



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2023 – 07:06 am BST

PDB ID : 7QZ1
Title : Formate dehydrogenase from Starkeya novella
Authors : Pontillo, N.; Slotboom, D.J.; Guskov, A.
Deposited on : 2022-01-30
Resolution : 2.10 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 : 1.8.4, CSD as541be (2020)
Xtrriage (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

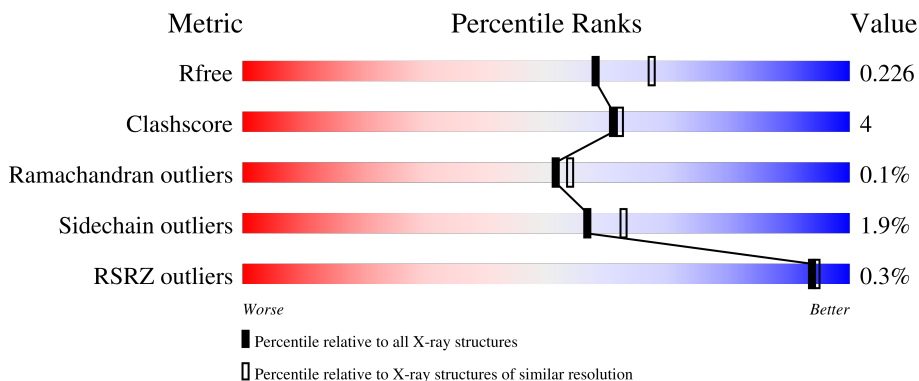
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	421	 78% 10% 12%
1	B	421	 78% 11% 11%
1	C	421	 76% 12% 12%
1	D	421	 74% 14% 12%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12267 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
			Total	C	N	O	S			
1	A	372	Total 2915	C 1851	N 509	O 543	S 12	0	1	0
1	B	375	Total 2922	C 1857	N 508	O 545	S 12	0	0	0
1	C	370	Total 2912	C 1850	N 507	O 543	S 12	0	2	0
1	D	371	Total 2900	C 1843	N 504	O 541	S 12	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP D7A8L2
A	2	SER	-	expression tag	UNP D7A8L2
A	403	ALA	-	expression tag	UNP D7A8L2
A	404	LEU	-	expression tag	UNP D7A8L2
A	405	GLU	-	expression tag	UNP D7A8L2
A	406	VAL	-	expression tag	UNP D7A8L2
A	407	LEU	-	expression tag	UNP D7A8L2
A	408	PHE	-	expression tag	UNP D7A8L2
A	409	GLN	-	expression tag	UNP D7A8L2
A	410	GLY	-	expression tag	UNP D7A8L2
A	411	PRO	-	expression tag	UNP D7A8L2
A	412	HIS	-	expression tag	UNP D7A8L2
A	413	HIS	-	expression tag	UNP D7A8L2
A	414	HIS	-	expression tag	UNP D7A8L2
A	415	HIS	-	expression tag	UNP D7A8L2
A	416	HIS	-	expression tag	UNP D7A8L2
A	417	HIS	-	expression tag	UNP D7A8L2
A	418	HIS	-	expression tag	UNP D7A8L2
A	419	HIS	-	expression tag	UNP D7A8L2
A	420	HIS	-	expression tag	UNP D7A8L2
A	421	HIS	-	expression tag	UNP D7A8L2

