0/0	0/0/0/0
5	ACT	A	312	-	-	0/0/0/0	0/0/0/0
5	ACT	A	313	-	-	0/0/0/0	0/0/0/0
6	BCN	A	314	-	-	0/10/10/10	0/0/0/0
6	BCN	A	315	-	-	0/10/10/10	0/0/0/0
7	0Y3	B	306	2	-	0/84/94/94	0/5/5/5
4	PEG	B	307	-	-	0/4/4/4	0/0/0/0
4	PEG	B	308	-	-	0/4/4/4	0/0/0/0
4	PEG	B	309	-	-	0/4/4/4	0/0/0/0
5	ACT	B	310	-	-	0/0/0/0	0/0/0/0
6	BCN	B	311	-	-	0/10/10/10	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	306	0Y3	C2-S1	-8.18	1.64	1.76
7	B	306	0Y3	C63-S60	-8.01	1.64	1.76
7	B	306	0Y3	O56-N55	-7.10	1.28	1.41
7	B	306	0Y3	O17-N16	-6.98	1.28	1.41
7	B	306	0Y3	S1-N16	-6.29	1.56	1.70
7	B	306	0Y3	S60-N55	-6.11	1.57	1.70
7	B	306	0Y3	O17-C19	-2.44	1.42	1.46

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	306	0Y3	C19-O17-N16	3388.93	127.30	112.41
7	B	306	0Y3	C57-O56-N55	2666.83	124.12	112.41
7	B	306	0Y3	O17-N16-S1	15.29	122.05	105.96
7	B	306	0Y3	O56-N55-S60	12.11	118.70	105.96
7	B	306	0Y3	O61-S60-O62	-8.10	104.98	119.41
7	B	306	0Y3	O15-S1-O14	-7.70	105.68	119.41
6	A	314	BCN	C1-N1-C5	4.24	122.86	112.34
6	A	315	BCN	C1-N1-C3	3.77	121.69	112.34
7	B	306	0Y3	C63-S60-N55	3.64	114.57	102.13
6	B	311	BCN	C1-N1-C3	3.55	121.16	112.34
6	B	311	BCN	C5-N1-C3	3.27	119.36	111.44
6	A	315	BCN	C5-N1-C3	3.25	119.31	111.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	314	BCN	C1-N1-C3	3.21	120.31	112.34
6	B	311	BCN	C1-N1-C5	2.88	119.48	112.34
7	B	306	0Y3	C37-C34-N33	2.76	123.52	117.13
7	B	306	0Y3	O56-N55-C54	2.76	120.08	111.46
6	A	315	BCN	C1-N1-C5	2.68	118.99	112.34
7	B	306	0Y3	C2-S1-N16	2.50	110.67	102.13
7	B	306	0Y3	C27-N28-C29	2.47	127.84	122.81
7	B	306	0Y3	O35-C34-C37	-2.36	116.88	120.98
6	A	314	BCN	C5-N1-C3	2.22	116.82	111.44
7	B	306	0Y3	C45-N44-C43	2.14	127.02	122.16
7	B	306	0Y3	C50-N49-C48	2.06	127.01	122.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	164/164 (100%)	2.29	90 (54%) 0 0	1, 15, 35, 49	0
1	B	164/164 (100%)	2.31	88 (53%) 0 0	0, 14, 31, 42	0
All	All	328/328 (100%)	2.30	178 (54%) 0 0	0, 15, 35, 49	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	173	ALA	9.0
1	A	113	ASP	8.3
1	B	183	GLY	8.0
1	B	173	ALA	7.1
1	B	237	SER	6.3
