



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 29, 2024 – 04:32 AM EDT

PDB ID : 3MPR  
Title : Crystal Structure of endonuclease/exonuclease/phosphatase family protein from *Bacteroides thetaiotaomicron*, Northeast Structural Genomics Consortium Target BtR318A  
Authors : Kuzin, A.; Su, M.; Seetharaman, J.; Mao, M.; Xiao, R.; Ciccocanti, C.; Lee, D.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2010-04-27  
Resolution : 1.90 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](mailto: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>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

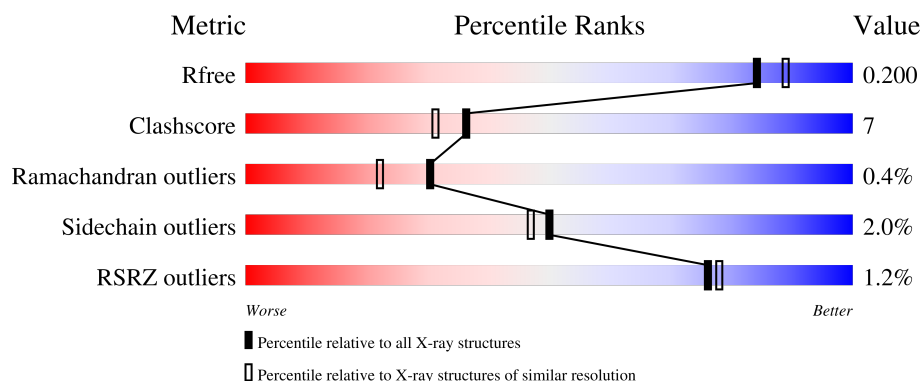
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	298	
1	B	298	
1	C	298	
1	D	298	

Validation Pipeline (wwPDB-VP) : 2.39

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
2	ACY	A	1311	-	-	X	-
2	ACY	D	1311	-	-	X	-
3	BR	D	301	-	-	X	-
4	UNL	A	455	-	-	X	-
5	PEG	C	306	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10382 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 Putative endonuclease/exonuclease/phosphatase family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	Se	0	2	0
			2307	1469	398	430	5	5			
1	B	271	Total	C	N	O	S	Se	0	1	0
			2213	1413	376	415	5	4			
1	C	281	Total	C	N	O	S	Se	0	3	0
			2302	1468	397	427	5	5			
1	D	275	Total	C	N	O	S	Se	0	8	0
			2271	1447	384	430	6	4			

There are 32 discrepancies between the modelled and reference sequences:

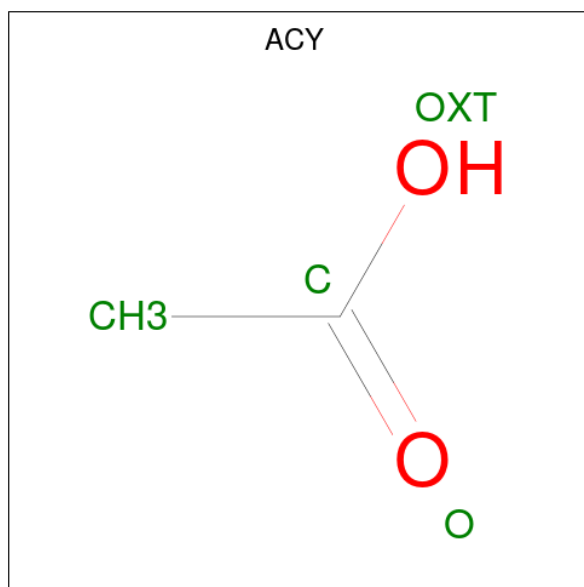
Chain	Residue	Modelled	Actual	Comment	Reference
A	291	LEU	-	expression tag	UNP Q8A183
A	292	GLU	-	expression tag	UNP Q8A183
A	293	HIS	-	expression tag	UNP Q8A183
A	294	HIS	-	expression tag	UNP Q8A183
A	295	HIS	-	expression tag	UNP Q8A183
A	296	HIS	-	expression tag	UNP Q8A183
A	297	HIS	-	expression tag	UNP Q8A183
A	298	HIS	-	expression tag	UNP Q8A183
B	291	LEU	-	expression tag	UNP Q8A183
B	292	GLU	-	expression tag	UNP Q8A183
B	293	HIS	-	expression tag	UNP Q8A183
B	294	HIS	-	expression tag	UNP Q8A183
B	295	HIS	-	expression tag	UNP Q8A183
B	296	HIS	-	expression tag	UNP Q8A183
B	297	HIS	-	expression tag	UNP Q8A183
B	298	HIS	-	expression tag	UNP Q8A183
C	291	LEU	-	expression tag	UNP Q8A183
C	292	GLU	-	expression tag	UNP Q8A183
C	293	HIS	-	expression tag	UNP Q8A183
C	294	HIS	-	expression tag	UNP Q8A183