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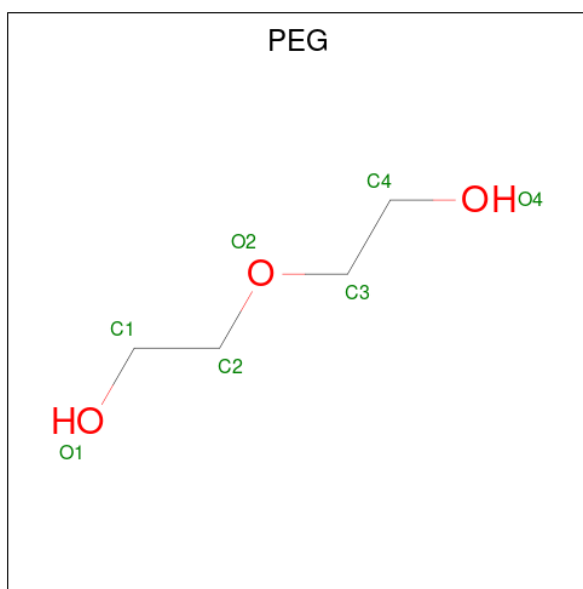
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP D7A8L2
B	2	SER	-	expression tag	UNP D7A8L2
B	403	ALA	-	expression tag	UNP D7A8L2
B	404	LEU	-	expression tag	UNP D7A8L2
B	405	GLU	-	expression tag	UNP D7A8L2
B	406	VAL	-	expression tag	UNP D7A8L2
B	407	LEU	-	expression tag	UNP D7A8L2
B	408	PHE	-	expression tag	UNP D7A8L2
B	409	GLN	-	expression tag	UNP D7A8L2
B	410	GLY	-	expression tag	UNP D7A8L2
B	411	PRO	-	expression tag	UNP D7A8L2
B	412	HIS	-	expression tag	UNP D7A8L2
B	413	HIS	-	expression tag	UNP D7A8L2
B	414	HIS	-	expression tag	UNP D7A8L2
B	415	HIS	-	expression tag	UNP D7A8L2
B	416	HIS	-	expression tag	UNP D7A8L2
B	417	HIS	-	expression tag	UNP D7A8L2
B	418	HIS	-	expression tag	UNP D7A8L2
B	419	HIS	-	expression tag	UNP D7A8L2
B	420	HIS	-	expression tag	UNP D7A8L2
B	421	HIS	-	expression tag	UNP D7A8L2
C	1	MET	-	initiating methionine	UNP D7A8L2
C	2	SER	-	expression tag	UNP D7A8L2
C	403	ALA	-	expression tag	UNP D7A8L2
C	404	LEU	-	expression tag	UNP D7A8L2
C	405	GLU	-	expression tag	UNP D7A8L2
C	406	VAL	-	expression tag	UNP D7A8L2
C	407	LEU	-	expression tag	UNP D7A8L2
C	408	PHE	-	expression tag	UNP D7A8L2
C	409	GLN	-	expression tag	UNP D7A8L2
C	410	GLY	-	expression tag	UNP D7A8L2
C	411	PRO	-	expression tag	UNP D7A8L2
C	412	HIS	-	expression tag	UNP D7A8L2
C	413	HIS	-	expression tag	UNP D7A8L2
C	414	HIS	-	expression tag	UNP D7A8L2
C	415	HIS	-	expression tag	UNP D7A8L2
C	416	HIS	-	expression tag	UNP D7A8L2
C	417	HIS	-	expression tag	UNP D7A8L2
C	418	HIS	-	expression tag	UNP D7A8L2
C	419	HIS	-	expression tag	UNP D7A8L2
C	420	HIS	-	expression tag	UNP D7A8L2
C	421	HIS	-	expression tag	UNP D7A8L2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP D7A8L2
D	2	SER	-	expression tag	UNP D7A8L2
D	403	ALA	-	expression tag	UNP D7A8L2
D	404	LEU	-	expression tag	UNP D7A8L2
D	405	GLU	-	expression tag	UNP D7A8L2
D	406	VAL	-	expression tag	UNP D7A8L2
D	407	LEU	-	expression tag	UNP D7A8L2
D	408	PHE	-	expression tag	UNP D7A8L2
D	409	GLN	-	expression tag	UNP D7A8L2
D	410	GLY	-	expression tag	UNP D7A8L2
D	411	PRO	-	expression tag	UNP D7A8L2
D	412	HIS	-	expression tag	UNP D7A8L2
D	413	HIS	-	expression tag	UNP D7A8L2
D	414	HIS	-	expression tag	UNP D7A8L2
D	415	HIS	-	expression tag	UNP D7A8L2
D	416	HIS	-	expression tag	UNP D7A8L2
D	417	HIS	-	expression tag	UNP D7A8L2
D	418	HIS	-	expression tag	UNP D7A8L2
D	419	HIS	-	expression tag	UNP D7A8L2
D	420	HIS	-	expression tag	UNP D7A8L2
D	421	HIS	-	expression tag	UNP D7A8L2

