Full wwPDB X-ray Structure Validation Report (i)

Jan 9, 2023 – 12:27 pm GMT

PDB ID	:	7QON
Title	:	Monoclinic triose phosphate isomerase from Fasciola hepatica.
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Deposited on	:	2021-12-24
Resolution	:	1.51 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 (i) 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 (i)) were used in the production of this report:

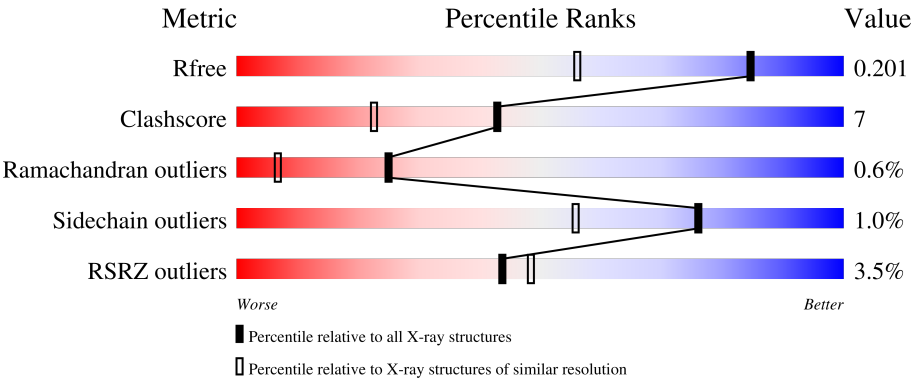
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 1.51 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}	130704	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

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 <=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	AAA	253	3% 88% 11%
1	BBB	253	2% 90% 9%
1	CCC	253	4% 85% 13%
1	DDD	253	4% 87% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NA	AAA	302	-	-	-	X
4	EDO	CCC	301	-	-	X	-
4	EDO	DDD	301	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 18399 atoms, of which 8772 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 Triosephosphate isomerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	251	Total	C	H	N	O	S	55	25	0
			4223	1322	2143	366	381	11			
1	BBB	252	Total	C	H	N	O	S	55	29	0
			4284	1341	2179	368	385	11			
1	CCC	252	Total	C	H	N	O	S	60	43	0
			4442	1393	2250	381	407	11			
1	DDD	251	Total	C	H	N	O	S	55	25	0
			4222	1327	2136	363	385	11			

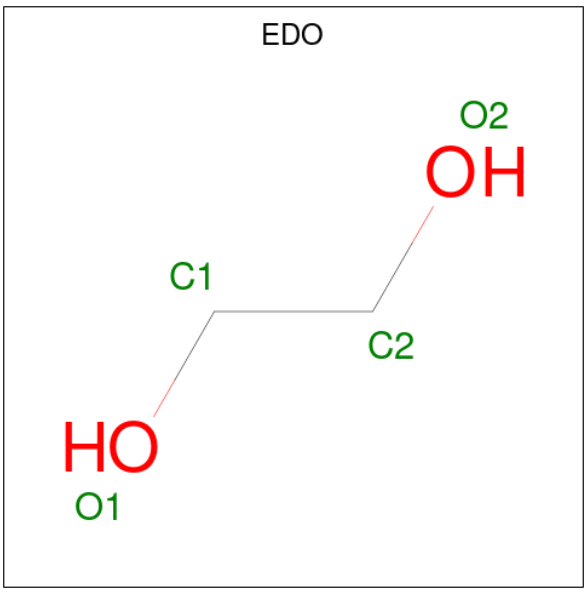
- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	5	Total	Na	0	0
			5	5		
2	BBB	5	Total	Na	0	0
			5	5		
2	CCC	9	Total	Na	0	0
			9	9		
2	DDD	2	Total	Na	0	0
			2	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