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Chain	Residue	Modelled	Actual	Comment	Reference
C	295	HIS	-	expression tag	UNP Q8A183
C	296	HIS	-	expression tag	UNP Q8A183
C	297	HIS	-	expression tag	UNP Q8A183
C	298	HIS	-	expression tag	UNP Q8A183
D	291	LEU	-	expression tag	UNP Q8A183
D	292	GLU	-	expression tag	UNP Q8A183
D	293	HIS	-	expression tag	UNP Q8A183
D	294	HIS	-	expression tag	UNP Q8A183
D	295	HIS	-	expression tag	UNP Q8A183
D	296	HIS	-	expression tag	UNP Q8A183
D	297	HIS	-	expression tag	UNP Q8A183
D	298	HIS	-	expression tag	UNP Q8A183

- Molecule 2 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			4	2	2		

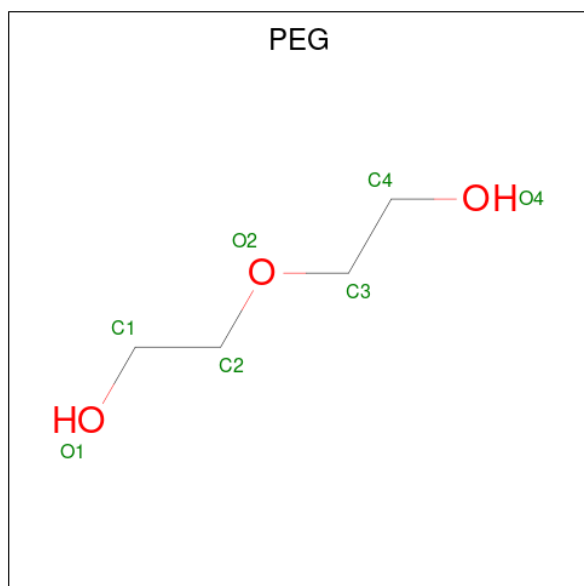
- Molecule 3 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	Br	0	0
			5	5		
3	B	3	Total	Br	0	0
			3	3		
3	C	3	Total	Br	0	0
			3	3		
3	D	3	Total	Br	0	0
			3	3		

- Molecule 4 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		

- Molecule 5 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
5	C	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	1
			14	8	6		

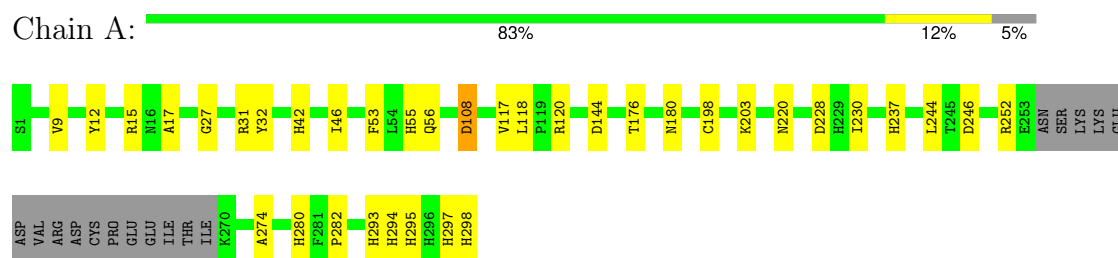
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	354	Total	O	0	0
			354	354		
6	B	304	Total	O	0	0
			304	304		
6	C	300	Total	O	0	0
			300	300		
6	D	264	Total	O	0	0
			264	264		