1	B	213	GLY	6.1
1	A	213	GLY	6.1
1	B	255	PRO	6.0
1	A	183	GLY	6.0
1	A	209	LEU	5.8
1	A	224	ALA	5.7
1	A	172	VAL	5.6
1	B	236	HIS	5.4
1	A	231	ALA	5.3
1	B	174	GLU	5.3
1	B	109	THR	5.3
1	A	251	THR	5.3
1	B	251	THR	5.2
1	B	113	ASP	5.1
1	A	112	GLY	5.1
1	B	269	GLY	5.1
1	B	131	ASP	4.9
1	B	190	HIS	4.6
1	B	250	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	249	ARG	4.5
1	A	159	VAL	4.3
1	A	255	PRO	4.3
1	B	107	PHE	4.1
1	A	145	PHE	4.1
1	B	153	PRO	4.1
1	B	254	PRO	4.1
1	A	174	GLU	4.0
1	B	159	VAL	4.0
1	A	236	HIS	4.0
1	A	207	ASP	4.0
1	B	268	TYR	3.9
1	A	254	PRO	3.8
1	A	208	GLU	3.8
1	B	175	HIS	3.7
1	B	191	ALA	3.7
1	A	200	GLY	3.7
1	B	180	PRO	3.7
1	A	131	ASP	3.7
1	A	124	TRP	3.7
1	A	132	LEU	3.7
1	A	217	GLY	3.6
1	A	216	VAL	3.6
1	B	224	ALA	3.6
1	B	242	ALA	3.6
1	A	128	TYR	3.5
1	B	114	LEU	3.5
1	B	238	SER	3.5
1	B	266	HIS	3.5
1	B	209	LEU	3.4
1	B	215	GLY	3.4
1	B	233	GLY	3.4
1	A	242	ALA	3.4
1	A	196	PRO	3.4
1	A	215	GLY	3.3
1	A	120	ASN	3.3
1	B	128	TYR	3.3
1	B	244	MET	3.3
1	B	160	TYR	3.3
1	A	266	HIS	3.3
1	B	231	ALA	3.3
1	A	177	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	200	GLY	3.2
1	B	259	ASP	3.2
1	B	172	VAL	3.2
1	B	248	TYR	3.2
1	B	145	PHE	3.2
1	A	190	HIS	3.2
1	A	152	THR	3.1
1	A	193	PRO	3.1
1	A	127	ASN	3.0
1	B	176	GLY	3.0
1	B	118	HIS	3.0
1	A	180	PRO	3.0
1	B	249	ARG	3.0
1	A	176	GLY	3.0
1	A	212	LEU	2.9
1	B	141	PHE	2.9
1	A	257	HIS	2.9
1	B	193	PRO	2.9
1	A	244	MET	2.9
1	B	139	ASP	2.9
1	A	197	GLY	2.8
1	B	253	GLY	2.8
1	A	246	PRO	2.8
1	B	142	ALA	2.8
1	A	233	GLY	2.8
1	B	212	LEU	2.8
1	A	194	PRO	2.8
1	A	232	LEU	2.8
1	A	160	TYR	2.7
1	B	152	THR	2.7
1	A	121	ILE	2.7
1	B	208	GLU	2.7
1	B	207	ASP	2.7
1	A	153	PRO	2.7
1	A	106	GLY	2.7
1	A	225	ALA	2.7
1	B	192	PHE	2.7
1	B	221	PHE	2.7
1	A	133	PRO	2.7
1	A	237	SER	2.7
1	A	218	TYR	2.6
1	A	268	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	112	GLY	2.6
1	A	239	VAL	2.6
1	A	269	GLY	2.6
1	B	119	HIS	2.6
1	B	182	ASP	2.6
1	B	214	LYS	2.6
1	B	228	PHE	2.5
1	A	259	ASP	2.5
1	B	148	TRP	2.5
1	B	121	ILE	2.5
1	B	166	ILE	2.5
1	B	197	GLY	2.5
1	A	158	ARG	2.5
1	B	163	ASP	2.5
1	B	126	GLN	2.5
1	A	175	HIS	2.5
