



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:20 PM UTC

PDB ID : 7JH0 / pdb_00007jh0
Title : Crystallographic structure of glyceraldehyde-3-phosphate dehydrogenase from Schistosoma mansoni
Authors : Boreiko, S.; Silva, M.; Iulek, J.
Deposited on : 2020-07-20
Resolution : 2.51 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

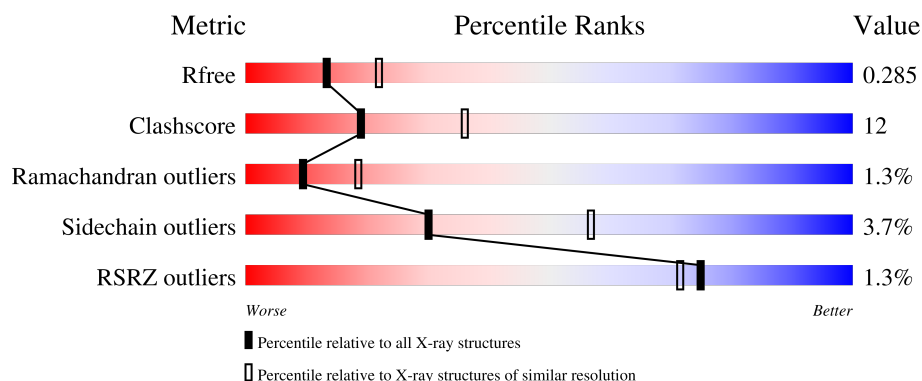
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	338	
1	B	338	
1	C	338	
2	D	338	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10188 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.

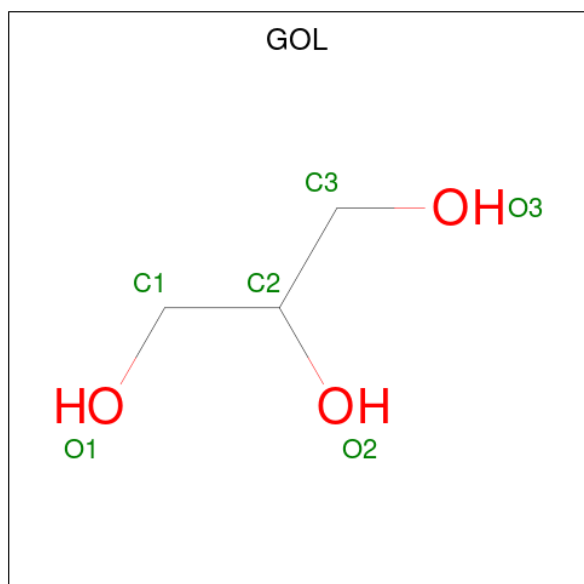
- Molecule 1 is a protein called Glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	P	S	0	2	0
			2512	1580	429	488	1	14			
1	B	338	Total	C	N	O	P	S	0	3	0
			2476	1549	431	482	1	13			
1	C	338	Total	C	N	O	P	S	0	1	0
			2481	1559	429	478	1	14			

- Molecule 2 is a protein called Glyceraldehyde-3-phosphate dehydrogenase.

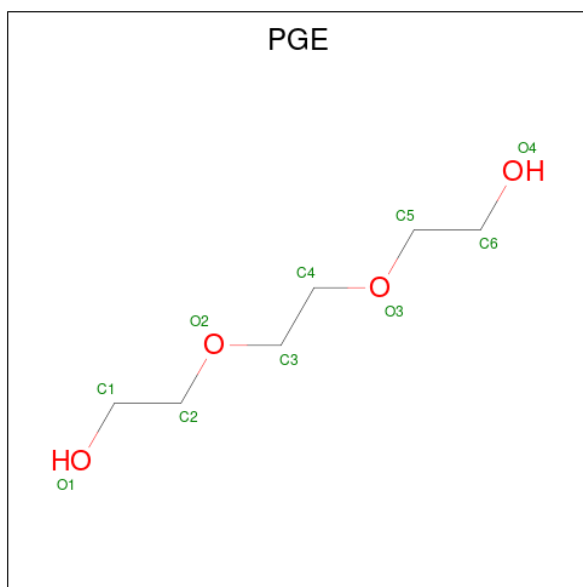
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	338	Total	C	N	O	S	0	0	0
			2466	1551	426	476	13			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



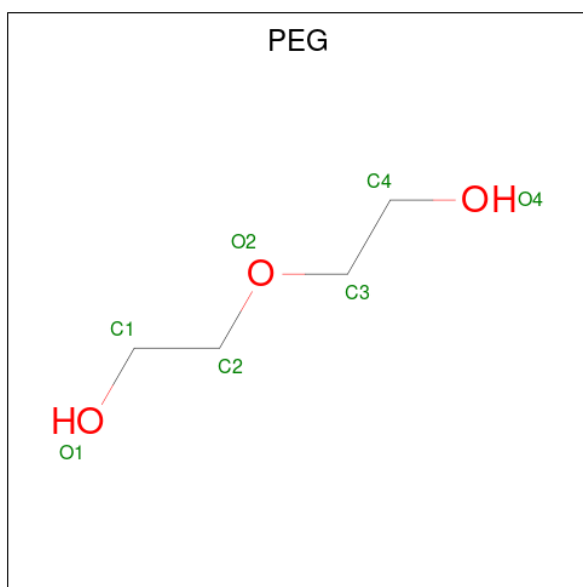
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



