



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 12:35 AM GMT

PDB ID : 2GUG  
Title : NAD-dependent formate dehydrogenase from Pseudomonas sp.101 in complex with formate  
Authors : Filippova, E.V.; Polyakov, K.M.; Tikhonova, T.V.; Boiko, K.M.; Tishkov, V.I.; Popov, V.O.  
Deposited on : 2006-04-30  
Resolution : 2.28 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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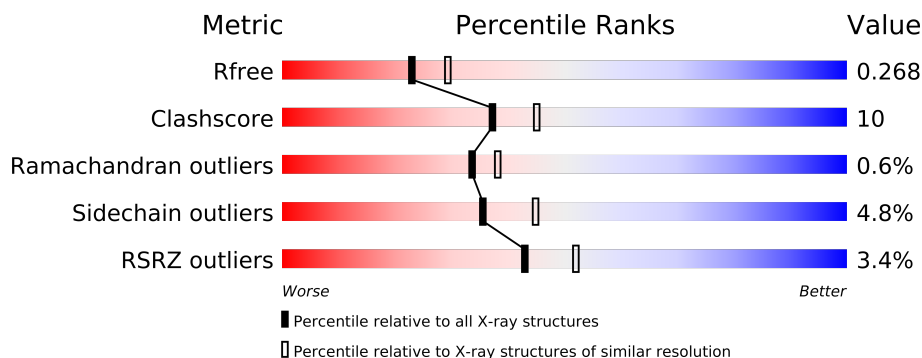
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
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) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.28 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	3861 (2.30-2.26)
Clashscore	79885	4801 (2.30-2.26)
Ramachandran outliers	78287	4729 (2.30-2.26)
Sidechain outliers	78261	4728 (2.30-2.26)
RSRZ outliers	66119	3864 (2.30-2.26)

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	401	
1	B	401	
1	C	401	
1	D	401	

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	FMT	C	401	-	X
4	PEG	A	476	-	X
4	PEG	A	477	-	X
4	PEG	C	482	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11994 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.

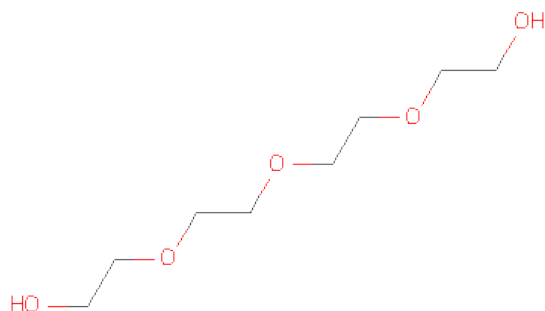
- Molecule 1 is a protein called Formate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	2	0
			2884	1824	510	536	14			
1	B	369	Total	C	N	O	S	0	2	0
			2906	1838	510	544	14			
1	C	369	Total	C	N	O	S	0	1	0
			2901	1836	507	544	14			
1	D	362	Total	C	N	O	S	0	0	0
			2837	1797	496	530	14			

There are 4 discrepancies between the modelled and reference sequences:

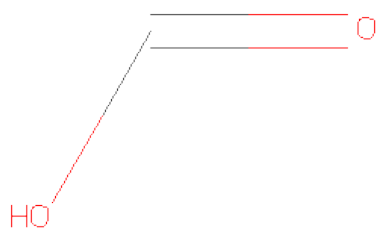
Chain	Residue	Modelled	Actual	Comment	Reference
A	354	OCS	CYS	MODIFIED RESIDUE	UNP P33160
B	354	OCS	CYS	MODIFIED RESIDUE	UNP P33160
C	354	OCS	CYS	MODIFIED RESIDUE	UNP P33160
D	354	OCS	CYS	MODIFIED RESIDUE	UNP P33160

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		
2	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula:  $\text{CH}_2\text{O}_2$ ).



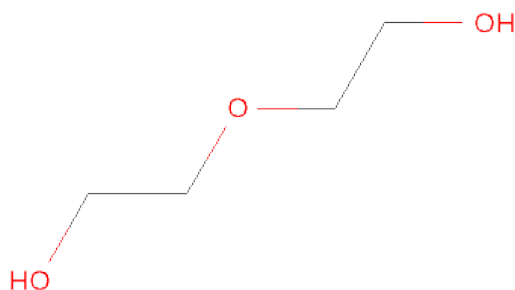
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	112	Total	O	0	0
			112	112		
5	B	106	Total	O	0	0
			106	106		

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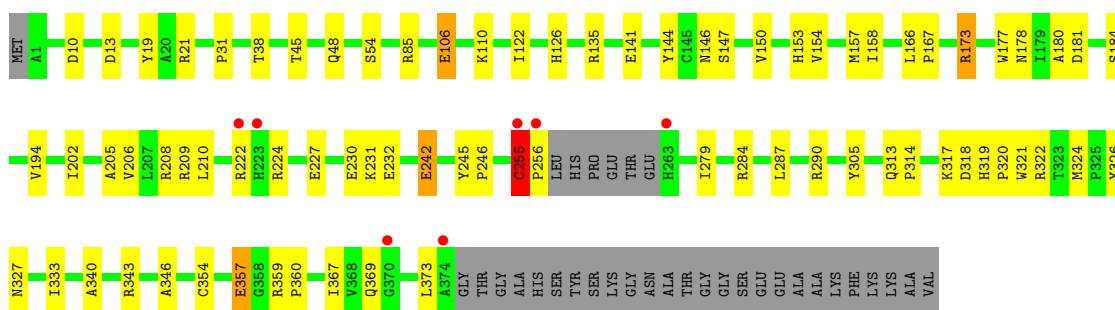
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	87	Total	O	0	0
			87	87		
5	D	84	Total	O	0	0
			84	84		

### 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 ( $RSRZ > 2$ ). 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.