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



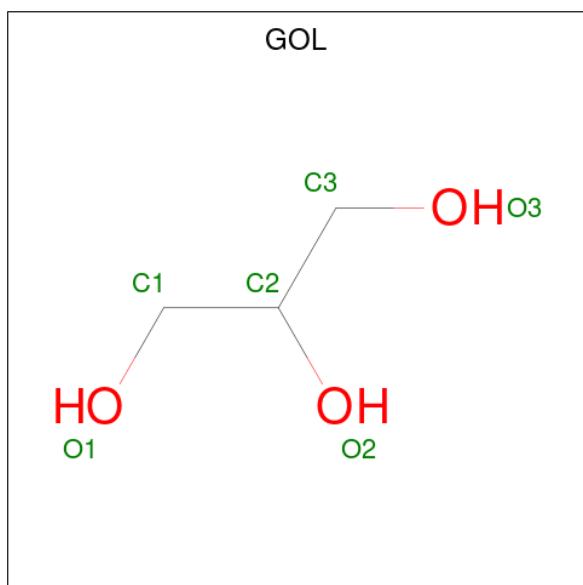
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

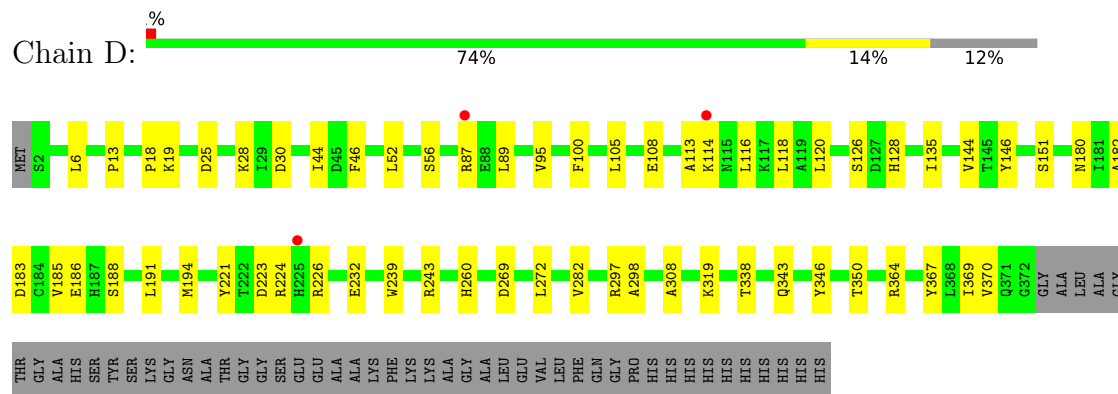
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Cl 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	167	Total O 167 167	0	0
6	B	115	Total O 115 115	0	0
6	C	121	Total O 121 121	0	0
6	D	98	Total O 98 98	0	0

- Molecule 1: Formate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.26Å 59.48Å 122.67Å 79.89° 85.41° 63.15°	Depositor
Resolution (Å)	52.87 – 2.10 52.87 – 2.10	Depositor EDS
% Data completeness (in resolution range)	91.5 (52.87-2.10) 86.5 (52.87-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.176 , 0.224 0.181 , 0.226	Depositor DCC
R_{free} test set	3749 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtrriage
Anisotropy	0.319	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12267	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.41	0/2989	0.62	0/4069
1	B	0.38	0/2996	0.59	0/4080
1	C	0.39	0/2989	0.60	0/4070
1	D	0.37	0/2974	0.59	0/4050
All	All	0.39	0/11948	0.60	0/16269

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	2915	0	2868	27	0
1	B	2922	0	2877	23	0
1	C	2912	0	2866	31	0
1	D	2900	0	2853	32	0
2	A	14	0	20	1	0
2	B	7	0	10	0	0
3	A	30	0	40	2	0
3	B	6	0	8	0	0
3	C	30	0	40	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	24	0	32	0	0
4	A	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	B	2	0	0	0	0
6	A	167	0	0	1	0
6	B	115	0	0	0	0
6	C	121	0	0	0	0
6	D	98	0	0	0	0
All	All	12267	0	11614	104	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 4.