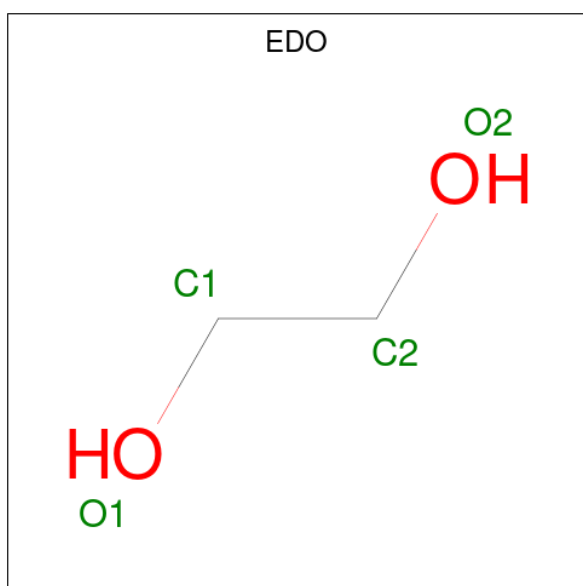
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

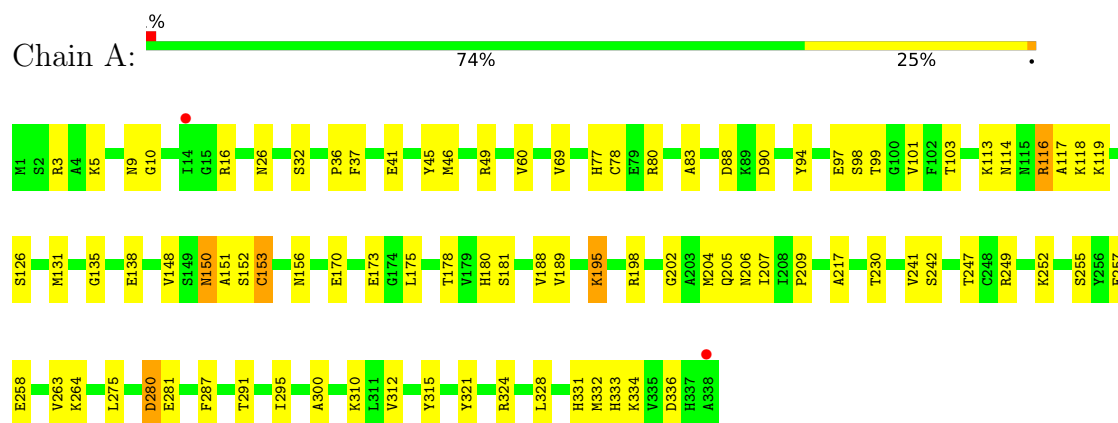
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	45	Total 45	O 45	0	0
7	B	57	Total 57	O 57	0	0
7	C	49	Total 49	O 49	0	0
7	D	52	Total 52	O 52	0	0

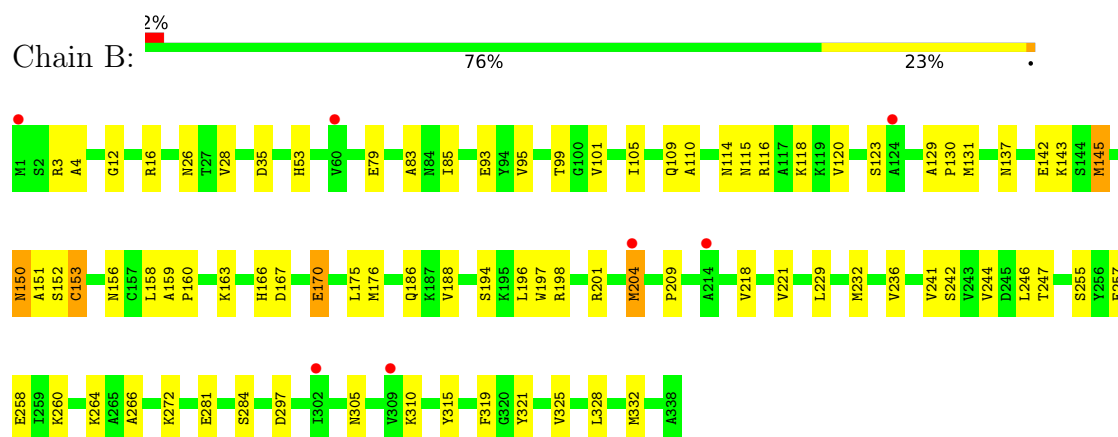
3 Residue-property plots [i](#)

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.

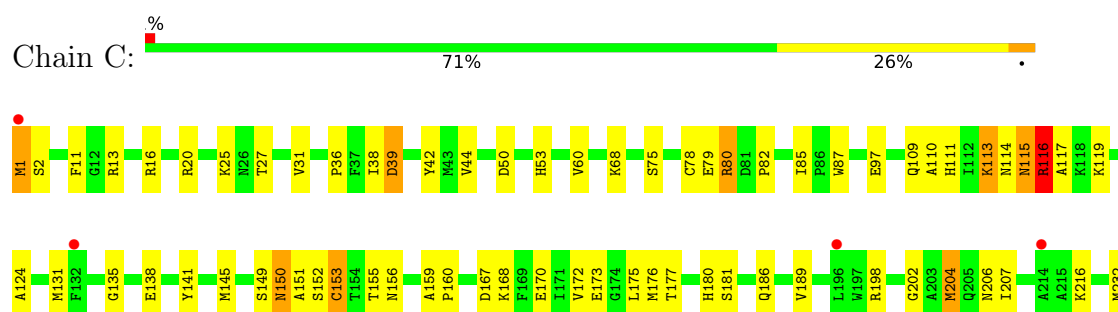
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