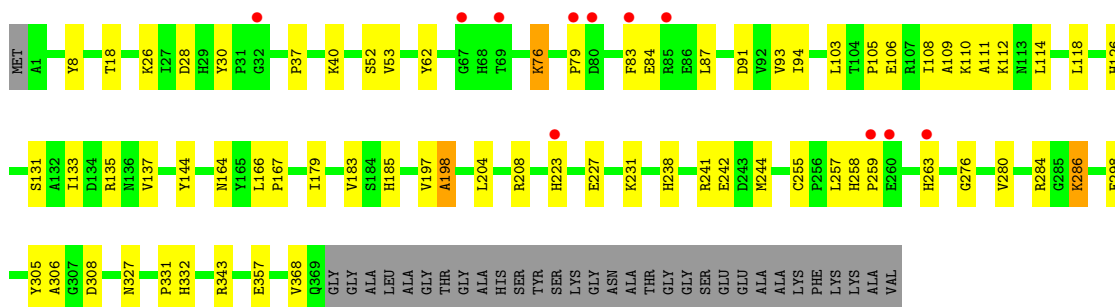
- Molecule 1: Formate dehydrogenase

Chain A:



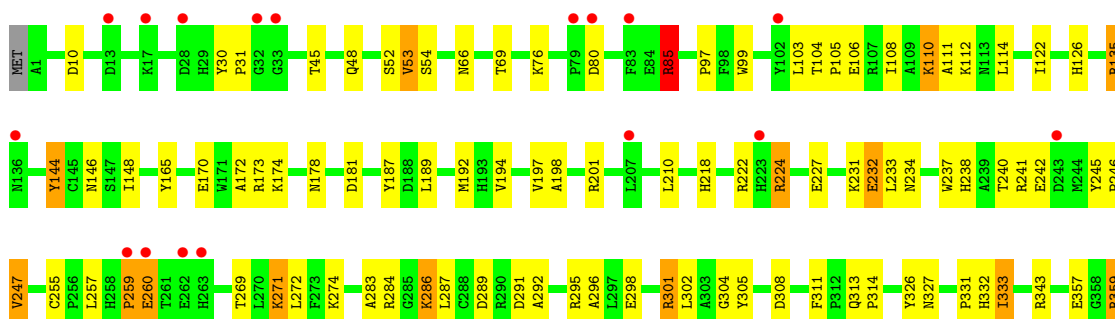
- Molecule 1: Formate dehydrogenase

Chain B:



- Molecule 1: Formate dehydrogenase

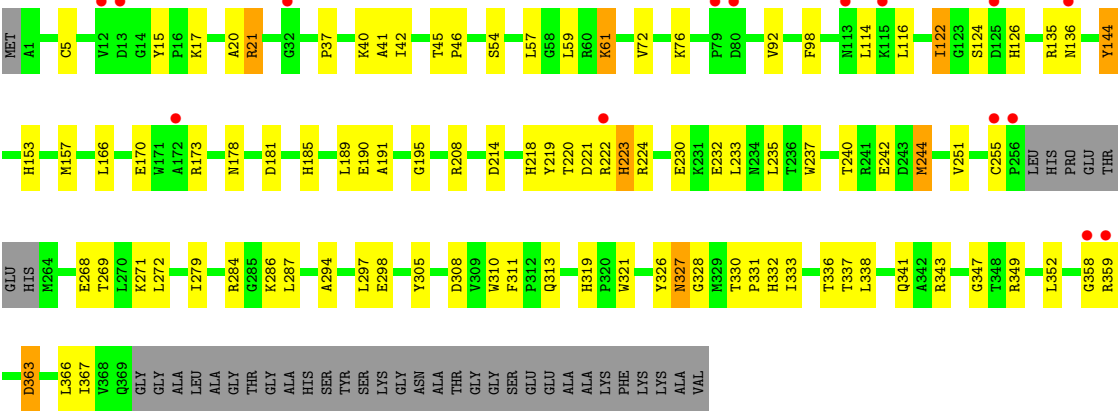
Chain C:





● Molecule 1: Formate dehydrogenase

Chain D:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.00Å 54.98Å 128.91Å 90.00° 95.74° 90.00°	Depositor
Resolution (Å)	100.00 – 2.28 16.10 – 2.28	Depositor EDS
% Data completeness (in resolution range)	97.5 (100.00-2.28) 97.8 (16.10-2.28)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.00 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.196 , 0.269 0.197 , 0.268	Depositor DCC
$R_{free}$ test set	3696 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.8	Xtriage
Anisotropy	0.874	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 30.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 73290 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11994	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.96	0/2956	0.94	2/4025 (0.0%)
1	B	0.96	0/2980	0.90	0/4062
1	C	0.93	2/2970 (0.1%)	0.90	4/4049 (0.1%)
1	D	0.95	0/2897	0.88	3/3947 (0.1%)
All	All	0.95	2/11803 (0.0%)	0.91	9/16083 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	165	TYR	CD2-CE2	5.34	1.47	1.39
1	C	232	GLU	CG-CD	5.12	1.59	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	343	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	A	255	CYS	N-CA-C	5.83	126.75	111.00
1	C	85	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	C	343	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	D	21	ARG	NE-CZ-NH1	-5.21	117.69	120.30
1	D	244	MET	CG-SD-CE	-5.10	92.04	100.20
1	C	333	ILE	CB-CA-C	-5.08	101.45	111.60
1	A	373	LEU	CA-CB-CG	5.07	126.96	115.30
1	C	301	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 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	2884	0	2844	65	0
1	B	2906	0	2857	39	0
1	C	2901	0	2850	68	0
1	D	2837	0	2796	61	0
2	A	13	0	18	0	0
2	D	13	0	18	5	0
3	A	3	0	1	2	0
3	B	3	0	1	0	0
3	C	3	0	1	1	0
4	A	21	0	30	24	0
4	B	7	0	10	0	0
4	C	14	0	20	0	0
5	A	112	0	0	2	0
5	B	106	0	0	3	0
5	C	87	0	0	1	0
5	D	84	0	0	3	0
All	All	11994	0	11446	232	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 10.