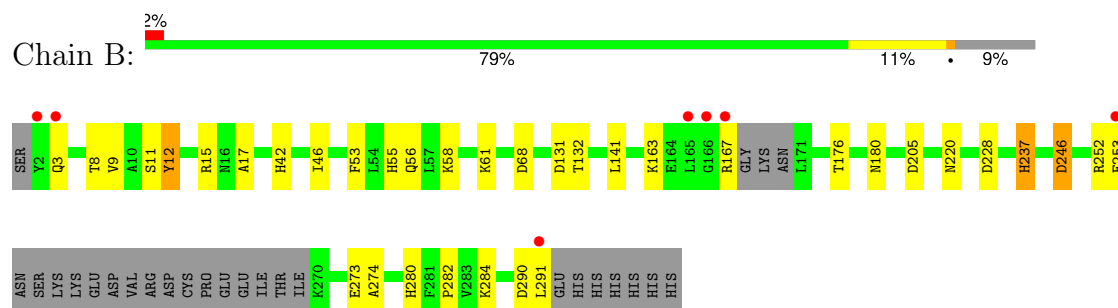
### 3 Residue-property plots

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.

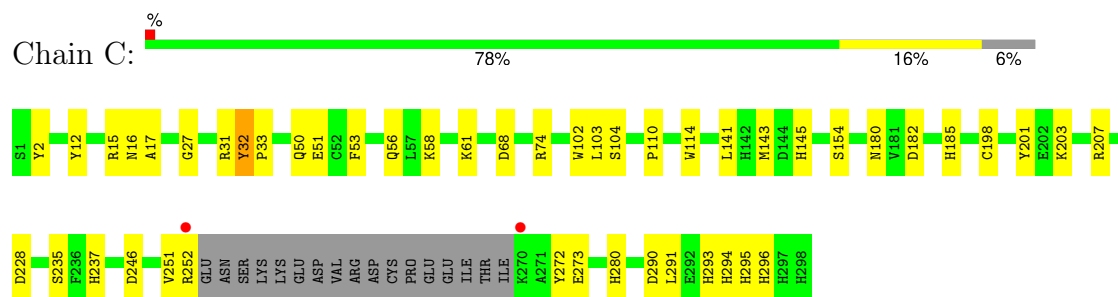
- Molecule 1: Putative endonuclease/exonuclease/phosphatase family protein



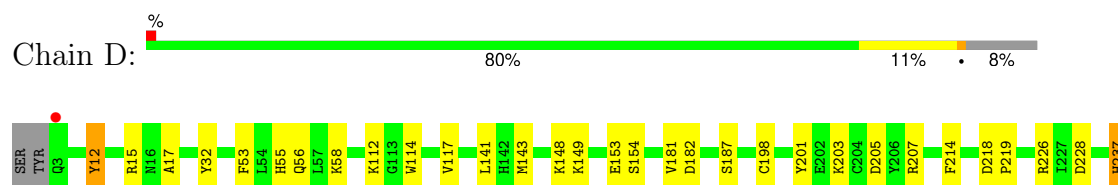
- Molecule 1: Putative endonuclease/exonuclease/phosphatase family protein



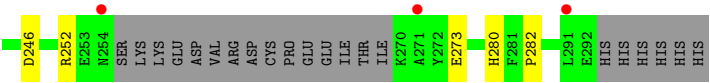
- Molecule 1: Putative endonuclease/exonuclease/phosphatase family protein