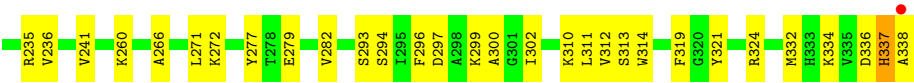


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

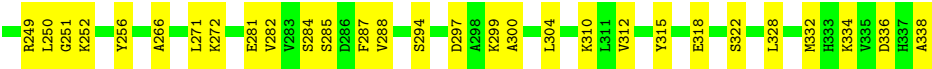
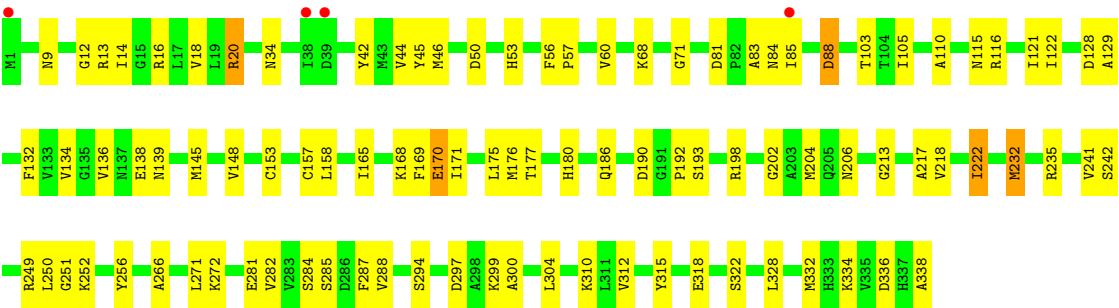


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase





● Molecule 2: Glyceraldehyde-3-phosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	80.12Å 80.12Å 417.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	57.76 – 2.51 57.76 – 2.51	Depositor EDS
% Data completeness (in resolution range)	100.0 (57.76-2.51) 100.0 (57.76-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.213 , 0.273 0.225 , 0.285	Depositor DCC
R_{free} test set	1967 reflections (3.83%)	wwPDB-VP
Wilson B-factor (Å ²)	63.4	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 65.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.087 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.080 for h,-h-k,-l	Depositor
Outliers	1 of 51375 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10188	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CSP, CSD, PGE, PEG, EDO

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	0.33	0/2560	0.75	0/3473
1	B	0.32	0/2526	0.74	0/3433
1	C	0.37	1/2521 (0.0%)	0.77	1/3422 (0.0%)
2	D	0.35	0/2504	0.75	2/3407 (0.1%)
All	All	0.34	1/10111 (0.0%)	0.75	3/13735 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	116	ARG	CA-C	7.34	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	222	ILE	CA-C-N	6.12	126.01	119.28
2	D	222	ILE	C-N-CA	6.12	126.01	119.28
1	C	116	ARG	N-CA-C	5.27	116.53	108.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2512	0	2430	68	0
1	B	2476	0	2353	60	0
1	C	2481	0	2378	65	0
2	D	2466	0	2353	67	0
3	A	6	0	8	1	0
3	B	6	0	8	1	0
4	A	10	0	14	2	0
4	B	10	0	14	2	0
5	B	7	0	10	1	0
5	D	7	0	10	3	0
6	C	4	0	6	1	0
7	A	45	0	0	5	0
7	B	57	0	0	6	0
7	C	49	0	0	1	0
7	D	52	0	0	0	0
All	All	10188	0	9584	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 12.

