Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 01:34 AM EDT

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 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:

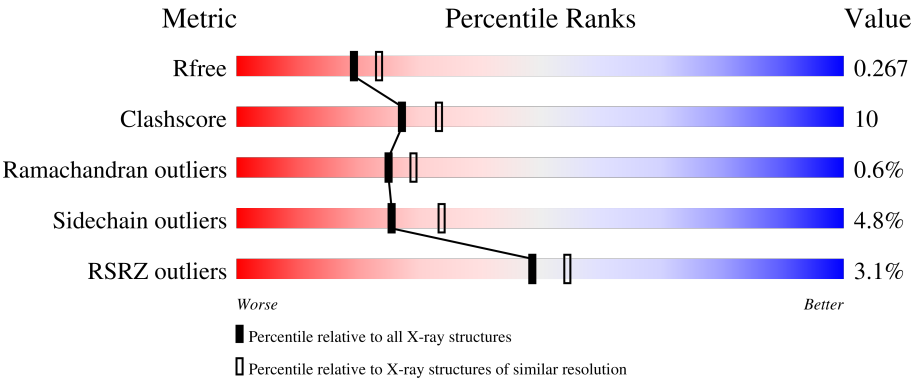
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (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 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 <=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	401	2% 73% 18% • 8%
1	B	401	2% 74% 17% • 8%
1	C	401	4% 68% 20% • 8%
1	D	401	4% 66% 22% • 10%

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	FMT	A	479	-	-	X	-
4	PEG	A	476	-	-	X	-
4	PEG	A	477	-	-	X	-

2 Entry composition (i)

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

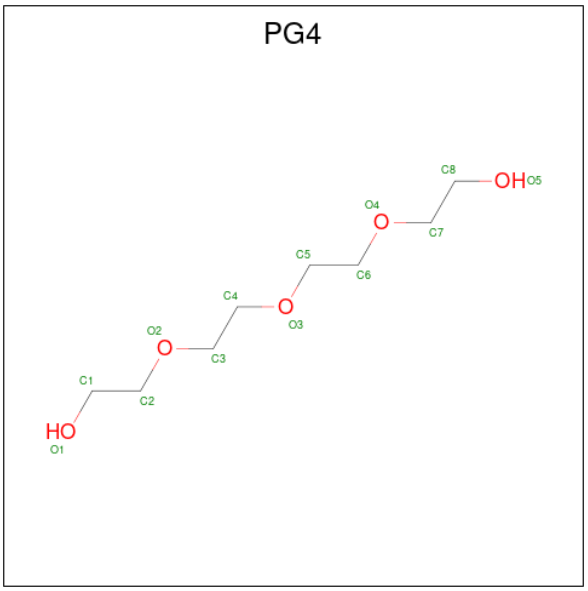
- Molecule 1 is a protein called Formate dehydrogenase.

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:

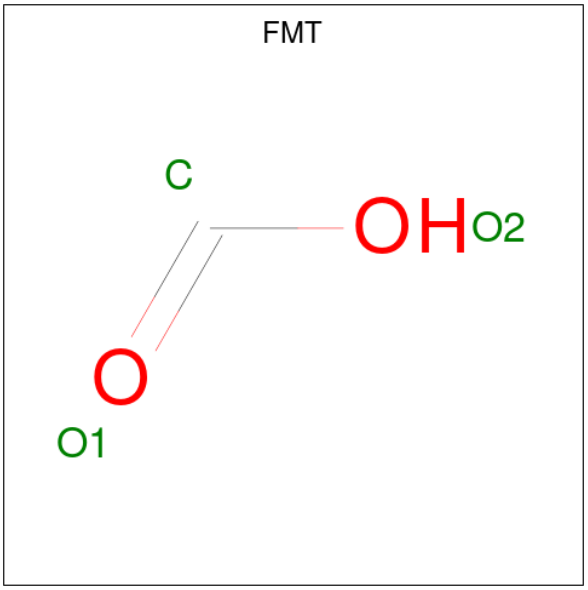
Chain	Residue	Modelled	Actual	Comment	Reference
A	354	OCS	CYS	modified residue	UNP P33160
B	354	OCS	CYS	modified residue	UNP P33160
C	354	OCS	CYS	modified residue	UNP P33160
D	354	OCS	CYS	modified residue	UNP P33160