- Molecule 1: Putative endonuclease/exonuclease/phosphatase family protein







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.64Å 103.14Å 79.81Å 90.00° 103.39° 90.00°	Depositor
Resolution (Å)	39.47 – 1.90 39.47 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.47-1.90) 99.4 (39.47-1.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.50 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.6.1_357, REFMAC	Depositor
R, $R_{free}$	0.156 , 0.204 0.153 , 0.200	Depositor DCC
$R_{free}$ test set	4744 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.2	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10382	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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: UNL, BR, PEG, ACY

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	0.36	0/2377	0.54	0/3204
1	B	0.37	0/2271	0.54	0/3061
1	C	0.33	0/2375	0.52	0/3202
1	D	0.34	0/2350	0.52	0/3166
All	All	0.35	0/9373	0.53	0/12633

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	2307	0	2173	26	0
1	B	2213	0	2086	33	0
1	C	2302	0	2176	47	0
1	D	2271	0	2156	23	0
2	A	8	0	6	3	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	8	0	6	2	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	0	0	0
3	C	3	0	0	2	0
3	D	3	0	0	2	0
4	A	8	0	0	2	0
5	C	21	0	30	8	0
6	A	354	0	0	5	0
6	B	304	0	0	8	0
6	C	300	0	0	2	0
6	D	264	0	0	3	0
All	All	10382	0	8639	127	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 7.