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:B:232:MET:HE2	1:C:310:LYS:HD3	1.47	0.95
1:C:114:ASN:O	1:C:115:ASN:ND2	2.01	0.92
2:D:148:VAL:HG21	2:D:332:MET:HE1	1.52	0.90
1:C:332:MET:O	1:C:336:ASP:N	2.06	0.88
2:D:110:ALA:O	2:D:116:ARG:NH1	2.07	0.88
1:A:148:VAL:HG21	1:A:332:MET:HE1	1.57	0.86
1:A:49:ARG:HH12	1:C:282:VAL:HG12	1.42	0.85
1:A:249:ARG:HD2	2:D:249:ARG:HD2	1.61	0.82
1:C:152:SER:O	1:C:156:ASN:ND2	2.16	0.76
1:B:110:ALA:O	1:B:116:ARG:NH1	2.20	0.74
1:C:279:GLU:O	1:C:299:LYS:NZ	2.19	0.74
1:B:297:ASP:OD2	1:C:198:ARG:NH2	2.20	0.72
1:B:201:ARG:O	7:B:501:HOH:O	2.07	0.72
1:B:153:CSP:O1P	7:B:502:HOH:O	2.10	0.69
1:B:196:LEU:HA	4:B:403:PGE:H62	1.76	0.68
1:B:131:MET:HE3	1:B:151:ALA:HA	1.75	0.67
1:B:266:ALA:O	7:B:503:HOH:O	2.11	0.67
1:C:113:LYS:O	1:C:116:ARG:HD3	1.94	0.67
1:C:1:MET:HG2	1:C:2:SER:H	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LYS:NZ	7:A:503:HOH:O	2.28	0.65
2:D:297:ASP:HB3	2:D:312:VAL:HG23	1.79	0.65
1:C:202:GLY:O	1:C:206:ASN:ND2	2.26	0.65
1:A:198:ARG:HD2	3:A:401:GOL:H12	1.77	0.65
1:A:310:LYS:HB2	2:D:175:LEU:HD13	1.79	0.64
1:A:83:ALA:O	1:A:116:ARG:NH2	2.25	0.64
1:B:158:LEU:HD22	1:B:176:MET:HG3	1.80	0.64
1:B:163:LYS:O	1:B:163:LYS:HG3	1.97	0.63
1:B:83:ALA:HA	1:B:116:ARG:HH12	1.62	0.62
1:C:36:PRO:HA	1:C:78:CYS:HB2	1.82	0.62
1:A:204:MET:HE2	1:B:188:VAL:HG12	1.82	0.62
1:B:150:ASN:O	1:B:150:ASN:ND2	2.30	0.62
1:A:180:HIS:ND1	1:A:181:SER:O	2.27	0.61
1:C:294:SER:OG	1:C:313:SER:OG	2.18	0.61
1:A:83:ALA:C	1:A:116:ARG:HH22	2.09	0.60
2:D:299:LYS:HA	5:D:401:PEG:H31	1.82	0.60
1:A:198:ARG:NH1	2:D:297:ASP:OD2	2.34	0.60
1:B:3:ARG:NH1	7:B:508:HOH:O	2.34	0.60
2:D:20:ARG:NH1	2:D:53:HIS:HB3	2.16	0.59
2:D:136:VAL:HG11	2:D:222:ILE:HG12	1.84	0.59
1:B:12:GLY:O	1:B:16:ARG:HG3	2.02	0.59
1:A:60:VAL:HG13	1:A:69:VAL:HG22	1.84	0.58
2:D:20:ARG:NH1	2:D:53:HIS:O	2.36	0.58
1:B:198:ARG:NH2	7:B:509:HOH:O	2.35	0.58
1:C:44:VAL:HG13	1:C:60:VAL:HG12	1.84	0.58
2:D:13:ARG:NH1	2:D:50:ASP:OD2	2.36	0.58
2:D:68:LYS:HE3	2:D:71:GLY:HA2	1.85	0.58
1:C:141:TYR:HE2	1:C:336:ASP:OD1	1.87	0.58
1:B:137:ASN:HD21	1:B:221:VAL:HG12	1.70	0.57
1:C:302:ILE:HG22	1:C:310:LYS:HD2	1.84	0.57
1:B:99:THR:HB	1:B:101:VAL:HG22	1.86	0.57
1:A:198:ARG:HH11	1:A:209:PRO:HG2	1.69	0.56
1:A:230:THR:HG22	2:D:304:LEU:HD13	1.88	0.56
1:B:218:VAL:HG11	1:B:229:LEU:HD12	1.86	0.56
2:D:134:VAL:HA	2:D:138:GLU:HB3	1.86	0.56
1:A:150:ASN:ND2	1:A:150:ASN:O	2.38	0.56
1:A:242:SER:HB2	1:A:315:TYR:CZ	2.42	0.56
1:B:158:LEU:HD11	1:B:246:LEU:HD22	1.88	0.55
1:C:294:SER:HG	1:C:313:SER:HG	1.48	0.55
1:B:123:SER:O	1:B:321:TYR:OH	2.18	0.55
1:C:297:ASP:HB3	1:C:312:VAL:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:170:GLU:O	2:D:251:GLY:N	2.37	0.55
2:D:132:PHE:HZ	2:D:145:MET:HE1	1.71	0.55
1:B:4:ALA:HB3	1:B:28:VAL:HG12	1.89	0.54
2:D:83:ALA:HA	2:D:116:ARG:HH12	1.72	0.54
1:A:328:LEU:HG	1:A:332:MET:HE3	1.88	0.54
1:B:130:PRO:HG2	1:B:145:MET:HE2	1.88	0.54
1:A:97:GLU:OE2	1:A:99:THR:OG1	2.20	0.53
1:C:111:HIS:O	1:C:116:ARG:HG3	2.08	0.53
1:B:209:PRO:HG3	1:C:314:TRP:HZ2	1.74	0.53
2:D:334:LYS:O	2:D:338:ALA:HB3	2.09	0.53
1:C:296:PHE:HE1	1:C:311:LEU:HD22	1.74	0.52
2:D:44:VAL:HG13	2:D:60:VAL:HG12	1.92	0.52
1:A:202:GLY:O	1:A:206:ASN:ND2	2.39	0.52
1:A:10:GLY:O	1:A:98:SER:OG	2.18	0.52
1:C:153:CSP:HA	1:C:321:TYR:CD1	2.45	0.51
2:D:242:SER:HB2	2:D:315:TYR:CZ	2.46	0.51
1:C:87:TRP:HB2	1:C:116:ARG:HB2	1.92	0.51
1:B:85:ILE:O	1:B:116:ARG:NH2	2.34	0.51
1:B:158:LEU:HD13	1:B:244:VAL:HG11	1.91	0.51