All (104) 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:125:GLY:N	1:A:143:GLU:OE1	2.21	0.67
1:D:226:ARG:HD2	1:D:239:TRP:CG	2.32	0.65
1:D:95:VAL:HG21	1:D:105:LEU:HD11	1.83	0.61
1:B:259:LEU:HB2	1:B:286:ARG:HG3	1.82	0.60
1:C:93:ASP:OD1	1:C:117:LYS:NZ	2.35	0.59
1:A:19:LYS:N	1:A:19:LYS:HD2	2.18	0.59
1:B:125:GLY:N	1:B:143:GLU:OE1	2.31	0.59
1:C:334:HIS:NE2	3:C:504:GOL:H2	2.18	0.58
1:D:120:LEU:HD23	1:D:350:THR:HG23	1.85	0.58
1:C:19:LYS:HD3	1:C:20:THR:HG23	1.85	0.58
1:B:185:VAL:HA	1:B:188:SER:HB3	1.86	0.57
1:D:272:LEU:HD13	1:D:298:ALA:HB2	1.85	0.57
1:D:144:VAL:HG11	1:D:346:TYR:HA	1.86	0.57
1:D:118:LEU:HG	1:D:120:LEU:HD13	1.85	0.57
1:A:320:ASP:OD2	1:B:114:LYS:NZ	2.38	0.56
1:D:185:VAL:HA	1:D:188:SER:HB3	1.87	0.56
1:D:126:SER:HB3	1:D:369:ILE:HD13	1.89	0.55
1:D:128:HIS:H	1:D:128:HIS:CD2	2.24	0.55
1:D:191:LEU:O	1:D:194:MET:HB2	2.06	0.55
1:C:296:VAL:HA	1:C:326:MET:CE	2.38	0.54
1:C:286:ARG:HB2	1:C:289:LEU:HD13	1.89	0.53
1:C:223:ASP:OD1	1:C:224:ARG:N	2.39	0.53
1:C:272:LEU:HD13	1:C:298:ALA:HB2	1.91	0.53
1:D:95:VAL:HG22	1:D:116:LEU:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:ASP:OD1	1:D:224:ARG:N	2.39	0.53
1:D:25:ASP:N	1:D:25:ASP:OD1	2.43	0.52
1:B:96:ILE:HG12	1:B:120:LEU:HB3	1.91	0.52
1:A:334:HIS:NE2	3:A:507:GOL:H2	2.25	0.52
1:D:30:ASP:OD1	1:D:30:ASP:N	2.43	0.52
1:B:272:LEU:HD13	1:B:298:ALA:HB2	1.92	0.51
1:A:358:PHE:HB3	3:A:505:GOL:H31	1.91	0.51
1:A:120:LEU:HD11	1:A:353:ILE:HD13	1.93	0.51
1:B:115:ASN:O	1:B:117:LYS:HG3	2.11	0.51
1:D:226:ARG:HD2	1:D:239:TRP:CD2	2.45	0.51
1:C:148:ASN:O	1:C:152:VAL:HG23	2.11	0.50
1:C:137:ARG:CZ	1:D:224:ARG:HE	2.25	0.50
1:C:144:VAL:HG11	1:C:346:TYR:HA	1.93	0.50
1:A:144:VAL:HG11	1:A:346:TYR:HA	1.94	0.50
1:D:180:ASN:HB3	1:D:183:ASP:OD2	2.12	0.50
1:D:44:ILE:HD12	1:D:46:PHE:O	2.12	0.49
1:C:291:ASP:HB3	1:C:294:ALA:HB3	1.94	0.49
1:B:2:SER:N	1:B:69:GLY:O	2.45	0.49
1:B:126:SER:HB3	1:B:369:ILE:HD13	1.94	0.49
1:C:136:ASP:OD2	1:D:260:HIS:NE2	2.42	0.49
1:B:124:ILE:HD12	1:B:148:ASN:OD1	2.13	0.48
1:C:368:LEU:HD22	1:C:371:GLN:HB2	1.95	0.48
1:B:228:PRO:HB2	1:B:231:VAL:HG23	1.96	0.48
1:A:4:LYS:NZ	1:A:88:GLU:OE1	2.43	0.47
1:A:327:LYS:HD2	1:A:328:TRP:H	1.79	0.47
1:C:282:VAL:HA	1:C:308:ALA:O	2.15	0.47
1:C:171:HIS:HE1	1:C:175[A]:ARG:CZ	2.28	0.47
1:A:23:ARG:HD3	1:C:189:TYR:CE1	2.50	0.47
1:B:168:ILE:HB	1:B:169:PRO:HD3	1.96	0.47
1:D:108:GLU:OE1	1:D:108:GLU:N	2.41	0.47
1:D:221:TYR:OH	1:D:232:GLU:OE2	2.29	0.47
1:B:371:GLN:OE1	1:B:371:GLN:HA	2.15	0.46