All (232) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:255:CYS:SG	1:A:256:PRO:HD3	1.81	1.20
1:A:202:ILE:HD11	4:A:476:PEG:H31	1.25	1.12
1:C:271:LYS:NZ	1:C:272:LEU:HG	1.66	1.08
1:D:122:ILE:HD11	1:D:144:TYR:H	1.23	1.01
1:A:150:VAL:HG21	4:A:476:PEG:H21	1.42	0.99
1:C:232:GLU:HB2	5:C:514:HOH:O	1.66	0.94
1:C:271:LYS:HZ1	1:C:272:LEU:HG	1.30	0.89
1:B:241:ARG:NH1	1:B:255:CYS:SG	2.48	0.87
1:C:97:PRO:HG2	3:C:401:FMT:H	1.57	0.86
1:A:205:ALA:HA	4:A:477:PEG:H22	1.57	0.85
1:D:294:ALA:O	1:D:298:GLU:HG2	1.78	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:202:ILE:HD11	4:A:476:PEG:C3	2.07	0.82
1:A:31:PRO:HG3	4:A:477:PEG:H41	1.59	0.82
1:A:287:LEU:HD23	1:A:287:LEU:O	1.79	0.81
1:A:122:ILE:HG21	4:A:476:PEG:H41	1.69	0.74
1:D:122:ILE:HD11	1:D:144:TYR:N	2.02	0.74
1:C:271:LYS:HZ2	1:C:272:LEU:HG	1.50	0.74
1:A:209:ARG:HH12	4:A:477:PEG:C3	2.01	0.74
1:A:205:ALA:CA	4:A:477:PEG:H22	2.17	0.73
1:C:85:ARG:HB3	1:C:85:ARG:HH11	1.53	0.73
1:C:224:ARG:HD2	1:C:237:TRP:CD2	2.25	0.71
1:C:144:TYR:CZ	1:C:201:ARG:HG2	2.26	0.70
1:C:286:LYS:HE2	1:C:311:PHE:CE2	2.26	0.70
1:C:224:ARG:HD2	1:C:237:TRP:CE2	2.26	0.70
1:A:45:THR:O	1:A:48:GLN:HG3	1.93	0.69
1:A:122:ILE:HD12	1:A:146:ASN:OD1	1.93	0.68
2:D:480:PG4:H22	5:D:550:HOH:O	1.94	0.67
1:A:242:GLU:CD	1:A:242:GLU:H	1.98	0.66
1:C:257:LEU:HB2	1:C:284:ARG:HG3	1.78	0.65
1:C:170:GLU:OE1	1:C:173:ARG:NH2	2.30	0.64
1:A:209:ARG:HH12	4:A:477:PEG:H32	1.62	0.63
1:C:170:GLU:OE1	1:C:174:LYS:HE3	1.99	0.63
1:A:209:ARG:HH12	4:A:477:PEG:H31	1.64	0.62
1:C:271:LYS:NZ	1:C:272:LEU:CG	2.54	0.62
1:D:170:GLU:OE2	1:D:173:ARG:NH2	2.30	0.62
1:C:45:THR:O	1:C:48:GLN:HG3	1.99	0.62
1:D:153:HIS:O	1:D:157:MET:HG3	2.00	0.60
1:C:85:ARG:HB3	1:C:85:ARG:NH1	2.16	0.60
1:D:326:TYR:HE2	2:D:480:PG4:H71	1.66	0.60
1:A:290:ARG:HD2	1:A:320:PRO:CG	2.33	0.59
1:D:218:HIS:HB3	1:D:244:MET:CE	2.33	0.59
1:A:177:TRP:O	1:A:178:ASN:C	2.37	0.59
1:A:208[B]:ARG:HE	4:A:477:PEG:H21	1.66	0.59
1:D:326:TYR:CE2	2:D:480:PG4:H71	2.38	0.59
1:A:178:ASN:HB3	1:A:181:ASP:OD2	2.03	0.59
1:D:185:HIS:ND1	2:D:480:PG4:H21	2.18	0.58
1:B:126:HIS:H	1:B:126:HIS:CD2	2.22	0.57
1:D:166:LEU:CD1	1:D:328:GLY:HA2	2.35	0.57
1:A:287:LEU:C	1:A:287:LEU:HD23	2.24	0.57
1:A:153:HIS:O	1:A:157:MET:HG3	2.05	0.57
1:A:245:TYR:HB2	1:A:246:PRO:HD3	1.87	0.57
1:B:106:GLU:O	1:B:109:ALA:HB3	2.05	0.56
1:C:170:GLU:CD	1:C:173:ARG:HH21	2.08	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:230:GLU:HA	1:D:235:LEU:HD12	1.87	0.56
1:C:135:ARG:HD3	1:C:135:ARG:N	2.19	0.56
1:C:289:ASP:HB3	1:C:292:ALA:HB3	1.88	0.56
1:C:291:ASP:O	1:C:295:ARG:HG3	2.04	0.56
1:C:271:LYS:HZ1	1:C:272:LEU:CG	2.12	0.55
1:C:110:LYS:O	1:C:112:LYS:N	2.39	0.55
1:A:180:ALA:O	1:A:184:SER:HB3	2.07	0.55
1:B:305:TYR:O	1:B:327:ASN:HA	2.07	0.54
1:D:218:HIS:HB3	1:D:244:MET:HE1	1.90	0.54
1:C:305:TYR:O	1:C:327:ASN:HA	2.07	0.54
1:A:147:SER:HA	4:A:476:PEG:H32	1.89	0.54
1:A:359:ARG:HG3	1:A:360:PRO:HD2	1.89	0.54
1:A:31:PRO:CB	4:A:477:PEG:H11	2.38	0.54
1:B:227:GLU:O	1:B:231:LYS:HD3	2.06	0.54
3:A:479:FMT:H	4:A:476:PEG:H22	1.90	0.54
1:C:126:HIS:H	1:C:126:HIS:CD2	2.23	0.54
1:A:318:ASP:HB3	5:A:534:HOH:O	2.06	0.53
1:D:251:VAL:O	1:D:279:ILE:HA	2.08	0.53
1:D:222:ARG:HB3	1:D:223:HIS:CD2	2.43	0.53
1:B:8:TYR:O	1:B:52:SER:HA	2.09	0.53
1:C:80:ASP:O	1:C:85:ARG:NH2	2.41	0.53
1:A:359:ARG:HG3	1:A:360:PRO:CD	2.39	0.53
1:A:21:ARG:HD3	1:C:187:TYR:CE2	2.44	0.53
1:B:111:ALA:HB1	1:B:114:LEU:HB2	1.89	0.52
1:D:135:ARG:NH1	1:D:135:ARG:O	2.41	0.52
1:C:10:ASP:OD2	1:C:54:SER:OG	2.24	0.52