2:D:318:GLU:O	2:D:322:SER:OG	2.24	0.51
1:A:9:ASN:O	1:A:98:SER:OG	2.29	0.51
2:D:186:GLN:OE1	2:D:235:ARG:HD3	2.11	0.50
1:B:257:GLU:HA	1:B:260:LYS:HD3	1.93	0.50
1:B:255:SER:H	1:B:258:GLU:HG3	1.75	0.50
1:C:131:MET:HG2	1:C:149:SER:HB3	1.94	0.50
1:B:186:GLN:HG2	7:B:501:HOH:O	2.11	0.50
1:C:39:ASP:OD1	1:C:39:ASP:N	2.35	0.50
1:C:79:GLU:HB2	1:C:85:ILE:HG12	1.93	0.50
1:A:103:THR:O	1:A:126:SER:OG	2.21	0.49
1:B:95:VAL:HB	1:B:120:VAL:HG22	1.95	0.49
2:D:9:ASN:OD1	2:D:34:ASN:ND2	2.45	0.49
1:C:38:ILE:HD11	2:D:192:PRO:HB3	1.95	0.49
1:C:135:GLY:H	1:C:138:GLU:HB2	1.77	0.49
1:A:175:LEU:HD13	2:D:310:LYS:HB2	1.94	0.49
2:D:132:PHE:CZ	2:D:145:MET:HE1	2.47	0.49
1:A:16:ARG:HD2	1:A:46:MET:HB3	1.95	0.48
1:A:188:VAL:HG12	1:A:204:MET:HE1	1.95	0.48
1:C:82:PRO:HB3	1:C:111:HIS:CE1	2.48	0.48
1:A:60:VAL:HG22	1:A:69:VAL:HG13	1.94	0.48
1:C:13:ARG:HH11	1:C:16:ARG:HH22	1.62	0.48
1:C:296:PHE:CE1	1:C:311:LEU:HD22	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:299:LYS:HD3	5:D:401:PEG:H22	1.96	0.48
1:B:242:SER:HB2	1:B:315:TYR:CZ	2.48	0.48
1:C:186:GLN:OE1	1:C:235:ARG:HD3	2.12	0.48
1:A:324:ARG:NH2	7:A:508:HOH:O	2.46	0.48
1:A:77:HIS:HA	4:A:402:PGE:H5	1.95	0.48
1:B:93:GLU:HG2	1:B:118:LYS:HB2	1.96	0.48
1:A:263:VAL:HG13	1:A:275:LEU:HD21	1.96	0.48
1:B:175:LEU:HD13	1:C:310:LYS:HB2	1.95	0.48
1:C:124:ALA:O	1:C:149:SER:OG	2.23	0.48
1:A:41:GLU:HG2	1:B:197:TRP:HH2	1.79	0.48
2:D:213:GLY:O	2:D:217:ALA:N	2.46	0.47
2:D:300:ALA:HB3	2:D:312:VAL:HG21	1.95	0.47
1:A:287:PHE:HE1	1:A:295:ILE:HG21	1.79	0.47
1:C:13:ARG:HH12	1:C:50:ASP:CG	2.22	0.47
2:D:138:GLU:OE2	2:D:139:ASN:ND2	2.47	0.47
1:A:135:GLY:H	1:A:138:GLU:CD	2.23	0.47
1:B:105:ILE:O	1:B:109:GLN:HG2	2.14	0.47
1:A:281:GLU:HB3	2:D:198:ARG:HG3	1.97	0.47
1:A:36:PRO:HA	1:A:78:CYS:HB2	1.97	0.47
1:B:142:GLU:O	1:B:145:MET:HG3	2.14	0.47
1:B:163:LYS:O	1:B:167:ASP:HB2	2.14	0.47
1:A:280:ASP:N	1:A:280:ASP:OD1	2.47	0.47
1:C:152:SER:O	1:C:155:THR:HG22	2.14	0.47
4:B:403:PGE:H22	4:B:403:PGE:H4	1.52	0.47
1:C:20:ARG:HD3	6:C:401:EDO:H22	1.97	0.47
1:C:260:LYS:HE2	1:C:277:TYR:OH	2.14	0.47
1:C:189:VAL:HB	2:D:13:ARG:HD2	1.97	0.47
2:D:266:ALA:HB1	2:D:271:LEU:HD12	1.97	0.46
1:B:310:LYS:HB2	1:C:175:LEU:HD13	1.97	0.46
1:A:10:GLY:HA3	1:A:99:THR:HG23	1.97	0.46
1:B:93:GLU:HG3	1:B:118:LYS:HD3	1.97	0.46
1:A:113:LYS:HG2	1:A:114:ASN:OD1	2.15	0.46
1:A:131:MET:HE1	1:A:217:ALA:HB1	1.96	0.46
1:C:300:ALA:HB3	1:C:312:VAL:HG21	1.97	0.46
2:D:158:LEU:HD23	2:D:218:VAL:HG21	1.98	0.46
1:A:152:SER:O	1:A:156:ASN:ND2	2.40	0.46
1:A:188:VAL:HG23	1:A:189:VAL:HG22	1.96	0.46
1:B:328:LEU:HG	1:B:332:MET:HE3	1.98	0.46
1:C:68:LYS:NZ	7:C:503:HOH:O	2.37	0.46
1:C:337:HIS:O	1:C:338:ALA:HB2	2.16	0.46
1:A:3:ARG:NH2	1:A:26:ASN:O	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:202:GLY:O	2:D:206:ASN:ND2	2.49	0.45
2:D:282:VAL:HG21	2:D:287:PHE:HZ	1.82	0.45
1:A:198:ARG:NH1	1:A:209:PRO:HG2	2.31	0.45
1:B:166:HIS:CE1	1:B:170:GLU:HG3	2.51	0.45
1:B:236:VAL:HG11	1:C:236:VAL:HG11	1.98	0.45
1:C:42:TYR:HE2	2:D:193:SER:H	1.63	0.45
1:B:79:GLU:HB2	1:B:85:ILE:HG12	1.97	0.45
2:D:165:ILE:HB	2:D:171:ILE:HD11	1.98	0.45
2:D:176:MET:HG2	2:D:177:THR:N	2.32	0.45
1:B:3:ARG:HH22	1:B:26:ASN:C	2.24	0.45
1:C:116:ARG:CG	1:C:117:ALA:H	2.30	0.45
1:C:302:ILE:HG22	1:C:310:LYS:HB3	1.99	0.45
2:D:105:ILE:H	2:D:128:ASP:CG	2.25	0.45
2:D:168:LYS:O	2:D:252:LYS:HE2	2.17	0.45
2:D:83:ALA:HB2	2:D:110:ALA:HB1	1.99	0.44
1:A:205:GLN:HG3	7:A:505:HOH:O	2.17	0.44