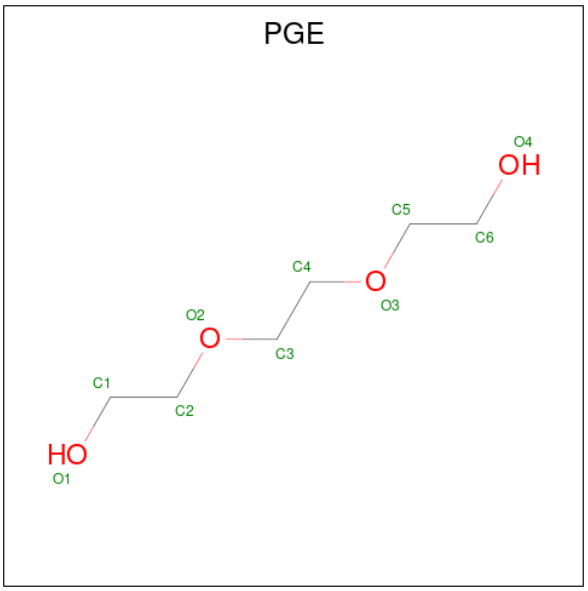
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	3	Total	Cl	0	0
			3	3		
3	BBB	2	Total	Cl	0	0
			2	2		
3	CCC	2	Total	Cl	0	0
			2	2		
3	DDD	2	Total	Cl	0	0
			2	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
4	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
4	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
4	CCC	1	Total	C	H	O	1	0
			10	2	6	2		
4	DDD	1	Total	C	H	O	1	0
			10	2	6	2		
4	DDD	1	Total	C	H	O	1	0
			10	2	6	2		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	BBB	1	Total C H O 24 6 14 4	1	0
5	DDD	1	Total C H O 24 6 14 4	1	0

- Molecule 6 is water.

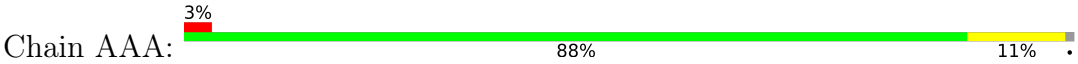
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	276	Total O 276 276	0	0
6	BBB	294	Total O 294 294	0	0
6	CCC	257	Total O 257 257	0	0
6	DDD	263	Total O 263 263	0	0

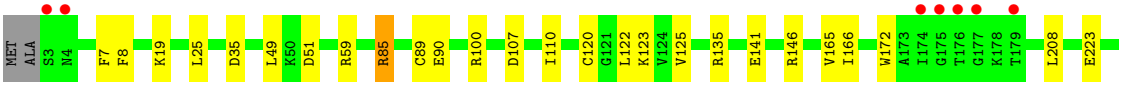
3 Residue-property plots (i)

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: Triosephosphate isomerase

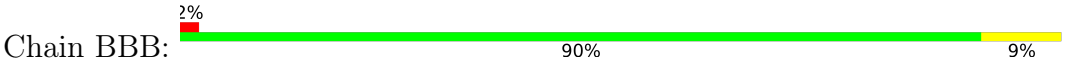
Chain AAA:





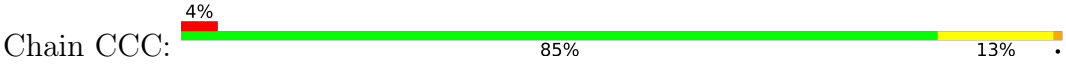
• Molecule 1: Triosephosphate isomerase

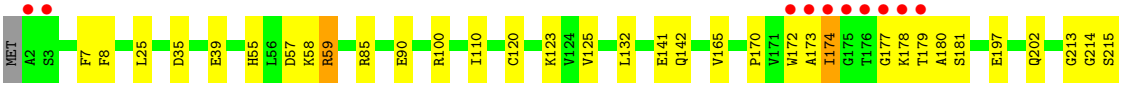
Chain BBB:

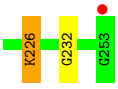


• Molecule 1: Triosephosphate isomerase

Chain CCC:

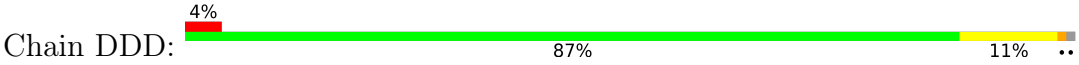


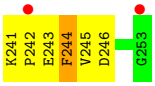




• Molecule 1: Triosephosphate isomerase

Chain DDD:




K241
P242
E243
F244
V245
D246
G253

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	42.39Å 110.46Å 118.14Å 90.00° 97.37° 90.00°	Depositor
Resolution (Å)	51.81 – 1.51 51.76 – 1.51	Depositor EDS
% Data completeness (in resolution range)	99.1 (51.81-1.51) 99.1 (51.76-1.51)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 1.51Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.165 , 0.193 0.175 , 0.201	Depositor DCC
R_{free} test set	8336 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	20.7	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 49.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	18399	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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: EDO, NA, PGE, CL