1:A:17:TYR:CD1	1:A:56:SER:HB2	2.51	0.46
1:A:185:VAL:HG11	1:C:338:THR:HG23	1.97	0.46
1:A:338:THR:HG23	1:C:185:VAL:HG11	1.98	0.46
1:D:364:ARG:HB2	1:D:367:TYR:CD2	2.51	0.45
1:A:227:LEU:HD13	1:A:231:VAL:HG11	1.99	0.44
1:A:86:GLU:OE2	1:A:112:LYS:NZ	2.41	0.44
1:A:181:ILE:O	1:A:185:VAL:HG22	2.17	0.44
1:C:114:LYS:HE2	1:C:114:LYS:HB2	1.74	0.44
1:B:233:LYS:HD3	1:B:233:LYS:HA	1.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:PHE:CE1	1:B:108:GLU:HG3	2.53	0.44
1:C:260:HIS:HB3	1:C:261:PRO:HD2	1.99	0.44
1:A:172:ASP:CG	1:C:175[A]:ARG:HH22	2.20	0.43
1:B:17:TYR:CD1	1:B:18:PRO:HD2	2.54	0.43
1:C:29:ILE:O	1:C:38:LEU:HD22	2.19	0.43
1:B:288:LYS:HE2	1:B:313:PHE:CZ	2.53	0.43
1:A:89:LEU:HG	1:A:113:ALA:HB2	2.01	0.43
1:D:182:ALA:O	1:D:186:GLU:HB2	2.19	0.43
1:B:10:TYR:O	1:B:54:SER:HA	2.19	0.43
1:C:39:PRO:HG2	1:C:345:ARG:O	2.19	0.43
1:C:124:ILE:HD12	1:C:148:ASN:OD1	2.18	0.42
1:B:310:ASP:O	1:B:334:HIS:HA	2.19	0.42
1:A:101:TRP:CE2	2:A:502:PEG:H21	2.55	0.42
1:C:191:LEU:O	1:C:194:MET:HB2	2.18	0.42
1:C:203:ARG:HH12	3:C:502:GOL:H32	1.85	0.42
1:D:282:VAL:HA	1:D:308:ALA:O	2.19	0.42
1:D:13:PRO:HG2	1:D:18:PRO:HD3	2.01	0.42
1:B:197:GLY:HA2	1:B:220:HIS:O	2.20	0.42
1:D:135:ILE:HD13	1:D:135:ILE:HA	1.86	0.42
1:A:327:LYS:HG3	1:A:328:TRP:CE2	2.55	0.41
1:D:269:ASP:CG	1:D:297:ARG:HH21	2.22	0.41
1:C:331:MET:HE3	1:C:331:MET:HB3	1.92	0.41
1:B:95:VAL:HG23	1:B:116:LEU:HD13	2.02	0.41
1:D:52:LEU:N	1:D:343:GLN:OE1	2.50	0.41
1:D:6:LEU:HB3	1:D:95:VAL:HG12	2.02	0.41
1:A:25:ASP:HB2	6:A:667:HOH:O	2.20	0.41
1:C:296:VAL:HG22	1:C:326:MET:HE3	2.02	0.41
1:D:89:LEU:HG	1:D:113:ALA:HB2	2.02	0.41
1:A:175[A]:ARG:HH22	1:C:172:ASP:CG	2.24	0.41
1:A:120:LEU:HD11	1:A:353:ILE:CD1	2.51	0.41
1:A:132:GLN:NE2	1:A:136:ASP:OD1	2.53	0.40
1:B:359:GLU:OE1	1:B:361:ARG:NH1	2.53	0.40
1:A:8:VAL:HA	1:A:75:THR:O	2.22	0.40
1:C:64:TYR:HB2	1:C:351:ARG:NH2	2.37	0.40
1:D:87:ARG:HE	1:D:87:ARG:HB3	1.65	0.40
1:D:100:PHE:CE2	1:D:338:THR:HB	2.56	0.40
1:A:364:ARG:HB2	1:A:367:TYR:CD2	2.57	0.40
1:B:148:ASN:O	1:B:152:VAL:HG23	2.21	0.40
1:C:94:VAL:HG13	1:C:118:LEU:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	371/421 (88%)	360 (97%)	11 (3%)	0	100	100
1	B	373/421 (89%)	362 (97%)	11 (3%)	0	100	100
1	C	370/421 (88%)	357 (96%)	11 (3%)	2 (0%)	29	26
1	D	369/421 (88%)	352 (95%)	17 (5%)	0	100	100
All	All	1483/1684 (88%)	1431 (96%)	50 (3%)	2 (0%)	51	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	201	ALA
1	C	200	ALA