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



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

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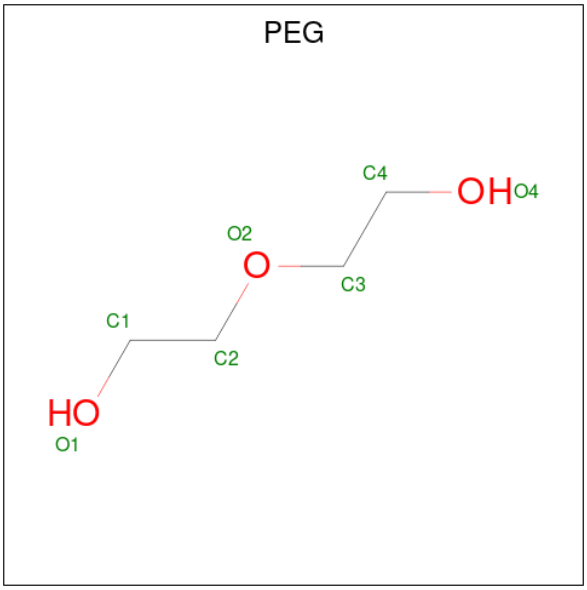
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 3 1 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 5 is water.

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

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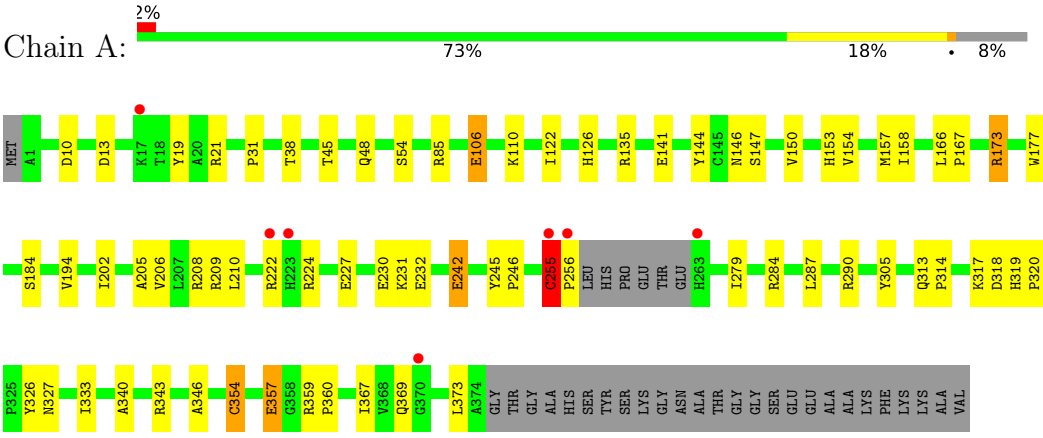
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	87	Total O 87 87	0	0
5	D	84	Total O 84 84	0	0

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.

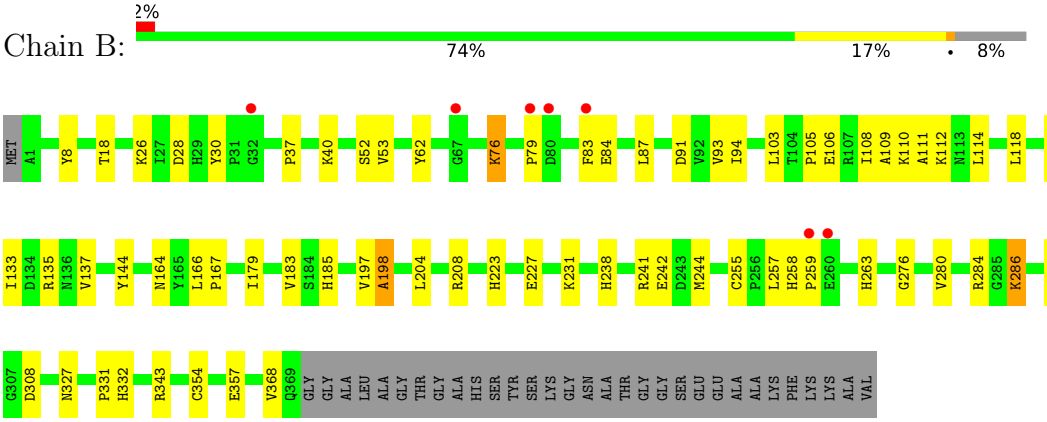
• Molecule 1: Formate dehydrogenase

Chain A:



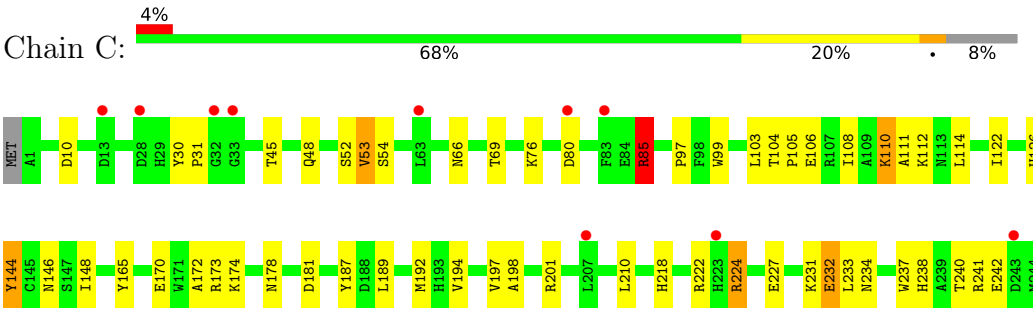
• Molecule 1: Formate dehydrogenase

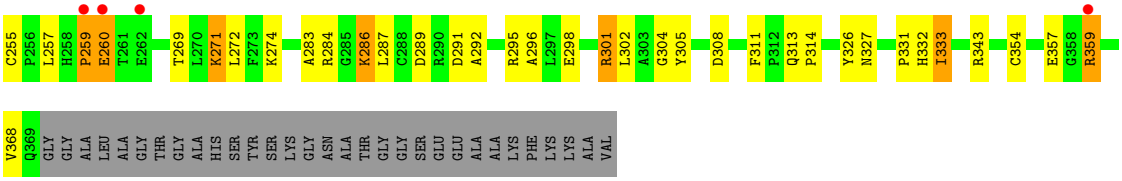
Chain B:



• Molecule 1: Formate dehydrogenase

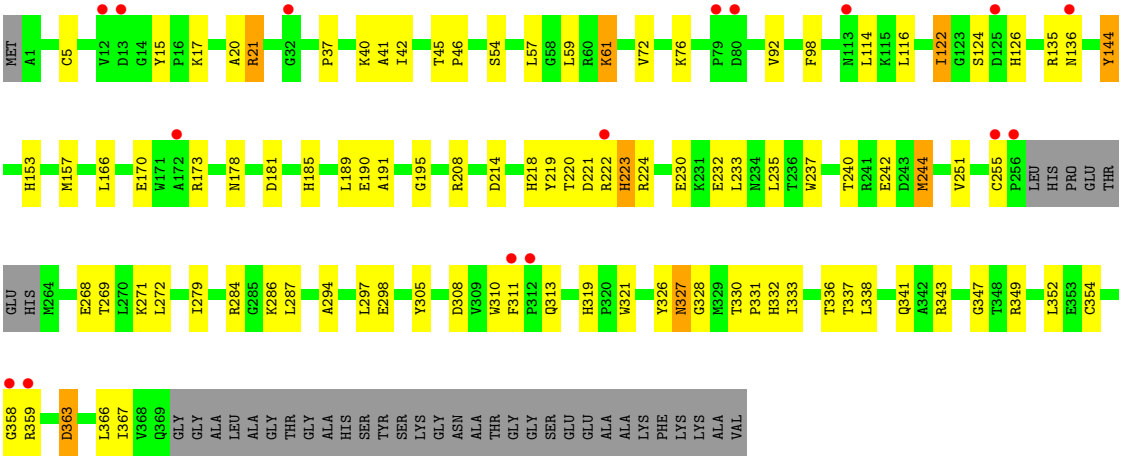
Chain C:





• Molecule 1: Formate dehydrogenase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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) 97.9 (16.10-2.28)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.00 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.269 0.197 , 0.267	Depositor DCC
R_{free} test set	3696 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	32.8	Xtriage
Anisotropy	0.874	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 40.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11994	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PG4, OCS, PEG, FMT

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(^{o})	Ideal(^{o})
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 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	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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (232) 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: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	Interatomic distance (Å)	Clash overlap (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:HH11	1:C:85:ARG:HB3	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:A:178:ASN:HB3	1:A:181:ASP:OD2	2.03	0.59
1:D:326:TYR:CE2	2:D:480:PG4:H71	2.38	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:HD23	1:A:287:LEU:C	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:GLU:CD	1:C:173:ARG:HH21	2.08	0.56
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:C:305:TYR:O	1:C:327:ASN:HA	2.07	0.54
1:D:218:HIS:HB3	1:D:244:MET:HE1	1.90	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:CD2	1:C:126:HIS:H	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:21:ARG:HD3	1:C:187:TYR:CE2	2.44	0.53
1:A:359:ARG:HG3	1:A:360:PRO:CD	2.39	0.53
1:B:111:ALA:HB1	1:B:114:LEU:HB2	1.89	0.52
1:D:135:ARG:O	1:D:135:ARG:NH1	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:H	1:D:126:HIS:CD2	2.26	0.52
1:A:146:ASN:O	1:A:150:VAL:HG23	2.10	0.51
1:C:304:GLY:HA2	1:C:326:TYR:O	2.11	0.51
1:D:191:ALA:HA	1:D:214:ASP: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
1:D:219:TYR:N	1:D:244:MET:HE1	2.25	0.51
2:D:480:PG4:H41	5:D:550:HOH:O	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:194:VAL:HG11	1:A:210:LEU:CD1	2.43	0.49
1:A:354:OCS:OD2	1:A:359:ARG:HG2	2.12	0.49
1:B:164:ASN:OD1	1:B:167:PRO:HG2	2.13	0.48
1:B:204:LEU:O	1:B:208[B]:ARG:HG3	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:5:CYS:O	1:D:72:VAL:HA	2.14	0.48
1:D:195:GLY:HA2	1:D:218:HIS:O	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:O	1:D:220:THR:HG23	2.11	0.48
1:A:106:GLU:CD	1:A:106:GLU:H	2.18	0.47
1:C:197:VAL:O	1:C:198:ALA:HB3	2.15	0.47
1:D:15:TYR:CD1	1:D:54:SER:HB2	2.49	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:94:ILE:HA	1:B:118:LEU:O	2.14	0.47
1:B:308:ASP:HB2	1:B:331:PRO:O	2.15	0.47