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	AAA	0.65	0/2190	0.73	0/2947
1	BBB	0.66	0/2230	0.73	0/2999
1	CCC	0.69	0/2317	0.76	0/3120
1	DDD	0.67	0/2189	0.75	0/2947
All	All	0.67	0/8926	0.74	0/12013

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	DDD	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	DDD	240	LEU	Mainchain

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	AAA	2080	2143	2158	18	0
1	BBB	2105	2179	2199	32	0
1	CCC	2192	2250	2268	44	1
1	DDD	2086	2136	2148	29	0
2	AAA	5	0	0	0	0
2	BBB	5	0	0	0	0
2	CCC	9	0	0	0	0
2	DDD	2	0	0	0	0
3	AAA	3	0	0	0	0
3	BBB	2	0	0	0	0
3	CCC	2	0	0	0	0
3	DDD	2	0	0	0	0
4	BBB	12	18	18	4	0
4	CCC	4	6	6	4	0
4	DDD	8	12	12	5	1
5	BBB	10	14	14	0	0
5	DDD	10	14	14	0	0
6	AAA	276	0	0	1	0
6	BBB	294	0	0	4	0
6	CCC	257	0	0	13	0
6	DDD	263	0	0	3	0
All	All	9627	8772	8837	118	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (118) 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:BBB:58[A]:LYS:HG3	6:CCC:406:HOH:O	1.20	1.29
1:CCC:58[B]:LYS:NZ	6:CCC:401:HOH:O	1.67	1.27
1:BBB:58[B]:LYS:NZ	6:BBB:401:HOH:O	1.68	1.26
1:CCC:173[A]:ALA:HB1	1:CCC:178[A]:LYS:HB3	1.27	1.14
1:CCC:174[B]:ILE:HD11	1:CCC:214[B]:GLY:HA3	1.47	0.95
1:BBB:57[B]:ASP:OD1	6:BBB:402:HOH:O	1.82	0.95
1:BBB:58[A]:LYS:CG	6:CCC:406:HOH:O	1.87	0.94
1:DDD:243[B]:GLU:O	1:DDD:245:VAL:N	2.02	0.93
1:CCC:174[B]:ILE:CD1	1:CCC:214[B]:GLY:HA2	2.04	0.87
1:CCC:174[B]:ILE:CD1	1:CCC:214[B]:GLY:CA	2.53	0.85
1:CCC:174[B]:ILE:HD13	1:CCC:214[B]:GLY:HA2	1.60	0.83
1:CCC:174[B]:ILE:HD11	1:CCC:214[B]:GLY:CA	2.07	0.83
1:DDD:85[B]:ARG:NH2	1:DDD:120[B]:CYS:SG	2.53	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:58[A]:LYS:CD	1:CCC:58[A]:LYS:HG2	2.10	0.81
1:CCC:170:PRO:HD2	1:CCC:213[B]:GLY:O	1.82	0.80
1:DDD:222:LYS:H	4:DDD:301:EDO:H21	1.45	0.78
1:CCC:85[B]:ARG:NH2	1:CCC:120[B]:CYS:SG	2.57	0.77
1:AAA:85[B]:ARG:NH1	1:AAA:120[B]:CYS:SG	2.56	0.77
1:DDD:241[B]:LYS:O	6:DDD:401:HOH:O	2.02	0.77
1:DDD:222:LYS:N	4:DDD:301:EDO:H21	2.01	0.75
1:CCC:173[A]:ALA:CB	1:CCC:178[A]:LYS:HB3	2.12	0.73
1:BBB:58[A]:LYS:HD3	1:CCC:58[A]:LYS:HG2	1.70	0.73
1:CCC:174[B]:ILE:CD1	1:CCC:214[B]:GLY:HA3	2.18	0.72