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	309/342 (90%)	302 (98%)	7 (2%)	50	55
1	B	309/342 (90%)	304 (98%)	5 (2%)	62	69
1	C	310/342 (91%)	307 (99%)	3 (1%)	76	82
1	D	308/342 (90%)	299 (97%)	9 (3%)	42	46
All	All	1236/1368 (90%)	1212 (98%)	24 (2%)	57	63

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	19	LYS
1	A	42	LYS
1	A	146	TYR
1	A	301	SER
1	A	326	MET
1	A	327	LYS
1	B	146	TYR
1	B	149	SER
1	B	224	ARG
1	B	320	ASP
1	B	327	LYS
1	C	63	LYS
1	C	146	TYR
1	C	218	LYS
1	D	19	LYS
1	D	28	LYS
1	D	56	SER
1	D	114	LYS
1	D	146	TYR
1	D	151	SER
1	D	243	ARG
1	D	319	LYS
1	D	370	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	371	GLN
1	C	68	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](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	507	-	5,5,5	0.71	0	5,5,5	1.16	0
3	GOL	C	502	-	5,5,5	1.02	0	5,5,5	0.87	0
2	PEG	B	501	-	6,6,6	0.29	0	5,5,5	0.10	0
3	GOL	C	503	-	5,5,5	0.96	0	5,5,5	0.91	0
3	GOL	C	501	-	5,5,5	0.82	0	5,5,5	0.93	0
3	GOL	C	504	-	5,5,5	0.76	0	5,5,5	1.15	0
3	GOL	A	503	-	5,5,5	1.01	0	5,5,5	1.08	0
3	GOL	C	505	-	5,5,5	1.43	1 (20%)	5,5,5	0.66	0
3	GOL	A	506	-	5,5,5	0.55	0	5,5,5	1.08	0
2	PEG	A	501	-	6,6,6	0.21	0	5,5,5	0.10	0
3	GOL	B	504	-	5,5,5	0.75	0	5,5,5	0.98	0
3	GOL	D	501	-	5,5,5	0.93	0	5,5,5	0.95	0
2	PEG	A	502	-	6,6,6	0.21	0	5,5,5	0.13	0
3	GOL	D	502	-	5,5,5	0.65	0	5,5,5	1.20	1 (20%)
3	GOL	A	504	-	5,5,5	1.12	0	5,5,5	0.86	0
3	GOL	D	503	-	5,5,5	0.90	0	5,5,5	1.18	1 (20%)
3	GOL	A	505	-	5,5,5	0.96	0	5,5,5	0.87	0
3	GOL	D	504	-	5,5,5	0.87	0	5,5,5	0.95	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	507	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	502	-	-	1/4/4/4	-
2	PEG	B	501	-	-	3/4/4/4	-
3	GOL	C	503	-	-	4/4/4/4	-
3	GOL	C	501	-	-	3/4/4/4	-
3	GOL	C	504	-	-	4/4/4/4	-
3	GOL	A	503	-	-	2/4/4/4	-
3	GOL	C	505	-	-	2/4/4/4	-
3	GOL	A	506	-	-	2/4/4/4	-
2	PEG	A	501	-	-	2/4/4/4	-
3	GOL	B	504	-	-	1/4/4/4	-
3	GOL	D	501	-	-	0/4/4/4	-
2	PEG	A	502	-	-	3/4/4/4	-
3	GOL	D	502	-	-	2/4/4/4	-
3	GOL	A	504	-	-	1/4/4/4	-
3	GOL	D	503	-	-	0/4/4/4	-
3	GOL	A	505	-	-	2/4/4/4	-
3	GOL	D	504	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	505	GOL	O2-C2	-2.14	1.37	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	GOL	C3-C2-C1	-2.16	103.30	111.70
3	D	503	GOL	C3-C2-C1	-2.05	103.75	111.70