1:A:357:GLU:HG3	1:A:357:GLU:O	2.09	0.52
1:D:166:LEU:HD12	1:D:328:GLY:HA2	1.92	0.52
1:C:286:LYS:HE2	1:C:311:PHE:CZ	2.44	0.52
1:D:126:HIS:CD2	1:D:126:HIS:H	2.26	0.52
1:A:146:ASN:O	1:A:150:VAL:HG23	2.10	0.51
1:D:191:ALA:HA	1:D:214:ASP:O	2.11	0.51
1:C:304:GLY:HA2	1:C:326:TYR:O	2.11	0.51
1:A:146:ASN:HB3	1:A:340:ALA:HB1	1.92	0.51
1:C:170:GLU:OE2	1:C:173:ARG:NH2	2.41	0.51
1:D:218:HIS:C	1:D:244:MET:HE1	2.31	0.51
2:D:480:PG4:H41	5:D:550:HOH:O	2.11	0.51
1:D:219:TYR:N	1:D:244:MET:HE1	2.25	0.51
1:C:111:ALA:HB1	1:C:114:LEU:HB2	1.93	0.51
1:A:319:HIS:O	1:A:322:ARG:HG3	2.11	0.51
1:A:202:ILE:O	1:A:206:VAL:HG23	2.10	0.50
1:C:222:ARG:HH22	1:C:241:ARG:HH12	1.60	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:322:ARG:HD3	1:C:172:ALA:O	2.11	0.50
1:C:259:PRO:O	1:C:260:GLU:HB2	2.12	0.50
1:A:255:CYS:SG	1:A:256:PRO:CD	2.76	0.49
1:B:108:ILE:HG22	1:B:135:ARG:HD3	1.94	0.49
1:B:280:VAL:HA	1:B:306:ALA:O	2.12	0.49
1:D:61:LYS:HE2	1:D:61:LYS:HB3	1.55	0.49
1:A:354:OCS:OD2	1:A:359:ARG:HG2	2.12	0.49
1:A:194:VAL:HG11	1:A:210:LEU:CD1	2.43	0.49
1:B:204:LEU:O	1:B:208[B]:ARG:HG3	2.13	0.48
1:B:164:ASN:OD1	1:B:167:PRO:HG2	2.13	0.48
1:D:218:HIS:CB	1:D:244:MET:HE1	2.43	0.48
1:D:284:ARG:HH22	1:D:313:GLN:NE2	2.11	0.48
1:D:195:GLY:HA2	1:D:218:HIS:O	2.14	0.48
1:D:5:CYS:O	1:D:72:VAL:HA	2.14	0.48
1:A:290:ARG:HD2	1:A:320:PRO:HG3	1.94	0.48
1:B:179:ILE:HG23	1:D:333:ILE:HG22	1.96	0.48
1:D:297:LEU:HD11	1:D:305:TYR:HB3	1.96	0.48
1:D:220:THR:HG23	1:D:220:THR:O	2.11	0.48
1:A:106:GLU:CD	1:A:106:GLU:H	2.18	0.47
1:D:15:TYR:CD1	1:D:54:SER:HB2	2.49	0.47
1:C:197:VAL:O	1:C:198:ALA:HB3	2.15	0.47
1:B:94:ILE:HA	1:B:118:LEU:O	2.14	0.47
1:A:227:GLU:HG2	1:A:231:LYS:HD3	1.97	0.47
1:A:305:TYR:O	1:A:327:ASN:HA	2.15	0.47
1:B:308:ASP:HB2	1:B:331:PRO:O	2.15	0.47
1:A:126:HIS:H	1:A:126:HIS:CD2	2.33	0.47
1:B:263:HIS:CE1	1:B:286:LYS:HG2	2.51	0.46
1:C:170:GLU:CD	1:C:173:ARG:NH2	2.67	0.46
1:D:223:HIS:N	1:D:223:HIS:CD2	2.82	0.46
1:D:114:LEU:HD11	1:D:116:LEU:O	2.15	0.46
1:A:205:ALA:CB	4:A:477:PEG:H22	2.45	0.46
1:C:103:LEU:HA	1:C:103:LEU:HD23	1.82	0.46
1:B:79:PRO:O	1:B:84:GLU:HG2	2.16	0.46
1:C:246:PRO:O	1:C:274:LYS:HG3	2.16	0.46
1:B:183:VAL:O	1:D:338:LEU:HG	2.16	0.45
1:D:337:THR:O	1:D:341:GLN:HG3	2.17	0.45
1:B:308:ASP:O	1:B:332:HIS:HA	2.16	0.45
1:D:124:SER:HB3	1:D:367:ILE:HD13	1.98	0.45
1:B:257:LEU:HB2	1:B:284:ARG:HG3	1.97	0.45
1:D:37:PRO:HB3	1:D:347:GLY:HA2	1.98	0.45
1:B:166:LEU:HB2	1:B:167:PRO:HD3	1.98	0.45
1:B:76:LYS:HA	1:B:83:PHE:HB3	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:105:PRO:HB3	1:B:131:SER:OG	2.16	0.45
1:C:227:GLU:O	1:C:231:LYS:HG3	2.16	0.45
1:B:53:VAL:HG21	5:B:546:HOH:O	2.17	0.45
1:D:221:ASP:H	1:D:237:TRP:HZ3	1.64	0.45
1:D:284:ARG:HH12	1:D:313:GLN:HE22	1.65	0.44
1:C:255:CYS:O	1:C:283:ALA:HB1	2.17	0.44
1:C:257:LEU:CB	1:C:284:ARG:HG3	2.46	0.44
1:A:326:TYR:HE2	4:A:480:PEG:H21	1.81	0.44
1:A:173:ARG:HD3	5:A:487:HOH:O	2.18	0.44
1:A:19:TYR:CZ	1:A:48:GLN:HA	2.53	0.44
1:C:178:ASN:HB3	1:C:181:ASP:OD2	2.17	0.44
1:A:205:ALA:HA	4:A:477:PEG:C2	2.39	0.44
1:C:245:TYR:N	1:C:246:PRO:CD	2.80	0.44
1:A:321:TRP:HA	1:A:324:MET:SD	2.58	0.44
1:A:31:PRO:CG	4:A:477:PEG:H41	2.39	0.44
1:C:255:CYS:HB2	1:C:287:LEU:HD13	1.98	0.44
1:B:93:VAL:HG23	1:B:114:LEU:HD13	2.00	0.44
1:B:185:HIS:HE1	5:B:571:HOH:O	2.00	0.44
1:C:222:ARG:NH2	1:C:241:ARG:HH12	2.16	0.44
1:D:284:ARG:HA	1:D:284:ARG:NE	2.32	0.44
1:C:296:ALA:HB1	1:C:302:LEU:HG	1.99	0.44
1:A:343:ARG:O	1:A:346:ALA:HB3	2.18	0.44