1:BBB:58[A]:LYS:HE3	6:CCC:402:HOH:O	1.90	0.71
1:DDD:243[B]:GLU:C	1:DDD:245:VAL:N	2.35	0.69
1:CCC:179[A]:THR:HG23	1:CCC:215[A]:SER:O	1.94	0.67
1:BBB:58[A]:LYS:HD2	1:CCC:58[A]:LYS:HG2	1.75	0.67
1:BBB:58[A]:LYS:HD2	1:CCC:58[A]:LYS:NZ	2.10	0.67
1:CCC:90[B]:GLU:OE2	6:CCC:402:HOH:O	2.14	0.66
1:CCC:179[A]:THR:CG2	1:CCC:215[A]:SER:O	2.46	0.64
1:DDD:29:LEU:HD13	1:DDD:244[B]:PHE:HD2	1.65	0.61
1:DDD:100:ARG:CZ	1:DDD:110[B]:ILE:HD13	2.30	0.60
1:BBB:39[B]:GLU:HG2	4:BBB:302:EDO:H22	1.84	0.59
1:BBB:58[A]:LYS:HD2	1:CCC:58[A]:LYS:HZ2	1.65	0.59
1:DDD:243[B]:GLU:O	1:DDD:244[B]:PHE:C	2.40	0.59
1:CCC:141[B]:GLU:HG2	6:CCC:561:HOH:O	2.03	0.58
1:AAA:166[B]:ILE:HD12	1:AAA:208:LEU:CD2	2.34	0.57
4:CCC:301:EDO:H12	6:CCC:481:HOH:O	2.04	0.57
1:BBB:197:GLU:OE2	1:BBB:202[B]:GLN:NE2	2.38	0.56
1:CCC:170:PRO:CD	1:CCC:213[B]:GLY:O	2.52	0.56
1:BBB:197:GLU:HG3	1:BBB:202[B]:GLN:HG2	1.87	0.56
1:CCC:90[B]:GLU:HG3	6:CCC:406:HOH:O	2.04	0.56
1:AAA:166[B]:ILE:HD12	1:AAA:208:LEU:HD21	1.89	0.54
1:DDD:29:LEU:HD13	1:DDD:244[B]:PHE:CD2	2.44	0.53
1:DDD:107:ASP:OD2	1:DDD:146[A]:ARG:HD2	2.09	0.52
1:BBB:90[A]:GLU:HG2	6:CCC:410:HOH:O	2.11	0.51
1:CCC:39[B]:GLU:HG2	4:CCC:301:EDO:H21	1.93	0.50
1:BBB:166[B]:ILE:HD12	1:BBB:208:LEU:CD2	2.42	0.50
1:BBB:14:LYS:HD2	4:BBB:301:EDO:H12	1.92	0.50
1:BBB:123:LYS:HZ1	4:CCC:301:EDO:C1	2.25	0.49
1:BBB:58[A]:LYS:HE3	6:CCC:406:HOH:O	2.13	0.49
1:BBB:61:HIS:ND1	1:CCC:58[A]:LYS:HE3	2.28	0.49
1:BBB:107:ASP:OD2	1:BBB:146[B]:ARG:HD2	2.13	0.49
1:AAA:166[B]:ILE:CD1	1:AAA:208:LEU:HD21	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:222:LYS:HZ1	4:DDD:302:EDO:C2	2.27	0.47
1:BBB:139[A]:LYS:HD3	1:BBB:139[A]:LYS:HA	1.68	0.47
1:CCC:55:HIS:HE1	6:CCC:425:HOH:O	1.98	0.47
1:BBB:39[B]:GLU:HG2	4:BBB:302:EDO:C1	2.45	0.47
1:AAA:223:GLU:O	1:AAA:226[B]:LYS:HD2	2.16	0.46
1:DDD:6:LYS:HD3	1:DDD:39:GLU:HG3	1.97	0.46
1:DDD:44:VAL:HG22	1:DDD:49[B]:LEU:HD23	1.97	0.46
1:BBB:166[B]:ILE:HD12	1:BBB:208:LEU:HD21	1.97	0.46
1:CCC:197:GLU:HG3	1:CCC:202[B]:GLN:HG2	1.98	0.46
1:DDD:85[B]:ARG:NH2	1:DDD:120[B]:CYS:HG	2.14	0.46
1:DDD:223[B]:GLU:HG2	4:DDD:301:EDO:O2	2.16	0.46
1:BBB:8:PHE:O	1:BBB:232:GLY:HA3	2.15	0.46
1:BBB:59[B]:ARG:NH1	6:BBB:415:HOH:O	2.48	0.46