All (127) 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:274:ALA:H	1:B:220:ASN:HD22	1.13	0.92
1:A:220:ASN:HD22	1:B:274:ALA:H	1.18	0.92
1:C:252:ARG:HE	1:C:273:GLU:HB3	1.35	0.91
1:C:103:LEU:HD13	1:C:143[B]:MSE:HE1	1.64	0.80
1:C:235:SER:O	5:C:307[A]:PEG:H42	1.82	0.80
1:B:55:HIS:HD2	6:B:991:HOH:O	1.66	0.79
1:C:103:LEU:HD13	1:C:143[B]:MSE:CE	2.15	0.76
1:D:252:ARG:HB2	1:D:273:GLU:OE2	1.87	0.74
1:B:228:ASP:OD1	1:B:280:HIS:HD2	1.73	0.72
1:D:198[B]:CYS:SG	1:D:203:LYS:HD3	2.31	0.71
1:A:228:ASP:OD1	1:A:280:HIS:HD2	1.74	0.70
1:D:228:ASP:OD1	1:D:280:HIS:HD2	1.73	0.70
1:C:252:ARG:HH21	1:C:273:GLU:CD	1.94	0.70
1:A:42:HIS:HD2	6:A:768:HOH:O	1.75	0.69
6:B:1149:HOH:O	1:C:295:HIS:HB2	1.94	0.67
1:C:228:ASP:OD1	1:C:280:HIS:HD2	1.78	0.65
1:C:252:ARG:HH21	1:C:273:GLU:CG	2.09	0.65
1:A:274:ALA:H	1:B:220:ASN:ND2	1.91	0.64
1:B:280:HIS:HE1	6:B:599:HOH:O	1.81	0.63
1:B:61:LYS:HE2	1:B:68:ASP:OD1	2.01	0.61
1:D:181:VAL:HG21	1:D:187[B]:SER:OG	2.02	0.59
4:A:451:UNL:O	4:A:455:UNL:O	2.22	0.58
1:C:237:HIS:HB2	5:C:307[A]:PEG:H22	1.86	0.58
1:C:252:ARG:NH2	1:C:273:GLU:CD	2.56	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:LYS:HZ2	1:B:58:LYS:HB2	1.68	0.57
1:C:293:HIS:HD2	6:C:367:HOH:O	1.86	0.57
1:C:296:HIS:HE1	5:C:307[B]:PEG:O4	1.88	0.57
1:D:55:HIS:HD2	6:D:1089:HOH:O	1.87	0.56
1:C:2:TYR:CD1	1:C:291:LEU:HD13	2.40	0.56
1:B:290:ASP:O	1:B:291:LEU:HB2	2.06	0.55
1:B:205:ASP:OD2	1:B:237:HIS:HE1	1.89	0.55
1:A:294:HIS:HE1	6:A:442:HOH:O	1.88	0.55
1:A:220:ASN:ND2	1:B:274:ALA:H	1.98	0.55
1:A:237:HIS:HB2	5:C:306:PEG:H22	1.88	0.55
1:A:108:ASP:OD2	2:A:1311:ACY:H3	2.07	0.54
1:C:2:TYR:CG	1:C:291:LEU:HD22	2.43	0.54
1:B:11:SER:HB2	1:B:176:THR:HB	1.89	0.54
1:C:143[B]:MSE:HA	1:C:143[B]:MSE:HE2	1.90	0.54
1:B:58:LYS:HB2	1:B:58:LYS:NZ	2.23	0.54
1:C:203:LYS:NZ	3:C:301:BR:BR	2.96	0.54
1:D:112:LYS:HE2	1:D:117:VAL:O	2.08	0.54
4:A:455:UNL:O	4:A:457:UNL:O	2.25	0.54
1:B:42:HIS:HD2	6:B:766:HOH:O	1.90	0.53
1:D:205:ASP:OD2	1:D:237:HIS:HE1	1.91	0.53
1:C:145:HIS:HA	1:C:180:ASN:ND2	2.23	0.53
1:C:251:VAL:HG22	1:C:272:TYR:CE2	2.42	0.53
1:C:27:GLY:O	1:C:31:ARG:HG3	2.09	0.53
1:A:55:HIS:HD2	6:A:972:HOH:O	1.91	0.53
1:A:244:LEU:HB2	1:A:282:PRO:HG2	1.90	0.53
1:C:290:ASP:O	1:C:294:HIS:HD2	1.91	0.52
1:D:58[B]:LYS:HG2	6:D:777:HOH:O	2.10	0.51
1:A:108:ASP:CG	2:A:1311:ACY:H3	2.31	0.51
1:C:74:ARG:HD3	3:C:300:BR:BR	2.66	0.51
1:D:182:ASP:HA	1:D:226:ARG:O	2.09	0.51
1:C:198:CYS:HB3	1:C:203:LYS:HG3	1.93	0.50
1:C:2:TYR:HD1	1:C:291:LEU:HD13	1.77	0.50
1:D:12:TYR:CZ	1:D:282:PRO:HG3	2.47	0.49
1:D:148:LYS:O	1:D:148:LYS:HD3	2.12	0.49
1:D:187[A]:SER:HB2	3:D:301:BR:BR	2.67	0.49
1:A:293:HIS:HD2	6:A:809:HOH:O	1.95	0.49
1:D:205:ASP:OD2	1:D:237:HIS:CE1	2.66	0.48
1:A:117:VAL:HG23	1:A:118:LEU:HD13	1.95	0.48
1:C:58:LYS:HE3	1:C:58:LYS:HB2	1.66	0.48
1:C:252:ARG:HH21	1:C:273:GLU:HG2	1.76	0.48
1:B:131:ASP:HB3	1:C:2:TYR:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:306:PEG:H12	6:C:374:HOH:O	2.14	0.48
1:B:61:LYS:HG2	6:B:323:HOH:O	2.13	0.48