1:A:126:HIS:CD2	1:A:126:HIS:H	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:CD2	1:D:223:HIS:N	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:HD23	1:C:103:LEU:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:173:ARG:HD3	5:A:487:HOH:O	2.18	0.44
1:A:326:TYR:HE2	4:A:480:PEG:H21	1.81	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: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:A:321:TRP:HA	1:A:324:MET:SD	2.58	0.44
1:C:245:TYR:N	1:C:246:PRO:CD	2.80	0.44
1:A:31:PRO:CG	4:A:477:PEG:H41	2.39	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:255:CYS:HB2	1:C:287:LEU:HD13	1.98	0.44
1:C:222:ARG:NH2	1:C:241:ARG:HH12	2.16	0.44
1:D:284:ARG:NE	1:D:284:ARG:HA	2.32	0.44
1:A:343:ARG:O	1:A:346:ALA:HB3	2.18	0.44
1:C:296:ALA:HB1	1:C:302:LEU:HG	1.99	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: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:D:308:ASP:HB2	1:D:331:PRO:O	2.18	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:C:313:GLN:HA	1:C:314:PRO:C	2.38	0.43
1:D:178:ASN:HB3	1:D:181:ASP:OD2	2.18	0.43
1:C:283:ALA:O	1:C:284:ARG:HD2	2.18	0.43
1:D:57:LEU:HB2	1:D:59:LEU:HG	2.01	0.43
1:D:308:ASP:O	1:D:332:HIS:HA	2.19	0.43
1:B:79:PRO:HA	1:B:84:GLU:HG2	2.01	0.43
1:B:263:HIS:HE1	5:B:522:HOH:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:154:VAL:O	1:A:158:ILE:HG13	2.20	0.42
1:B:30:TYR:OH	1:B:343:ARG:HD2	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:B:276:GLY:HA3	1:D:20:ALA:O	2.20	0.41
1:C:122:ILE:HD12	1:C:146:ASN:OD1	2.20	0.41
1:D:45:THR:O	1:D:46:PRO:C	2.58	0.41
1:D:218:HIS:HB3	1:D:244:MET:HE2	2.02	0.41
1:D:308:ASP:HA	1:D:330:THR:O	2.20	0.41
1:D:310:TRP:CD1	1:D:310:TRP:N	2.89	0.41
1:D:363:ASP:HA	1:D:366:LEU:HD12	2.02	0.41
1:B:114:LEU:O	1:B:137:VAL:HG22	2.21	0.41
1:C:108:ILE:HG22	1:C:135:ARG:HG2	2.03	0.41
1:B:103:LEU:HD23	1:B:103:LEU:HA	1.91	0.41
1:A:224:ARG:HH21	1:A:230:GLU:CD	2.24	0.41
1:B:40:LYS:NZ	1:B:357:GLU:OE2	2.44	0.41
1:C:106:GLU:CD	1:C:106:GLU:H	2.24	0.41
1:D:41:ALA:O	1:D:349:ARG:HD3	2.21	0.41
1:D:98:PHE:CD2	1:D:336:THR:HB	2.56	0.41
1:D:208:ARG:HG2	1:D:233:LEU:HD11	2.02	0.41
1:C:30:TYR:O	1:C:31:PRO:C	2.57	0.41
1:C:189:LEU:O	1:C:192:MET:HB2	2.21	0.41
1:C:218:HIS:CE1	1:C:247:VAL:CG2	3.04	0.41
1:C:357:GLU:HB3	1:C:359:ARG:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:HIS:NE2	5:D:518:HOH:O	2.37	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:B:133:ILE:HG12	1:B:368:VAL:CG1	2.51	0.40
1:C:31:PRO:HG2	1:C:148:ILE:HD11	2.01	0.40
1:C:194:VAL:HG11	1:C:210:LEU:CD1	2.51	0.40
1:D:224:ARG:HG2	1:D:237:TRP:CD2	2.56	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: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:D:242:GLU:CD	1:D:242:GLU:H	2.24	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:HH11	1:D:21:ARG:HD2	1.73	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	365/401 (91%)	345 (94%)	16 (4%)	4 (1%)	14	14
1	B	368/401 (92%)	347 (94%)	20 (5%)	1 (0%)	41	49
1	C	367/401 (92%)	335 (91%)	30 (8%)	2 (0%)	29	34
1	D	357/401 (89%)	335 (94%)	21 (6%)	1 (0%)	41	49
All	All	1457/1604 (91%)	1362 (94%)	87 (6%)	8 (0%)	25	34