1:CCC:8:PHE:O	1:CCC:232:GLY:HA3	2.15	0.45
1:DDD:8:PHE:O	1:DDD:232:GLY:HA3	2.17	0.45
1:DDD:85[B]:ARG:HH21	1:DDD:120[B]:CYS:HG	1.65	0.45
1:DDD:100:ARG:NH1	1:DDD:110[B]:ILE:HD13	2.32	0.45
1:DDD:25:LEU:C	1:DDD:25:LEU:HD23	2.37	0.45
1:AAA:135[B]:ARG:HD2	1:AAA:172:TRP:CD2	2.52	0.44
1:CCC:59[B]:ARG:NH2	6:CCC:409:HOH:O	2.49	0.44
1:CCC:132:LEU:HD13	1:CCC:172[B]:TRP:HD1	1.82	0.44
1:AAA:8:PHE:O	1:AAA:232:GLY:HA3	2.17	0.44
1:DDD:28:THR:HG21	1:DDD:242[B]:PRO:HA	1.99	0.44
1:CCC:170:PRO:HB2	1:CCC:172[B]:TRP:CE3	2.53	0.44
1:BBB:253:GLY:N	6:BBB:403:HOH:O	2.19	0.44
1:DDD:242[B]:PRO:O	1:DDD:245:VAL:HG23	2.17	0.44
1:AAA:25:LEU:C	1:AAA:25:LEU:HD23	2.38	0.43
1:CCC:25:LEU:C	1:CCC:25:LEU:HD23	2.39	0.43
1:AAA:100:ARG:CZ	1:AAA:110[B]:ILE:HD13	2.49	0.43
1:AAA:90[B]:GLU:OE1	1:AAA:123:LYS:NZ	2.52	0.42
1:AAA:7:PHE:CZ	1:AAA:232:GLY:HA2	2.54	0.42
1:BBB:7:PHE:CZ	1:BBB:232:GLY:HA2	2.54	0.42
1:CCC:132:LEU:HA	1:CCC:172[B]:TRP:HB2	2.00	0.42
1:DDD:243[B]:GLU:O	1:DDD:246:ASP:N	2.52	0.42
1:BBB:25:LEU:C	1:BBB:25:LEU:HD23	2.40	0.42
1:CCC:55:HIS:CE1	6:CCC:425:HOH:O	2.71	0.42
1:CCC:7:PHE:CZ	1:CCC:232:GLY:HA2	2.55	0.42
1:AAA:19[A]:LYS:NZ	1:AAA:51:ASP:OD2	2.48	0.42
1:AAA:125:VAL:HA	1:AAA:165:VAL:O	2.20	0.42
1:AAA:141[B]:GLU:HG2	6:AAA:561:HOH:O	2.20	0.42
1:CCC:125:VAL:HA	1:CCC:165:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:100:ARG:CZ	1:CCC:110[B]:ILE:HD13	2.50	0.41
1:DDD:220:ASN:CA	4:DDD:301:EDO:H22	2.50	0.41
1:CCC:180[A]:ALA:C	1:CCC:181[A]:SER:O	2.57	0.41
1:AAA:107:ASP:OD2	1:AAA:146[A]:ARG:HD2	2.20	0.41
1:CCC:39[B]:GLU:HG2	4:CCC:301:EDO:C2	2.51	0.41
1:BBB:39[B]:GLU:HG2	4:BBB:302:EDO:C2	2.49	0.41
1:BBB:125:VAL:HA	1:BBB:165:VAL:O	2.19	0.41
1:DDD:125:VAL:HA	1:DDD:165:VAL:O	2.20	0.41
1:AAA:49[A]:LEU:HG	1:AAA:89:CYS:SG	2.61	0.41
1:CCC:90[B]:GLU:OE1	1:CCC:123:LYS:NZ	2.49	0.41
1:DDD:7:PHE:CZ	1:DDD:232:GLY:HA2	2.56	0.40
1:DDD:141[A]:GLU:HG2	6:DDD:551:HOH:O	2.20	0.40
1:BBB:88:GLY:HA2	1:CCC:57[A]:ASP:OD1	2.21	0.40
1:AAA:85[A]:ARG:HG2	1:AAA:122:LEU:HD21	2.03	0.40
1:CCC:85[B]:ARG:HH21	1:CCC:120[B]:CYS:HG	1.70	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:142:GLN:HA	4:DDD:302:EDO:H12[2_455]	1.30	0.30