1:C:141:LEU:HD13	1:C:143[B]:MSE:HE3	1.96	0.48
1:B:42:HIS:HE1	1:B:246:ASP:OD2	1.97	0.48
1:C:182:ASP:OD1	1:C:185:HIS:HD2	1.97	0.47
1:B:17:ALA:H	1:B:56:GLN:NE2	2.12	0.47
1:A:17:ALA:H	1:A:56:GLN:NE2	2.12	0.47
1:A:53:PHE:H	1:A:56:GLN:NE2	2.12	0.47
1:D:148:LYS:HE3	3:D:301:BR:BR	2.71	0.46
1:A:117:VAL:O	1:A:118:LEU:HD12	2.16	0.46
1:C:16:ASN:HA	1:C:56:GLN:HE22	1.81	0.46
1:D:17:ALA:H	1:D:56:GLN:NE2	2.13	0.46
6:B:371:HOH:O	1:C:294:HIS:HE1	1.97	0.46
1:B:58:LYS:NZ	1:B:58:LYS:CB	2.80	0.45
1:B:205:ASP:OD2	1:B:237:HIS:CE1	2.67	0.45
1:C:104:SER:HA	1:C:114:TRP:CZ3	2.52	0.45
1:C:17:ALA:H	1:C:56:GLN:NE2	2.14	0.45
1:D:53:PHE:H	1:D:56:GLN:NE2	2.14	0.45
1:D:141:LEU:HD12	1:D:141:LEU:C	2.37	0.45
1:A:274:ALA:N	1:B:220:ASN:HD22	1.95	0.45
1:B:12:TYR:CZ	1:B:282:PRO:HG3	2.52	0.45
1:D:143:MSE:HE2	1:D:154:SER:HB3	1.99	0.44
1:A:9:VAL:HG12	1:A:46:ILE:HG23	1.99	0.44
1:C:201:TYR:CE2	1:C:207:ARG:HD3	2.53	0.43
1:B:9:VAL:HG12	1:B:46:ILE:HG23	2.00	0.43
1:B:131:ASP:HB3	1:C:2:TYR:CE1	2.52	0.43
1:C:102:TRP:CE2	1:C:110:PRO:HA	2.53	0.43
1:C:53:PHE:H	1:C:56:GLN:NE2	2.15	0.43
1:C:143[B]:MSE:HE1	1:C:154:SER:HB3	2.01	0.43
1:D:201:TYR:CE2	1:D:207:ARG:HD3	2.54	0.43
1:D:214:PHE:O	2:D:1311:ACY:H3	2.19	0.43
1:C:294:HIS:HA	5:C:307[B]:PEG:H42	2.00	0.42
1:C:61:LYS:HE2	1:C:68:ASP:OD1	2.20	0.42
2:A:1310:ACY:H1	6:B:358:HOH:O	2.20	0.42
1:C:50:GLN:O	1:C:51:GLU:HB2	2.20	0.42
1:A:120:ARG:CZ	1:A:144:ASP:HA	2.49	0.42
1:C:290:ASP:O	1:C:294:HIS:CD2	2.72	0.42
1:A:237:HIS:HB2	5:C:306:PEG:H31	2.01	0.42
1:A:295:HIS:HB2	6:A:990:HOH:O	2.20	0.41
1:B:55:HIS:HE1	6:B:992:HOH:O	2.04	0.41
1:B:290:ASP:O	1:B:291:LEU:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:CYS:HB3	1:A:203:LYS:HG3	2.01	0.41
1:B:53:PHE:H	1:B:56:GLN:NE2	2.17	0.41
1:B:8:THR:HG21	1:B:284:LYS:HE3	2.02	0.41
1:A:27:GLY:O	1:A:31:ARG:HG3	2.21	0.41
1:C:32:TYR:CG	1:C:33:PRO:HD3	2.56	0.41
1:C:237:HIS:CD2	5:C:306:PEG:H41	2.55	0.41
1:B:141:LEU:HD12	1:B:141:LEU:C	2.41	0.41
1:A:297:HIS:O	1:A:298:HIS:HD2	2.04	0.41
1:D:53:PHE:H	1:D:56:GLN:HE21	1.69	0.41
1:B:252:ARG:HG3	1:B:273:GLU:OE2	2.21	0.41
1:D:114:TRP:CZ2	1:D:153:GLU:HB3	2.56	0.40
1:D:218:ASP:HA	1:D:219:PRO:HD3	1.91	0.40
2:D:1311:ACY:H3	6:D:323:HOH:O	2.21	0.40
1:A:176:THR:HG22	1:A:230:ILE:HG12	2.02	0.40
1:B:53:PHE:H	1:B:56:GLN:HE21	1.68	0.40
1:C:2:TYR:CB	1:C:291:LEU:HD22	2.52	0.40
1:C:198:CYS:HB3	1:C:203:LYS:CG	2.50	0.40
1:B:163:LYS:O	1:B:167:ARG:HB2	2.21	0.40
1:C:141:LEU:C	1:C:141:LEU:HD12	2.42	0.40
1:B:3:GLN:HG3	1:B:132:THR:HG22	2.03	0.40
1:C:53:PHE:H	1:C:56:GLN:HE21	1.69	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	280/298 (94%)	272 (97%)	7 (2%)	1 (0%)	30	22
1	B	266/298 (89%)	258 (97%)	7 (3%)	1 (0%)	30	22
1	C	280/298 (94%)	271 (97%)	8 (3%)	1 (0%)	30	22
1	D	279/298 (94%)	272 (98%)	6 (2%)	1 (0%)	30	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1105/1192 (93%)	1073 (97%)	28 (2%)	4 (0%)	30 22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	15	ARG
1	D	15	ARG
1	A	15	ARG
1	B	15	ARG