1:A:208[A]:ARG:HH12	1:A:232:GLU:CD	2.21	0.44
1:A:208[B]:ARG:NE	4:A:477:PEG:H21	2.32	0.44
1:D:308:ASP:HB2	1:D:331:PRO:O	2.18	0.43
1:C:52:SER:O	1:C:53:VAL:C	2.54	0.43
1:C:76:LYS:HD3	1:C:99:TRP:CD1	2.52	0.43
1:B:238:HIS:CD2	1:B:244:MET:HG3	2.53	0.43
1:C:308:ASP:O	1:C:332:HIS:HA	2.18	0.43
1:D:178:ASN:HB3	1:D:181:ASP:OD2	2.18	0.43
1:C:313:GLN:HA	1:C:314:PRO:C	2.38	0.43
1:C:283:ALA:O	1:C:284:ARG:HD2	2.18	0.43
1:D:308:ASP:O	1:D:332:HIS:HA	2.19	0.43
1:D:57:LEU:HB2	1:D:59:LEU:HG	2.01	0.43
1:B:263:HIS:HE1	5:B:522:HOH:O	2.01	0.43
1:B:79:PRO:HA	1:B:84:GLU:HG2	2.01	0.43
1:D:268:GLU:HA	1:D:271:LYS:HD2	2.00	0.43
1:B:204:LEU:O	1:B:208[A]:ARG:HG3	2.19	0.43
1:B:133:ILE:HG12	1:B:368:VAL:HG13	2.00	0.43
1:A:166:LEU:HB2	1:A:167:PRO:HD3	2.01	0.42
1:A:31:PRO:HB3	4:A:477:PEG:H11	2.01	0.42
1:D:305:TYR:O	1:D:327:ASN:HA	2.18	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:197:VAL:O	1:B:198:ALA:HB3	2.19	0.42
1:C:104:THR:HB	1:C:105:PRO:HD2	2.01	0.42
1:C:269:THR:O	1:C:272:LEU:HB2	2.20	0.42
1:C:194:VAL:HG11	1:C:210:LEU:HD13	2.01	0.42
1:C:233:LEU:O	1:C:234:ASN:HB2	2.19	0.42
1:A:194:VAL:HG11	1:A:210:LEU:HD13	2.02	0.42
1:A:202:ILE:CD1	4:A:476:PEG:H42	2.49	0.42
1:C:331:PRO:O	1:C:333:ILE:HG12	2.20	0.42
1:B:30:TYR:OH	1:B:343:ARG:HD2	2.20	0.42
1:A:154:VAL:O	1:A:158:ILE:HG13	2.20	0.42
1:B:258:HIS:HB3	1:B:259:PRO:CD	2.49	0.42
1:B:37:PRO:HG2	1:B:343:ARG:O	2.20	0.41
1:C:218:HIS:ND1	1:C:238:HIS:NE2	2.63	0.41
1:D:92:VAL:HG11	1:D:352:LEU:HD21	2.02	0.41
3:A:479:FMT:H	4:A:476:PEG:C2	2.50	0.41
1:C:85:ARG:HH11	1:C:85:ARG:CB	2.28	0.41
1:D:189:LEU:O	1:D:190:GLU:C	2.59	0.41
1:D:218:HIS:HB3	1:D:244:MET:HE2	2.02	0.41
1:B:276:GLY:HA3	1:D:20:ALA:O	2.20	0.41
1:D:45:THR:O	1:D:46:PRO:C	2.58	0.41
1:C:122:ILE:HD12	1:C:146:ASN:OD1	2.20	0.41
1:D:308:ASP:HA	1:D:330:THR:O	2.20	0.41
1:D:363:ASP:HA	1:D:366:LEU:HD12	2.02	0.41
1:D:310:TRP:CD1	1:D:310:TRP:N	2.89	0.41
1:C:108:ILE:HG22	1:C:135:ARG:HG2	2.03	0.41
1:B:114:LEU:O	1:B:137:VAL:HG22	2.21	0.41
1:B:103:LEU:HA	1:B:103:LEU:HD23	1.91	0.41
1:D:98:PHE:CD2	1:D:336:THR:HB	2.56	0.41
1:C:106:GLU:CD	1:C:106:GLU:H	2.24	0.41
1:A:224:ARG:HH21	1:A:230:GLU:CD	2.24	0.41
1:D:41:ALA:O	1:D:349:ARG:HD3	2.21	0.41
1:D:208:ARG:HG2	1:D:233:LEU:HD11	2.02	0.41
1:B:40:LYS:NZ	1:B:357:GLU:OE2	2.44	0.41
1:D:332:HIS:NE2	5:D:518:HOH:O	2.37	0.41
1:C:218:HIS:CE1	1:C:247:VAL:CG2	3.04	0.41
1:C:30:TYR:O	1:C:31:PRO:C	2.57	0.41
1:C:357:GLU:HB3	1:C:359:ARG:HD3	2.03	0.41
1:C:189:LEU:O	1:C:192:MET:HB2	2.21	0.41
1:A:313:GLN:HA	1:A:314:PRO:C	2.41	0.41
1:A:141:GLU:HB3	1:A:367:ILE:HD11	2.02	0.40
1:D:224:ARG:HG2	1:D:237:TRP:CD2	2.56	0.40
1:B:133:ILE:HG12	1:B:368:VAL:CG1	2.51	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:194:VAL:HG11	1:C:210:LEU:CD1	2.51	0.40
1:C:31:PRO:HG2	1:C:148:ILE:HD11	2.01	0.40
1:D:286:LYS:HG2	1:D:311:PHE:CD1	2.57	0.40
1:D:319:HIS:ND1	1:D:321:TRP:HB2	2.36	0.40
1:A:202:ILE:HD11	4:A:476:PEG:C4	2.50	0.40
1:D:242:GLU:CD	1:D:242:GLU:H	2.24	0.40
1:A:10:ASP:OD2	1:A:54:SER:OG	2.31	0.40
1:C:240:THR:HB	1:C:242[A]:GLU:OE1	2.21	0.40
1:A:147:SER:CA	4:A:476:PEG:H32	2.51	0.40
1:A:279:ILE:O	1:A:305:TYR:HA	2.21	0.40
1:D:21:ARG:HD2	1:D:21:ARG:HH11	1.73	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	365/401 (91%)	345 (94%)	16 (4%)	4 (1%)	21	19
1	B	368/401 (92%)	347 (94%)	20 (5%)	1 (0%)	50	59
1	C	367/401 (92%)	335 (91%)	30 (8%)	2 (0%)	38	43
1	D	357/401 (89%)	335 (94%)	21 (6%)	1 (0%)	50	59
All	All	1457/1604 (91%)	1362 (94%)	87 (6%)	8 (0%)	33	43