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	AAA	274/253 (108%)	269 (98%)	4 (2%)	1 (0%)	34 13
1	BBB	279/253 (110%)	274 (98%)	4 (1%)	1 (0%)	34 13
1	CCC	293/253 (116%)	281 (96%)	9 (3%)	3 (1%)	15 3
1	DDD	274/253 (108%)	267 (97%)	4 (2%)	3 (1%)	14 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1120/1012 (111%)	1091 (97%)	21 (2%)	8 (1%)	25 5

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	DDD	244[A]	PHE
1	DDD	244[B]	PHE
1	AAA	35	ASP
1	CCC	35	ASP
1	CCC	177[A]	GLY
1	CCC	177[B]	GLY
1	DDD	35	ASP
1	BBB	35	ASP

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	AAA	231/207 (112%)	228 (99%)	3 (1%)	69 43
1	BBB	235/207 (114%)	233 (99%)	2 (1%)	78 60
1	CCC	243/207 (117%)	237 (98%)	6 (2%)	47 17
1	DDD	231/207 (112%)	228 (99%)	3 (1%)	69 43
All	All	940/828 (114%)	926 (98%)	14 (2%)	76 38

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	59	ARG
1	AAA	85[A]	ARG
1	AAA	85[B]	ARG
1	BBB	59[A]	ARG
1	BBB	59[B]	ARG
1	CCC	59[A]	ARG
1	CCC	59[B]	ARG

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Mol	Chain	Res	Type
1	CCC	174[A]	ILE
1	CCC	174[B]	ILE
1	CCC	226[A]	LYS
1	CCC	226[B]	LYS
1	DDD	59	ARG
1	DDD	141[A]	GLU
1	DDD	141[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 38 ligands modelled in this entry, 30 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
4	EDO	CCC	301	-	3,3,3	0.12	0	2,2,2	0.20	0
5	PGE	DDD	303	-	9,9,9	0.24	0	8,8,8	0.19	0
5	PGE	BBB	304	-	9,9,9	0.23	0	8,8,8	0.12	0
4	EDO	BBB	303	-	3,3,3	0.18	0	2,2,2	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	DDD	301	-	3,3,3	0.04	0	2,2,2	0.78	0
4	EDO	BBB	301	-	3,3,3	0.55	0	2,2,2	0.79	0
4	EDO	BBB	302	-	3,3,3	0.16	0	2,2,2	0.17	0
4	EDO	DDD	302	-	3,3,3	0.29	0	2,2,2	0.46	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	EDO	CCC	301	-	-	0/1/1/1	-
5	PGE	DDD	303	-	-	3/7/7/7	-
5	PGE	BBB	304	-	-	6/7/7/7	-
4	EDO	BBB	303	-	-	0/1/1/1	-
4	EDO	DDD	301	-	-	0/1/1/1	-
4	EDO	BBB	301	-	-	1/1/1/1	-
4	EDO	BBB	302	-	-	1/1/1/1	-
4	EDO	DDD	302	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	BBB	304	PGE	O3-C5-C6-O4
5	DDD	303	PGE	O3-C5-C6-O4
5	BBB	304	PGE	O2-C3-C4-O3
5	BBB	304	PGE	O1-C1-C2-O2
4	BBB	301	EDO	O1-C1-C2-O2
5	BBB	304	PGE	C3-C4-O3-C5
5	DDD	303	PGE	C3-C4-O3-C5
5	BBB	304	PGE	C6-C5-O3-C4
5	BBB	304	PGE	C4-C3-O2-C2
4	BBB	302	EDO	O1-C1-C2-O2
5	DDD	303	PGE	O2-C3-C4-O3

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	CCC	301	EDO	4	0
4	DDD	301	EDO	4	0
4	BBB	301	EDO	1	0
4	BBB	302	EDO	3	0
4	DDD	302	EDO	1	1