### 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	249/259 (96%)	243 (98%)	6 (2%)	44 39
1	B	238/259 (92%)	233 (98%)	5 (2%)	48 45
1	C	249/259 (96%)	246 (99%)	3 (1%)	67 68
1	D	248/259 (96%)	243 (98%)	5 (2%)	50 47
All	All	984/1036 (95%)	965 (98%)	19 (2%)	50 49

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	TYR
1	A	32	TYR
1	A	108	ASP
1	A	180	ASN
1	A	246	ASP
1	A	252	ARG
1	B	12	TYR
1	B	180	ASN
1	B	237	HIS
1	B	246	ASP
1	B	253	GLU

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Mol	Chain	Res	Type
1	C	12	TYR
1	C	32	TYR
1	C	246	ASP
1	D	12	TYR
1	D	32	TYR
1	D	149	LYS
1	D	237	HIS
1	D	246	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	16	ASN
1	A	30	GLN
1	A	42	HIS
1	A	55	HIS
1	A	56	GLN
1	A	159	GLN
1	A	170	ASN
1	A	180	ASN
1	A	185	HIS
1	A	220	ASN
1	A	280	HIS
1	A	293	HIS
1	A	294	HIS
1	B	3	GLN
1	B	16	ASN
1	B	30	GLN
1	B	37	GLN
1	B	42	HIS
1	B	55	HIS
1	B	56	GLN
1	B	159	GLN
1	B	220	ASN
1	B	237	HIS
1	B	280	HIS
1	C	16	ASN
1	C	30	GLN
1	C	42	HIS
1	C	56	GLN
1	C	170	ASN

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Mol	Chain	Res	Type
1	C	185	HIS
1	C	280	HIS
1	C	293	HIS
1	C	294	HIS
1	C	296	HIS
1	D	16	ASN
1	D	30	GLN
1	D	55	HIS
1	D	56	GLN
1	D	237	HIS
1	D	280	HIS

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 14 are monoatomic and 8 are unknown - leaving 9 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	$\# Z  > 2$
2	ACY	D	1310	-	3,3,3	0.88	0	3,3,3	0.64	0
2	ACY	D	1311	-	3,3,3	0.79	0	3,3,3	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ACY	B	1310	-	3,3,3	0.86	0	3,3,3	0.69	0
2	ACY	C	1310	-	3,3,3	0.85	0	3,3,3	0.67	0
5	PEG	C	306	-	6,6,6	0.64	0	5,5,5	1.43	0
2	ACY	A	1310	-	3,3,3	0.74	0	3,3,3	1.14	0
5	PEG	C	307[A]	-	6,6,6	0.68	0	5,5,5	1.26	0
5	PEG	C	307[B]	-	6,6,6	0.64	0	5,5,5	1.51	1 (20%)
2	ACY	A	1311	-	3,3,3	0.80	0	3,3,3	1.03	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
5	PEG	C	307[A]	-	-	1/4/4/4	-
5	PEG	C	306	-	-	1/4/4/4	-
5	PEG	C	307[B]	-	-	1/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	307[B]	PEG	O2-C3-C4	2.01	118.98	110.11