1	A	214	LYS	2.5
1	B	258	LYS	2.5
1	A	122	THR	2.5
1	B	127	ASN	2.5
1	A	161	SER	2.5
1	A	185	ASP	2.4
1	B	124	TRP	2.4
1	B	161	SER	2.4
1	B	144	ALA	2.4
1	B	147	LEU	2.4
1	A	191	ALA	2.4
1	A	143	ARG	2.4
1	B	216	VAL	2.4
1	A	199	GLN	2.4
1	A	204	PHE	2.4
1	A	248	TYR	2.4
1	B	171	GLY	2.3
1	A	119	HIS	2.3
1	A	181	PHE	2.3
1	B	170	PHE	2.3
1	B	225	ALA	2.3
1	B	223	VAL	2.3
1	A	228	PHE	2.3
1	B	243	LEU	2.3
1	B	257	HIS	2.3
1	A	136	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	250	PHE	2.3
1	B	110	PHE	2.3
1	A	227	GLU	2.2
1	A	243	LEU	2.2
1	A	223	VAL	2.2
1	A	114	LEU	2.2
1	B	194	PRO	2.2
1	A	147	LEU	2.2
1	A	142	ALA	2.2
1	A	179	TYR	2.2
1	A	155	THR	2.2
1	A	162	ARG	2.2
1	A	230	HIS	2.2
1	B	199	GLN	2.1
1	B	260	ASP	2.1
1	A	262	ASN	2.1
1	A	238	SER	2.1
1	B	137	ILE	2.1
1	B	265	ARG	2.1
1	B	177	ASP	2.0
1	A	198	ILE	2.0
1	A	118	HIS	2.0
1	B	203	HIS	2.0
1	B	226	HIS	2.0
1	A	163	ASP	2.0
1	B	123	TYR	2.0
1	B	181	PHE	2.0
1	A	234	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	CA	B	305	1/1	0.71	3.25	51,51,51,51	0
7	0Y3	B	306	78/78	0.47	1.24	32,38,49,50	0
3	CA	A	304	1/1	0.40	0.34	21,21,21,21	0
4	PEG	A	306	7/7	0.36	0.19	23,23,23,24	0
4	PEG	A	305	7/7	0.31	0.02	16,17,18,18	0
6	BCN	A	315	11/11	0.35	-1.04	41,41,41,41	0
4	PEG	A	309	7/7	0.30	-1.09	29,29,30,30	0
4	PEG	A	310	7/7	0.26	-1.17	2,2,2,3	0
3	CA	B	304	1/1	0.17	-1.19	25,25,25,25	0
4	PEG	A	308	7/7	0.25	-1.23	13,13,14,14	0
6	BCN	B	311	11/11	0.30	-1.42	38,38,38,38	0
6	BCN	A	314	11/11	0.30	-1.50	17,18,18,18	0
5	ACT	B	310	4/4	0.33	-1.73	10,10,10,10	0
5	ACT	A	313	4/4	0.24	-1.74	6,6,6,6	0
2	ZN	A	302	1/1	0.26	-1.89	15,15,15,15	0
5	ACT	A	312	4/4	0.23	-2.03	17,17,17,17	0
4	PEG	B	308	7/7	0.24	-2.09	5,5,6,6	0
4	PEG	B	307	7/7	0.34	-2.38	20,20,20,20	0
2	ZN	B	301	1/1	0.14	-2.66	17,17,17,17	0
2	ZN	B	302	1/1	0.15	-3.03	13,13,13,13	0
3	CA	A	303	1/1	0.13	-3.17	15,15,15,15	0
3	CA	B	303	1/1	0.06	-3.57	13,13,13,13	0
2	ZN	A	301	1/1	0.09	-4.68	16,16,16,16	0
4	PEG	B	309	7/7	0.20	-11.98	3,3,3,3	0
4	PEG	A	307	7/7	0.33	-	24,24,24,24	0
5	ACT	A	311	4/4	0.28	-	5,5,5,5	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.