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
1	A	333	ILE

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	307/328 (94%)	295 (96%)	12 (4%)	32	43
1	B	312/328 (95%)	297 (95%)	15 (5%)	25	34
1	C	311/328 (95%)	296 (95%)	15 (5%)	25	34
1	D	303/328 (92%)	285 (94%)	18 (6%)	19	24
All	All	1233/1312 (94%)	1173 (95%)	60 (5%)	25	33

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	D	287	LEU
1	D	327	ASN
1	D	359	ARG
1	D	363	ASP

Sometimes 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 (i)

There are no RNA molecules in this entry.

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

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	C	354	1	7,8,9	1.20	1 (14%)	6,11,13	1.83	2 (33%)
1	OCS	A	354	1	7,8,9	0.84	0	6,11,13	2.63	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	OCS	D	354	1	7,8,9	1.11	0	6,11,13	2.14	3 (50%)
1	OCS	B	354	1	7,8,9	1.20	1 (14%)	6,11,13	1.87	3 (50%)

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	C	354	1	-	0/4/7/9	-
1	OCS	A	354	1	-	0/4/7/9	-
1	OCS	D	354	1	-	0/4/7/9	-
1	OCS	B	354	1	-	3/4/7/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	354	OCS	CB-CA	-2.22	1.51	1.53
1	C	354	OCS	OD1-SG	-2.02	1.39	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	354	OCS	OD1-SG-CB	5.89	113.94	106.94
1	D	354	OCS	OD2-SG-CB	3.90	111.96	105.74
1	C	354	OCS	OD3-SG-CB	3.07	110.59	106.94
1	D	354	OCS	OD3-SG-CB	2.60	110.03	106.94
1	B	354	OCS	OD2-SG-CB	2.57	109.83	105.74
1	C	354	OCS	OD2-SG-CB	2.56	109.82	105.74
1	B	354	OCS	OD3-SG-CB	2.32	109.70	106.94
1	D	354	OCS	OD2-SG-OD3	-2.19	105.93	111.27
1	B	354	OCS	OD3-SG-OD1	-2.02	106.94	113.95

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	354	OCS	CA-CB-SG-OD2
1	B	354	OCS	CA-CB-SG-OD1
1	B	354	OCS	CA-CB-SG-OD3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	354	OCS	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	477	-	6,6,6	1.13	0	5,5,5	1.80	2 (40%)
3	FMT	C	401	-	2,2,2	0.47	0	1,1,1	0.32	0
4	PEG	A	480	-	6,6,6	0.56	0	5,5,5	1.03	0
4	PEG	C	483	-	6,6,6	0.43	0	5,5,5	0.48	0
4	PEG	C	482	-	6,6,6	0.66	0	5,5,5	0.48	0
4	PEG	A	476	-	6,6,6	0.77	0	5,5,5	0.91	0
2	PG4	D	480	-	12,12,12	0.76	0	11,11,11	0.92	1 (9%)
3	FMT	B	401	-	2,2,2	0.64	0	1,1,1	0.09	0
2	PG4	A	478	-	12,12,12	0.67	0	11,11,11	0.51	0
4	PEG	B	481	-	6,6,6	0.80	0	5,5,5	0.62	0
3	FMT	A	479	-	2,2,2	0.39	0	1,1,1	0.00	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	477	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	A	480	-	-	4/4/4/4	-
4	PEG	C	483	-	-	1/4/4/4	-
4	PEG	C	482	-	-	4/4/4/4	-
4	PEG	A	476	-	-	3/4/4/4	-
2	PG4	D	480	-	-	6/10/10/10	-
2	PG4	A	478	-	-	6/10/10/10	-
4	PEG	B	481	-	-	4/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	477	PEG	C3-O2-C2	2.75	125.19	113.29
4	A	477	PEG	O4-C4-C3	2.08	123.88	111.81
2	D	480	PG4	O3-C4-C3	2.00	119.43	110.39