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	CYS
1	C	260	GLU
1	A	317	LYS
1	A	242	GLU
1	B	198	ALA
1	D	358	GLY
1	C	259	PRO

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Mol	Chain	Res	Type
1	A	333	ILE

### 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	307/328 (94%)	295 (96%)	12 (4%)	43	56
1	B	312/328 (95%)	297 (95%)	15 (5%)	35	45
1	C	311/328 (95%)	296 (95%)	15 (5%)	35	45
1	D	303/328 (92%)	285 (94%)	18 (6%)	28	33
All	All	1233/1312 (94%)	1173 (95%)	60 (5%)	35	44

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASP
1	A	38	THR
1	A	85	ARG
1	A	106	GLU
1	A	110	LYS
1	A	135	ARG
1	A	144	TYR
1	A	173	ARG
1	A	222	ARG
1	A	284	ARG
1	A	357	GLU
1	A	369	GLN
1	B	18	THR
1	B	26	LYS
1	B	28[A]	ASP
1	B	28[B]	ASP
1	B	62	TYR
1	B	76	LYS
1	B	87	LEU
1	B	91	ASP
1	B	110	LYS

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Mol	Chain	Res	Type
1	B	112	LYS
1	B	144	TYR
1	B	223	HIS
1	B	242	GLU
1	B	286	LYS
1	B	298	GLU
1	C	53	VAL
1	C	66	ASN
1	C	69	THR
1	C	85	ARG
1	C	110	LYS
1	C	135	ARG
1	C	144	TYR
1	C	224	ARG
1	C	247	VAL
1	C	271	LYS
1	C	286	LYS
1	C	298	GLU
1	C	301	ARG
1	C	359	ARG
1	C	368	VAL
1	D	17	LYS
1	D	40	LYS
1	D	42	ILE
1	D	61	LYS
1	D	76	LYS
1	D	122	ILE
1	D	136	ASN
1	D	144	TYR
1	D	223	HIS
1	D	232	GLU
1	D	240	THR
1	D	255	CYS
1	D	269	THR
1	D	272	LEU
1	D	287	LEU
1	D	327	ASN
1	D	359	ARG
1	D	363	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	HIS
1	A	369	GLN
1	B	29	HIS
1	B	126	HIS
1	B	185	HIS
1	B	263	HIS
1	B	369	GLN
1	C	113	ASN
1	C	126	HIS
1	D	126	HIS
1	D	223	HIS
1	D	254	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
1	OCS	A	354	1	8,8,9	5.68	1 (12%)	9,11,13	1.74	1 (11%)
1	OCS	B	354	1	8,8,9	7.47	2 (25%)	9,11,13	1.78	2 (22%)
1	OCS	C	354	1	8,8,9	6.17	2 (25%)	9,11,13	2.60	3 (33%)
1	OCS	D	354	1	8,8,9	6.52	3 (37%)	9,11,13	2.20	3 (33%)

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
1	OCS	A	354	1	-	0/5/7/9	0/0/0/0
1	OCS	B	354	1	-	0/5/7/9	0/0/0/0
1	OCS	C	354	1	-	0/5/7/9	0/0/0/0
1	OCS	D	354	1	-	0/5/7/9	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	354	OCS	O-C	20.80	1.25	1.11
1	D	354	OCS	O-C	17.66	1.23	1.11
1	C	354	OCS	O-C	16.92	1.23	1.11
1	A	354	OCS	O-C	15.82	1.22	1.11
1	D	354	OCS	CB-SG	3.71	1.81	1.77
1	C	354	OCS	CB-SG	3.20	1.81	1.77
1	D	354	OCS	CA-C	2.87	1.53	1.48
1	B	354	OCS	CA-C	2.82	1.53	1.48

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	354	OCS	C-CA-N	-6.24	107.59	113.83
1	D	354	OCS	OD2-SG-CB	4.91	111.96	105.64
1	A	354	OCS	OD1-SG-CB	3.94	113.94	107.03
1	B	354	OCS	OD2-SG-CB	3.26	109.83	105.64
1	C	354	OCS	OD2-SG-CB	3.25	109.82	105.64
1	D	354	OCS	C-CA-N	-2.77	111.06	113.83
1	D	354	OCS	OD2-SG-OD3	-2.71	105.93	111.78
1	B	354	OCS	CA-CB-SG	-2.59	108.43	114.30
1	C	354	OCS	OD3-SG-CB	2.03	110.59	107.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

11 ligands are modelled in this entry.