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, 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	AAA	251/253 (99%)	-0.41	8 (3%) 47 52	17, 25, 49, 75	0
1	BBB	252/253 (99%)	-0.27	5 (1%) 65 70	15, 22, 42, 92	0
1	CCC	252/253 (99%)	-0.03	11 (4%) 34 38	16, 23, 50, 112	0
1	DDD	251/253 (99%)	-0.06	11 (4%) 34 38	18, 27, 58, 95	0
All	All	1006/1012 (99%)	-0.19	35 (3%) 44 48	15, 24, 52, 112	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	174[A]	ILE	10.5
1	CCC	2	ALA	10.0
1	BBB	2	ALA	8.1
1	CCC	175[A]	GLY	7.3
1	DDD	3	SER	6.9
1	DDD	29	LEU	6.2
1	BBB	175	GLY	5.6
1	DDD	253	GLY	5.1
1	CCC	172[A]	TRP	4.7
1	CCC	253	GLY	4.6
1	DDD	4	ASN	4.0
1	AAA	175	GLY	3.8
1	BBB	253	GLY	3.8
1	AAA	177	GLY	3.5
1	DDD	32	ALA	3.3
1	DDD	218	ALA	3.0
1	BBB	174	ILE	2.9
1	AAA	174	ILE	2.8
1	DDD	242[A]	PRO	2.8
1	CCC	3[A]	SER	2.7
1	AAA	176	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	DDD	177	GLY	2.5
1	AAA	3	SER	2.5
1	CCC	176[A]	THR	2.5
1	AAA	253	GLY	2.4
1	CCC	173[A]	ALA	2.4
1	AAA	179	THR	2.4
1	CCC	177[A]	GLY	2.3
1	BBB	177	GLY	2.1
1	DDD	175	GLY	2.1
1	CCC	178[A]	LYS	2.1
1	DDD	34	PRO	2.1
1	CCC	179[A]	THR	2.1
1	DDD	217	THR	2.1
1	AAA	4	ASN	2.0

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, 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	NA	CCC	308	1/1	0.48	0.18	67,67,67,67	0
2	NA	AAA	302	1/1	0.70	0.59	93,93,93,93	0
4	EDO	BBB	303	4/4	0.70	0.19	46,55,60,63	1
2	NA	BBB	307	1/1	0.80	0.12	69,69,69,69	0
2	NA	BBB	309	1/1	0.80	0.13	64,64,64,64	0
2	NA	CCC	307	1/1	0.81	0.21	64,64,64,64	0
5	PGE	DDD	303	10/10	0.81	0.09	42,53,55,56	1
5	PGE	BBB	304	10/10	0.85	0.10	51,59,70,74	1
2	NA	CCC	306	1/1	0.91	0.31	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	DDD	301	4/4	0.91	0.49	44,47,59,67	1
2	NA	CCC	310	1/1	0.92	0.09	49,49,49,49	0
3	CL	BBB	311	1/1	0.92	0.06	51,51,51,51	0
2	NA	AAA	304	1/1	0.92	0.06	52,52,52,52	0
4	EDO	BBB	301	4/4	0.93	0.16	25,38,43,50	1
2	NA	CCC	305	1/1	0.93	0.34	55,55,55,55	0
2	NA	DDD	304	1/1	0.93	0.05	27,27,27,27	0
4	EDO	DDD	302	4/4	0.93	0.23	35,45,57,62	1
2	NA	BBB	308	1/1	0.93	0.09	40,40,40,40	0
3	CL	DDD	307	1/1	0.93	0.05	42,42,42,42	0
2	NA	DDD	305	1/1	0.94	0.18	39,39,39,39	0
2	NA	BBB	306	1/1	0.94	0.15	38,38,38,38	0
2	NA	AAA	303	1/1	0.94	0.07	37,37,37,37	0
2	NA	CCC	304	1/1	0.95	0.07	52,52,52,52	0
2	NA	CCC	303	1/1	0.96	0.04	51,51,51,51	0
2	NA	CCC	309	1/1	0.96	0.09	43,43,43,43	0
4	EDO	BBB	302	4/4	0.96	0.09	24,35,64,65	1
3	CL	CCC	312	1/1	0.96	0.07	51,51,51,51	0
2	NA	AAA	305	1/1	0.97	0.13	56,56,56,56	0
4	EDO	CCC	301	4/4	0.97	0.15	25,37,50,61	1
3	CL	AAA	308	1/1	0.98	0.04	32,32,32,32	0
3	CL	AAA	307	1/1	0.98	0.04	42,42,42,42	0
3	CL	DDD	306	1/1	0.99	0.05	24,24,24,24	0
2	NA	AAA	301	1/1	0.99	0.05	22,22,22,22	0
2	NA	CCC	302	1/1	1.00	0.06	20,20,20,20	0
3	CL	BBB	310	1/1	1.00	0.10	19,19,19,19	0
3	CL	AAA	306	1/1	1.00	0.09	22,22,22,22	0
3	CL	CCC	311	1/1	1.00	0.11	21,21,21,21	0
2	NA	BBB	305	1/1	1.00	0.06	18,18,18,18	0

6.5 Other polymers (i)

There are no such residues in this entry.