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	506	GOL	O1-C1-C2-C3
3	A	507	GOL	O1-C1-C2-C3
3	C	503	GOL	C1-C2-C3-O3
3	C	504	GOL	C1-C2-C3-O3
3	C	505	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	D	502	GOL	C1-C2-C3-O3
3	D	504	GOL	O1-C1-C2-C3
3	D	504	GOL	C1-C2-C3-O3
3	D	504	GOL	O2-C2-C3-O3
2	B	501	PEG	C1-C2-O2-C3
3	C	505	GOL	O1-C1-C2-O2
2	A	501	PEG	O2-C3-C4-O4
3	A	503	GOL	C1-C2-C3-O3
3	A	504	GOL	O1-C1-C2-C3
3	A	505	GOL	O1-C1-C2-C3
3	A	507	GOL	C1-C2-C3-O3
3	C	502	GOL	O1-C1-C2-C3
3	C	503	GOL	O1-C1-C2-C3
3	C	504	GOL	O1-C1-C2-C3
3	A	506	GOL	O1-C1-C2-O2
3	A	507	GOL	O1-C1-C2-O2
3	A	507	GOL	O2-C2-C3-O3
3	C	504	GOL	O1-C1-C2-O2
3	C	504	GOL	O2-C2-C3-O3
3	D	504	GOL	O1-C1-C2-O2
2	A	501	PEG	O1-C1-C2-O2
2	A	502	PEG	O1-C1-C2-O2
2	B	501	PEG	O1-C1-C2-O2
3	C	501	GOL	O1-C1-C2-O2
3	D	502	GOL	O2-C2-C3-O3
3	A	503	GOL	O2-C2-C3-O3
3	C	503	GOL	O2-C2-C3-O3
2	B	501	PEG	C4-C3-O2-C2
2	A	502	PEG	C4-C3-O2-C2
3	C	501	GOL	C1-C2-C3-O3
3	C	503	GOL	O1-C1-C2-O2
3	C	501	GOL	O1-C1-C2-C3
2	A	502	PEG	O2-C3-C4-O4
3	A	505	GOL	O1-C1-C2-O2
3	B	504	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	507	GOL	1	0
3	C	502	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	504	GOL	1	0
2	A	502	PEG	1	0
3	A	505	GOL	1	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	372/421 (88%)	-0.33	0 100 100	27, 38, 50, 63	0
1	B	375/421 (89%)	-0.29	1 (0%) 94 94	30, 43, 59, 79	0
1	C	370/421 (87%)	-0.25	0 100 100	28, 45, 63, 73	0
1	D	371/421 (88%)	-0.20	3 (0%) 86 88	31, 47, 66, 80	0
All	All	1488/1684 (88%)	-0.27	4 (0%) 94 94	27, 43, 61, 80	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	225	HIS	3.6
1	B	375	LEU	3.0
1	D	87	ARG	2.4
1	D	114	LYS	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NA	A	509	1/1	0.80	0.24	45,45,45,45	0
3	GOL	C	502	6/6	0.81	0.16	45,53,59,62	0
2	PEG	A	502	7/7	0.82	0.17	37,44,50,52	0
3	GOL	A	507	6/6	0.82	0.26	40,45,49,52	0
3	GOL	C	505	6/6	0.86	0.13	41,45,45,46	0
2	PEG	A	501	7/7	0.86	0.19	48,51,55,56	0
3	GOL	A	503	6/6	0.87	0.16	56,57,60,61	0
3	GOL	C	503	6/6	0.87	0.21	63,65,67,69	0
3	GOL	A	504	6/6	0.90	0.12	38,41,43,44	0
3	GOL	D	503	6/6	0.90	0.19	56,57,58,59	0
3	GOL	B	504	6/6	0.90	0.16	47,50,51,53	0
3	GOL	C	501	6/6	0.91	0.11	57,58,63,63	0
3	GOL	A	505	6/6	0.91	0.13	49,53,56,57	0
3	GOL	D	502	6/6	0.92	0.15	42,47,51,52	0
2	PEG	B	501	7/7	0.92	0.15	42,44,48,55	0
3	GOL	D	501	6/6	0.92	0.17	48,48,53,53	0
3	GOL	C	504	6/6	0.94	0.21	45,47,48,49	0
3	GOL	A	506	6/6	0.94	0.10	44,44,49,49	0
3	GOL	D	504	6/6	0.95	0.15	48,50,53,59	0
5	CL	B	502	1/1	0.95	0.17	57,57,57,57	0
5	CL	B	503	1/1	0.95	0.10	63,63,63,63	0
4	NA	A	508	1/1	0.96	0.08	48,48,48,48	0
4	NA	C	506	1/1	0.97	0.10	49,49,49,49	0
4	NA	D	505	1/1	0.98	0.07	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.