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	477	PEG	O2-C3-C4-O4
4	A	480	PEG	O2-C3-C4-O4
4	B	481	PEG	O2-C3-C4-O4
2	D	480	PG4	O1-C1-C2-O2
4	A	476	PEG	O1-C1-C2-O2
4	A	476	PEG	O2-C3-C4-O4
4	C	482	PEG	O2-C3-C4-O4
2	D	480	PG4	O4-C7-C8-O5
4	A	480	PEG	C4-C3-O2-C2
2	A	478	PG4	C3-C4-O3-C5
4	B	481	PEG	C4-C3-O2-C2
4	C	482	PEG	C1-C2-O2-C3
4	B	481	PEG	O1-C1-C2-O2
2	A	478	PG4	O2-C3-C4-O3
2	D	480	PG4	C6-C5-O3-C4
2	D	480	PG4	O2-C3-C4-O3
2	D	480	PG4	C5-C6-O4-C7
4	C	482	PEG	O1-C1-C2-O2
2	A	478	PG4	C4-C3-O2-C2
4	A	477	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
2	A	478	PG4	C5-C6-O4-C7
4	A	476	PEG	C4-C3-O2-C2
4	B	481	PEG	C1-C2-O2-C3
4	A	480	PEG	C1-C2-O2-C3
2	D	480	PG4	O3-C5-C6-O4
4	C	482	PEG	C4-C3-O2-C2
2	A	478	PG4	O1-C1-C2-O2
4	C	483	PEG	O1-C1-C2-O2
2	A	478	PG4	C1-C2-O2-C3
4	A	480	PEG	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	477	PEG	13	0
3	C	401	FMT	1	0
4	A	480	PEG	1	0
4	A	476	PEG	10	0
2	D	480	PG4	5	0
3	A	479	FMT	2	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, 95^{th} 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	367/401 (91%)	-0.19	7 (1%)	66	72	18, 32, 48, 70	0
1	B	368/401 (91%)	-0.09	7 (1%)	66	72	21, 34, 51, 73	0
1	C	368/401 (91%)	-0.05	15 (4%)	37	42	19, 37, 53, 73	0
1	D	361/401 (90%)	0.02	16 (4%)	34	40	21, 38, 57, 72	0
All	All	1464/1604 (91%)	-0.08	45 (3%)	49	54	18, 35, 54, 73	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	263	HIS	6.5
1	A	256	PRO	6.2
1	B	260	GLU	5.9
1	B	259	PRO	4.8
1	C	259	PRO	4.7
1	A	370	GLY	4.3
1	D	80	ASP	4.1
1	C	80	ASP	3.9
1	D	256	PRO	3.7
1	C	223	HIS	3.6
1	B	80	ASP	3.4
1	D	255	CYS	3.4
1	D	136	ASN	2.9
1	B	32	GLY	2.8
1	C	260	GLU	2.8
1	D	12	VAL	2.8
1	C	32	GLY	2.8
1	D	13	ASP	2.7
1	A	222	ARG	2.6
1	B	83	PHE	2.6
1	C	13	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	172	ALA	2.6
1	B	67	GLY	2.6
1	D	125	ASP	2.6
1	C	33	GLY	2.6
1	B	79	PRO	2.5
1	D	359	ARG	2.5
1	A	255	CYS	2.5
1	D	358	GLY	2.5
1	C	262	GLU	2.4
1	D	79	PRO	2.4
1	A	223	HIS	2.3
1	D	32	GLY	2.3
1	D	222	ARG	2.3
1	C	243	ASP	2.2
1	A	17	LYS	2.1
1	D	113	ASN	2.1
1	C	83	PHE	2.1
1	C	28	ASP	2.1
1	C	63	LEU	2.1
1	C	359	ARG	2.1
1	D	311	PHE	2.1
1	C	207	LEU	2.0
1	D	312	PRO	2.0
1	C	136	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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
1	OCS	D	354	9/10	0.96	0.12	44,46,48,49	0
1	OCS	B	354	9/10	0.98	0.09	31,36,39,39	0
1	OCS	C	354	9/10	0.98	0.10	36,40,42,43	0
1	OCS	A	354	9/10	0.98	0.08	33,35,38,40	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
2	PG4	A	478	13/13	0.77	0.18	45,54,58,58	0
4	PEG	A	476	7/7	0.78	0.26	40,47,51,57	0
4	PEG	B	481	7/7	0.80	0.16	55,57,58,60	0
4	PEG	C	482	7/7	0.81	0.21	60,62,65,66	0
3	FMT	B	401	3/3	0.85	0.15	52,52,52,53	0
4	PEG	C	483	7/7	0.85	0.14	42,46,50,52	0
3	FMT	C	401	3/3	0.86	0.21	39,39,42,43	0
4	PEG	A	477	7/7	0.91	0.28	27,31,38,40	0
4	PEG	A	480	7/7	0.92	0.12	35,37,42,46	0
2	PG4	D	480	13/13	0.92	0.10	31,35,45,45	0
3	FMT	A	479	3/3	0.95	0.13	31,31,34,36	0

6.5 Other polymers (i)

There are no such residues in this entry.