1:A:300:ALA:O	2:D:232:MET:HE2	2.16	0.44
2:D:328:LEU:HG	2:D:332:MET:HE3	1.98	0.44
1:A:88:ASP:OD1	1:A:88:ASP:N	2.50	0.44
1:A:180:HIS:HA	1:A:242:SER:HB3	1.99	0.44
2:D:18:VAL:HA	2:D:322:SER:HB3	1.99	0.44
1:B:12:GLY:HA3	5:B:402:PEG:H42	2.00	0.44
2:D:12:GLY:O	2:D:16:ARG:HG3	2.17	0.44
1:B:159:ALA:HB3	1:B:160:PRO:HD3	1.99	0.44
1:C:79:GLU:OE2	1:C:80:ARG:NH2	2.51	0.44
1:C:119:LYS:HZ2	1:C:145:MET:C	2.25	0.44
1:A:113:LYS:O	1:A:116:ARG:HD2	2.17	0.44
1:A:151:ALA:O	1:A:321:TYR:OH	2.36	0.44
1:A:255:SER:OG	1:A:258:GLU:HB2	2.17	0.44
1:C:150:ASN:ND2	1:C:150:ASN:O	2.50	0.44
2:D:42:TYR:CZ	2:D:46:MET:HE3	2.52	0.44
1:A:99:THR:HB	1:A:101:VAL:HG22	2.00	0.44
1:C:159:ALA:HB3	1:C:160:PRO:HD3	2.01	0.43
2:D:88:ASP:OD1	2:D:88:ASP:N	2.27	0.43
2:D:128:ASP:OD1	2:D:129:ALA:N	2.51	0.43
1:B:204:MET:O	1:B:204:MET:HG3	2.17	0.43
1:A:198:ARG:NH2	2:D:281:GLU:HA	2.32	0.43
4:A:402:PGE:H2	4:A:402:PGE:H4	1.82	0.43
1:C:25:LYS:HB3	1:C:27:THR:HG23	2.01	0.43
2:D:285:SER:O	2:D:288:VAL:HG22	2.18	0.43
1:A:312:VAL:CG2	2:D:232:MET:HE1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:TYR:OH	1:A:333:HIS:HA	2.19	0.43
1:C:180:HIS:ND1	1:C:181:SER:O	2.34	0.43
1:A:32:SER:HB2	1:A:90:ASP:HB3	2.00	0.43
1:B:35:ASP:OD2	3:B:401:GOL:O3	2.34	0.42
1:A:37:PHE:HE1	1:A:80:ARG:HH22	1.67	0.42
1:A:153:CSP:O1P	7:A:501:HOH:O	2.20	0.42
1:C:151:ALA:O	1:C:321:TYR:OH	2.28	0.42
1:A:252:LYS:HB3	1:A:252:LYS:HE2	1.67	0.42
1:B:328:LEU:O	1:B:332:MET:HG3	2.19	0.42
2:D:103:THR:HA	2:D:122:ILE:HD13	2.00	0.42
2:D:81:ASP:HB3	2:D:84:ASN:ND2	2.33	0.42
2:D:157:CYS:O	2:D:294:SER:OG	2.33	0.42
1:B:305[B]:ASN:ND2	1:C:173:GLU:OE1	2.53	0.42
1:B:321:TYR:O	1:B:325:VAL:HG23	2.18	0.42
1:C:151:ALA:HB1	1:C:155:THR:HG21	2.01	0.42
1:B:129:ALA:HA	1:B:130:PRO:HD3	1.83	0.42
1:B:152:SER:O	1:B:156:ASN:ND2	2.33	0.42
1:A:291:THR:O	1:A:324:ARG:NH2	2.51	0.42
1:A:247:THR:HG23	2:D:175:LEU:HD12	2.02	0.42
1:B:281:GLU:O	2:D:45:TYR:OH	2.35	0.42
1:C:53:HIS:CE1	1:C:319:PHE:HB2	2.55	0.42
2:D:56:PHE:HA	2:D:57:PRO:HD3	1.81	0.42
2:D:121:ILE:HG13	2:D:148:VAL:CG2	2.49	0.42
1:C:266:ALA:O	1:C:271:LEU:HB2	2.20	0.41
1:A:195:LYS:NZ	7:A:507:HOH:O	2.44	0.41
1:B:284:SER:HB3	1:C:207:ILE:HB	2.02	0.41
1:C:293:SER:HG	1:C:324:ARG:HH11	1.59	0.41
1:A:45:TYR:OH	1:B:201:ARG:NH1	2.53	0.41
1:A:207:ILE:HB	2:D:284:SER:HB3	2.03	0.41
1:C:176:MET:HG2	1:C:177:THR:N	2.34	0.41
2:D:232:MET:H	2:D:232:MET:HG3	1.59	0.41
1:A:188:VAL:HA	1:A:204:MET:CE	2.50	0.41
2:D:242:SER:HB2	2:D:315:TYR:CE1	2.55	0.41
1:B:53:HIS:CE1	1:B:319:PHE:HB2	2.55	0.41
1:A:135:GLY:N	1:A:138:GLU:OE1	2.46	0.41
1:C:31:VAL:O	1:C:75:SER:N	2.52	0.41
1:C:110:ALA:O	1:C:116:ARG:NH2	2.45	0.41
2:D:85:ILE:O	2:D:116:ARG:NH2	2.47	0.41
2:D:256:TYR:CE2	5:D:401:PEG:H42	2.56	0.41
2:D:180:HIS:HA	2:D:242:SER:HB3	2.03	0.40
1:A:331:HIS:O	1:A:334:LYS:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:MET:HB2	1:B:204:MET:HE3	1.67	0.40
1:B:247:THR:HG23	1:C:175:LEU:HD12	2.04	0.40
2:D:169:PHE:O	2:D:251:GLY:N	2.53	0.40
1:A:173:GLU:OE2	1:A:249:ARG:HD3	2.22	0.40
1:B:198:ARG:NH1	1:C:297:ASP:OD2	2.54	0.40
1:A:116:ARG:HB2	1:A:117:ALA:H	1.77	0.40
1:C:204:MET:CE	2:D:204:MET:HB2	2.52	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	337/338 (100%)	316 (94%)	19 (6%)	2 (1%)	21	38
1	B	338/338 (100%)	306 (90%)	27 (8%)	5 (2%)	8	16
1	C	336/338 (99%)	298 (89%)	33 (10%)	5 (2%)	8	16
2	D	335/338 (99%)	299 (89%)	30 (9%)	6 (2%)	6	12
All	All	1346/1352 (100%)	1219 (91%)	109 (8%)	18 (1%)	9	18