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	307[A]	PEG	C4-C3-O2-C2
5	C	307[B]	PEG	C4-C3-O2-C2
5	C	306	PEG	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1311	ACY	2	0
5	C	306	PEG	4	0
2	A	1310	ACY	1	0
5	C	307[A]	PEG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	307[B]	PEG	2	0
2	A	1311	ACY	2	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	278/298 (93%)	-0.69	0	100	100	5, 13, 28, 71	1 (0%)
1	B	267/298 (89%)	-0.56	7 (2%)	57	59	7, 15, 33, 76	1 (0%)
1	C	277/298 (92%)	-0.39	2 (0%)	84	86	9, 18, 36, 71	2 (0%)
1	D	271/298 (90%)	-0.37	4 (1%)	71	74	8, 17, 37, 72	8 (2%)
All	All	1093/1192 (91%)	-0.50	13 (1%)	76	78	5, 15, 34, 76	12 (1%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	291	LEU	4.1
1	D	254	ASN	3.7
1	C	270	LYS	3.0
1	C	252	ARG	2.9
1	B	167	ARG	2.5
1	B	166	GLY	2.4
1	B	165	LEU	2.4
1	B	253	GLU	2.4
1	D	271	ALA	2.3
1	B	2	TYR	2.3
1	D	3	GLN	2.2
1	D	291	LEU	2.2
1	B	3	GLN	2.1

### 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

There are no monosaccharides 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. 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	UNL	A	457	1/-	0.72	0.22	39,39,39,39	0
4	UNL	A	452	1/-	0.77	0.17	36,36,36,36	0
2	ACY	C	1310	4/4	0.77	0.18	36,43,45,49	0
2	ACY	D	1310	4/4	0.78	0.18	47,49,49,51	0
4	UNL	A	450	1/-	0.80	0.19	30,30,30,30	0
2	ACY	B	1310	4/4	0.82	0.14	30,38,39,39	0
4	UNL	A	459	1/-	0.82	0.14	39,39,39,39	0
5	PEG	C	306	7/7	0.82	0.17	26,33,43,45	0
2	ACY	D	1311	4/4	0.86	0.16	34,42,44,48	0
4	UNL	A	455	1/-	0.87	0.17	26,26,26,26	0
3	BR	A	303	1/1	0.87	0.16	94,94,94,94	0
2	ACY	A	1310	4/4	0.87	0.15	15,33,34,41	0
2	ACY	A	1311	4/4	0.87	0.18	20,34,34,39	0
3	BR	A	302	1/1	0.89	0.13	92,92,92,92	0
4	UNL	A	451	1/-	0.90	0.11	21,21,21,21	0
4	UNL	A	454	1/-	0.91	0.17	30,30,30,30	0
5	PEG	C	307[A]	7/7	0.92	0.15	0,23,27,27	7
5	PEG	C	307[B]	7/7	0.92	0.15	16,22,26,27	7
4	UNL	A	460	1/-	0.94	0.09	27,27,27,27	0
3	BR	D	301	1/1	0.96	0.10	43,43,43,43	0
3	BR	A	301	1/1	0.97	0.19	50,50,50,50	0
3	BR	C	300	1/1	0.97	0.15	50,50,50,50	0
3	BR	D	300	1/1	0.97	0.23	67,67,67,67	0
3	BR	A	300	1/1	0.98	0.17	56,56,56,56	0
3	BR	B	301	1/1	0.99	0.21	52,52,52,52	0
3	BR	C	301	1/1	0.99	0.15	40,40,40,40	0
3	BR	D	299	1/1	0.99	0.08	26,26,26,26	0
3	BR	C	299	1/1	0.99	0.07	29,29,29,29	0
3	BR	A	299	1/1	1.00	0.04	20,20,20,20	0
3	BR	B	299	1/1	1.00	0.11	31,31,31,31	0
3	BR	B	300	1/1	1.00	0.04	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.