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	476	-	6,6,6	0.77	0	5,5,5	0.82	0
4	PEG	A	477	-	6,6,6	1.12	0	5,5,5	1.67	1 (20%)
2	PG4	A	478	-	12,12,12	0.68	0	11,11,11	0.49	0
3	FMT	A	479	-	2,2,2	0.38	0	1,1,1	0.03	0
4	PEG	A	480	-	6,6,6	0.56	0	5,5,5	0.92	0
3	FMT	B	401	-	2,2,2	0.60	0	1,1,1	0.10	0
4	PEG	B	481	-	6,6,6	0.79	0	5,5,5	0.50	0
3	FMT	C	401	-	2,2,2	0.51	0	1,1,1	0.25	0
4	PEG	C	482	-	6,6,6	0.66	0	5,5,5	0.40	0
4	PEG	C	483	-	6,6,6	0.43	0	5,5,5	0.38	0
2	PG4	D	480	-	12,12,12	0.77	0	11,11,11	0.87	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
4	PEG	A	476	-	-	0/4/4/4	0/0/0/0
4	PEG	A	477	-	-	0/4/4/4	0/0/0/0
2	PG4	A	478	-	-	0/10/10/10	0/0/0/0
3	FMT	A	479	-	-	0/0/0/0	0/0/0/0
4	PEG	A	480	-	-	0/4/4/4	0/0/0/0
3	FMT	B	401	-	-	0/0/0/0	0/0/0/0
4	PEG	B	481	-	-	0/4/4/4	0/0/0/0
3	FMT	C	401	-	-	0/0/0/0	0/0/0/0
4	PEG	C	482	-	-	0/4/4/4	0/0/0/0
4	PEG	C	483	-	-	0/4/4/4	0/0/0/0
2	PG4	D	480	-	-	0/10/10/10	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	A	477	PEG	C3-O2-C2	2.69	125.19	113.38

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	368/401 (91%)	-0.13	7 (1%) 64 72	18, 33, 48, 70	0
1	B	369/401 (92%)	-0.01	11 (2%) 48 57	21, 34, 51, 73	0
1	C	369/401 (92%)	0.04	17 (4%) 31 40	19, 37, 53, 73	0
1	D	362/401 (90%)	0.12	15 (4%) 35 45	21, 38, 57, 72	0
All	All	1468/1604 (91%)	0.00	50 (3%) 43 52	18, 35, 54, 73	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	263	HIS	7.1
1	A	256	PRO	6.9
1	B	260	GLU	6.4
1	B	259	PRO	5.3
1	D	80	ASP	5.2
1	C	259	PRO	4.9
1	C	80	ASP	4.6
1	D	255	CYS	4.1
1	C	260	GLU	4.0
1	A	370	GLY	3.9
1	D	12	VAL	3.9
1	B	80	ASP	3.6
1	C	32	GLY	3.6
1	C	223	HIS	3.4
1	D	79	PRO	3.4
1	D	256	PRO	3.3
1	D	359	ARG	3.1
1	D	113	ASN	2.9
1	B	32	GLY	2.9
1	C	13	ASP	2.9
1	D	125	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	136	ASN	2.9
1	A	222	ARG	2.8
1	C	33	GLY	2.7
1	C	243	ASP	2.6
1	D	222	ARG	2.6
1	D	13	ASP	2.6
1	D	32	GLY	2.6
1	C	262	GLU	2.6
1	B	67	GLY	2.5
1	C	263	HIS	2.5
1	C	83	PHE	2.5
1	A	255	CYS	2.5
1	D	172	ALA	2.4
1	C	79	PRO	2.4
1	B	263	HIS	2.4
1	B	83	PHE	2.4
1	B	69	THR	2.3
1	C	207	LEU	2.3
1	D	358	GLY	2.3
1	A	374	ALA	2.2
1	D	115	LYS	2.2
1	A	223	HIS	2.2
1	C	136	ASN	2.1
1	B	79	PRO	2.1
1	B	223	HIS	2.1
1	C	102	TYR	2.1
1	C	28	ASP	2.1
1	B	85	ARG	2.0
1	C	17	LYS	2.0

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

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
1	OCS	D	354	9/10	0.12	-0.65	44,46,48,49	0
1	OCS	C	354	9/10	0.09	-1.28	36,40,42,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	OCS	A	354	9/10	0.07	-1.58	33,35,38,40	0
1	OCS	B	354	9/10	0.09	-1.60	31,36,39,39	0

### 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( $\text{\AA}^2$ )	Q<0.9
4	PEG	A	476	7/7	0.23	15.61	40,47,51,57	0
4	PEG	A	477	7/7	0.29	10.53	27,31,38,40	0
3	FMT	C	401	3/3	0.19	4.70	39,39,42,43	0
4	PEG	C	482	7/7	0.19	3.64	60,62,65,66	0
3	FMT	B	401	3/3	0.15	1.85	52,52,52,53	0
4	PEG	A	480	7/7	0.12	0.83	35,37,42,46	0
4	PEG	B	481	7/7	0.13	0.32	55,57,58,60	0
3	FMT	A	479	3/3	0.11	0.17	31,31,34,36	0
2	PG4	A	478	13/13	0.16	0.09	45,54,58,58	0
4	PEG	C	483	7/7	0.11	-0.36	42,46,50,52	0
2	PG4	D	480	13/13	0.10	-0.58	31,35,45,45	0

### 6.5 Other polymers

There are no such residues in this entry.