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	115	ASN
1	A	170	GLU
1	B	170	GLU
1	B	241	VAL
1	C	241	VAL
2	D	115	ASN
2	D	190	ASP
2	D	241	VAL

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Mol	Chain	Res	Type
1	B	272	LYS
1	C	170	GLU
1	A	241	VAL
2	D	170	GLU
2	D	272	LYS
1	B	194	SER
1	C	113	LYS
1	C	167	ASP
1	C	172	VAL
2	D	14	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	261/280 (93%)	251 (96%)	10 (4%)	29	56
1	B	249/280 (89%)	243 (98%)	6 (2%)	43	70
1	C	250/280 (89%)	234 (94%)	16 (6%)	16	33
2	D	247/280 (88%)	242 (98%)	5 (2%)	48	75
All	All	1007/1120 (90%)	970 (96%)	37 (4%)	30	57

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	116	ARG
1	A	118	LYS
1	A	150	ASN
1	A	178	THR
1	A	195	LYS
1	A	257	GLU
1	A	264	LYS
1	A	280	ASP
1	A	336	ASP
1	B	114	ASN

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Mol	Chain	Res	Type
1	B	143	LYS
1	B	145	MET
1	B	150	ASN
1	B	204	MET
1	B	264	LYS
1	C	1	MET
1	C	11	PHE
1	C	39	ASP
1	C	80	ARG
1	C	97	GLU
1	C	109	GLN
1	C	115	ASN
1	C	116	ARG
1	C	150	ASN
1	C	168	LYS
1	C	204	MET
1	C	216	LYS
1	C	232	MET
1	C	272	LYS
1	C	334	LYS
1	C	337	HIS
2	D	20	ARG
2	D	88	ASP
2	D	232	MET
2	D	250	LEU
2	D	336	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	337	HIS
1	B	53	HIS
1	B	186	GLN
1	B	205	GLN
1	C	53	HIS
1	C	84	ASN
1	C	111	HIS
1	C	150	ASN
1	C	331	HIS
1	C	337	HIS
2	D	53	HIS
2	D	139	ASN

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Mol	Chain	Res	Type
2	D	306	ASN
2	D	333	HIS
2	D	337	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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	CSP	A	153	1	7,9,10	2.81	2 (28%)	4,12,14	2.24	1 (25%)
1	CSP	C	153	1	7,9,10	2.76	2 (28%)	4,12,14	3.92	3 (75%)
2	CSD	D	153	2	4,7,8	1.30	1 (25%)	1,8,10	1.71	0
1	CSP	B	153	1	7,9,10	2.89	2 (28%)	4,12,14	3.58	3 (75%)

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	CSP	A	153	1	-	0/0/8/10	-
1	CSP	C	153	1	-	0/0/8/10	-
2	CSD	D	153	2	-	1/2/6/8	-
1	CSP	B	153	1	-	0/0/8/10	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	153	CSP	P-O1P	5.64	1.59	1.46
1	A	153	CSP	P-O1P	5.38	1.58	1.46
1	C	153	CSP	P-O1P	5.27	1.58	1.46
1	A	153	CSP	P-O3P	-4.78	1.44	1.56
1	B	153	CSP	P-O2P	-4.77	1.44	1.56
1	C	153	CSP	P-O3P	-4.70	1.44	1.56
2	D	153	CSD	CA-N	-2.07	1.42	1.48

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	153	CSP	O2P-P-O1P	-6.78	95.95	112.90
1	B	153	CSP	O3P-P-O1P	-5.88	98.20	112.90
1	A	153	CSP	O2P-P-O1P	-4.21	102.36	112.90
1	B	153	CSP	CA-CB-SG	-3.13	105.32	112.49
1	C	153	CSP	CA-CB-SG	-2.99	105.64	112.49
1	B	153	CSP	O2P-P-O1P	2.56	119.31	112.90
1	C	153	CSP	O3P-P-O1P	2.10	118.16	112.90

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	153	CSD	CA-CB-SG-OD1

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	153	CSP	1	0
1	C	153	CSP	1	0
1	B	153	CSP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	$\# Z > 2$
6	EDO	C	401	-	3,3,3	0.07	0	2,2,2	0.08	0
3	GOL	A	401	-	5,5,5	0.08	0	5,5,5	0.21	0
4	PGE	B	403	-	9,9,9	0.16	0	8,8,8	0.10	0
3	GOL	B	401	-	5,5,5	0.09	0	5,5,5	0.32	0
5	PEG	D	401	-	6,6,6	0.14	0	5,5,5	0.07	0
4	PGE	A	402	-	9,9,9	0.14	0	8,8,8	0.10	0
5	PEG	B	402	-	6,6,6	0.09	0	5,5,5	0.15	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
6	EDO	C	401	-	-	0/1/1/1	-
3	GOL	A	401	-	-	4/4/4/4	-
4	PGE	B	403	-	-	5/7/7/7	-
3	GOL	B	401	-	-	3/4/4/4	-
5	PEG	D	401	-	-	3/4/4/4	-
4	PGE	A	402	-	-	3/7/7/7	-
5	PEG	B	402	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	GOL	O1-C1-C2-O2
3	A	401	GOL	O1-C1-C2-C3
3	A	401	GOL	C1-C2-C3-O3
3	A	401	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	B	403	PGE	C4-C3-O2-C2
4	A	402	PGE	O2-C3-C4-O3
5	B	402	PEG	O2-C3-C4-O4
3	B	401	GOL	O1-C1-C2-C3
4	B	403	PGE	O1-C1-C2-O2
5	D	401	PEG	O2-C3-C4-O4
3	B	401	GOL	O1-C1-C2-O2
5	D	401	PEG	O1-C1-C2-O2
4	A	402	PGE	O1-C1-C2-O2
4	B	403	PGE	C1-C2-O2-C3
4	A	402	PGE	C4-C3-O2-C2
4	B	403	PGE	C3-C4-O3-C5
5	D	401	PEG	C1-C2-O2-C3
4	B	403	PGE	O2-C3-C4-O3
3	B	401	GOL	O2-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	401	EDO	1	0
3	A	401	GOL	1	0
4	B	403	PGE	2	0
3	B	401	GOL	1	0
5	D	401	PEG	3	0
4	A	402	PGE	2	0
5	B	402	PEG	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

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, 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	337/338 (99%)	0.13	2 (0%) 85 83	46, 66, 95, 125	2 (0%)
1	B	337/338 (99%)	0.28	7 (2%) 63 59	46, 72, 98, 141	3 (0%)
1	C	337/338 (99%)	0.31	5 (1%) 72 68	45, 80, 116, 130	1 (0%)
2	D	337/338 (99%)	0.20	4 (1%) 76 73	48, 73, 107, 166	0
All	All	1348/1352 (99%)	0.23	18 (1%) 75 71	45, 73, 104, 166	6 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	132	PHE	4.2
2	D	39	ASP	3.4
1	B	1	MET	3.3
1	C	1	MET	2.9
2	D	38	ILE	2.7
1	B	124	ALA	2.6
1	C	338	ALA	2.6
1	B	214	ALA	2.6
2	D	1	MET	2.5
2	D	85	ILE	2.4
1	B	204	MET	2.2
1	B	302	ILE	2.2
1	B	309	VAL	2.1
1	A	14	ILE	2.1
1	B	60	VAL	2.1
1	A	338	ALA	2.1
1	C	196	LEU	2.0
1	C	214	ALA	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, 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(Å ²)	Q<0.9
2	CSD	D	153	8/9	0.80	0.14	63,68,80,83	0
1	CSP	C	153	10/11	0.87	0.12	70,85,103,104	0
1	CSP	A	153	10/11	0.91	0.10	60,71,101,104	0
1	CSP	B	153	10/11	0.91	0.10	78,83,98,99	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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(Å ²)	Q<0.9
4	PGE	A	402	10/10	0.80	0.14	98,106,109,110	0
4	PGE	B	403	10/10	0.81	0.13	78,80,85,85	0
5	PEG	B	402	7/7	0.82	0.16	77,79,84,86	0
6	EDO	C	401	4/4	0.82	0.17	66,67,69,72	0
3	GOL	A	401	6/6	0.84	0.13	79,81,84,86	0
5	PEG	D	401	7/7	0.86	0.12	63,64,66,66	0
3	GOL	B	401	6/6	0.88	0.13	69,71,74,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.