



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 03:08 am BST

PDB ID : 4C21
Title : L-Fucose Isomerase In Complex With Fucitol
Authors : Higgins, M.A.; Suits, M.D.L.; Marsters, C.; Boraston, A.B.
Deposited on : 2013-08-16
Resolution : 2.55 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 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 : 2.11
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) : 2.11

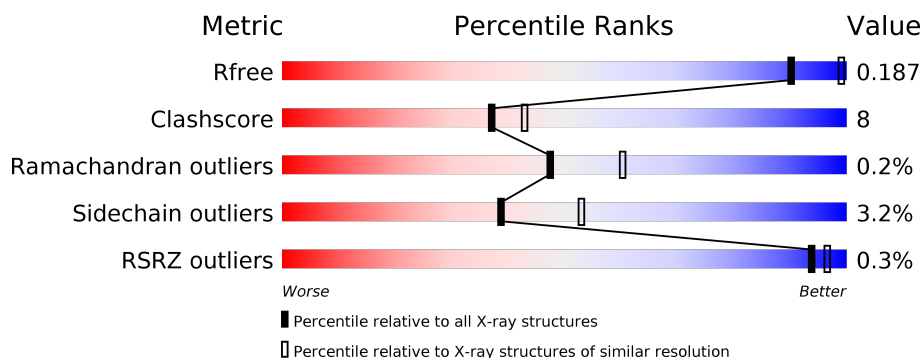
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	605	 83% 12% . .
1	B	605	 85% 14% .

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
4	EDO	B	1589	-	-	X	-
4	EDO	B	1591	-	-	X	-
4	EDO	B	1595	-	-	X	-
4	EDO	B	1596	-	-	-	X
4	EDO	B	1599	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10132 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 L-FUCOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	0	0	0
			4615	2918	800	869	28			
1	B	605	Total	C	N	O	S	0	0	0
			4749	3001	832	887	29			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	HIS	-	expression tag	UNP Q97N97
A	-15	HIS	-	expression tag	UNP Q97N97
A	-14	HIS	-	expression tag	UNP Q97N97
A	-13	HIS	-	expression tag	UNP Q97N97
A	-12	HIS	-	expression tag	UNP Q97N97
A	-11	SER	-	expression tag	UNP Q97N97
A	-10	SER	-	expression tag	UNP Q97N97
A	-9	GLY	-	expression tag	UNP Q97N97
A	-8	LEU	-	expression tag	UNP Q97N97
A	-7	VAL	-	expression tag	UNP Q97N97
A	-6	PRO	-	expression tag	UNP Q97N97
A	-5	ARG	-	expression tag	UNP Q97N97
A	-4	GLY	-	expression tag	UNP Q97N97
A	-3	ALA	-	expression tag	UNP Q97N97
A	-2	HIS	-	expression tag	UNP Q97N97
A	-1	MET	-	expression tag	UNP Q97N97
A	0	ALA	-	expression tag	UNP Q97N97
B	-16	HIS	-	expression tag	UNP Q97N97
B	-15	HIS	-	expression tag	UNP Q97N97
B	-14	HIS	-	expression tag	UNP Q97N97
B	-13	HIS	-	expression tag	UNP Q97N97
B	-12	HIS	-	expression tag	UNP Q97N97
B	-11	SER	-	expression tag	UNP Q97N97
B	-10	SER	-	expression tag	UNP Q97N97
B	-9	GLY	-	expression tag	UNP Q97N97

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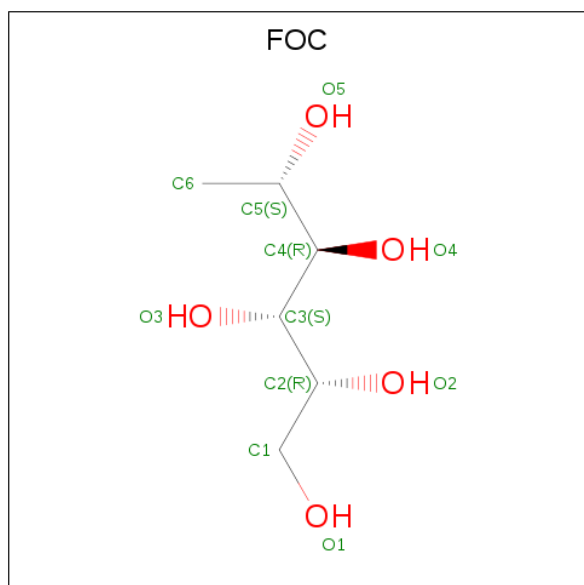
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	LEU	-	expression tag	UNP Q97N97
B	-7	VAL	-	expression tag	UNP Q97N97
B	-6	PRO	-	expression tag	UNP Q97N97
B	-5	ARG	-	expression tag	UNP Q97N97
B	-4	GLY	-	expression tag	UNP Q97N97
B	-3	ALA	-	expression tag	UNP Q97N97
B	-2	HIS	-	expression tag	UNP Q97N97
B	-1	MET	-	expression tag	UNP Q97N97
B	0	ALA	-	expression tag	UNP Q97N97

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mn 1 1	0	0
2	A	1	Total Mn 1 1	0	0

- Molecule 3 is FUCITOL (three-letter code: FOC) (formula: C₆H₁₄O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 11 6 5	0	0
3	B	1	Total C O 11 6 5	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

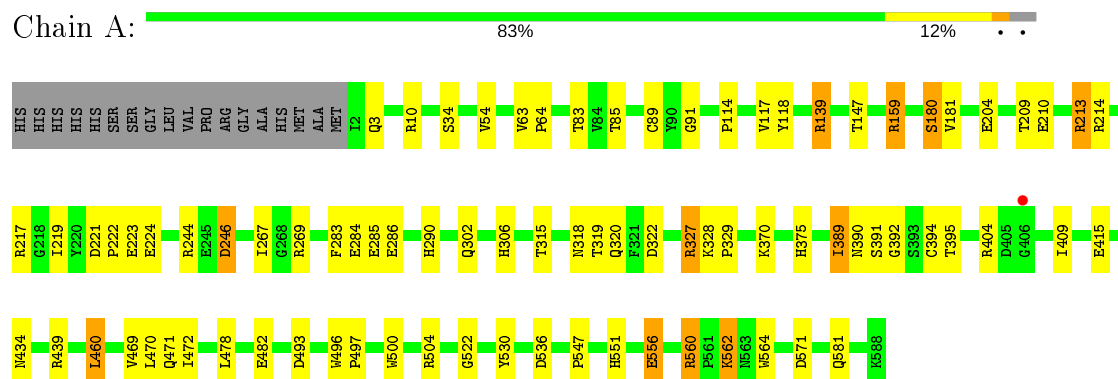
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	338	Total	O	0	0
			338	338		
5	B	342	Total	O	0	0
			342	342		

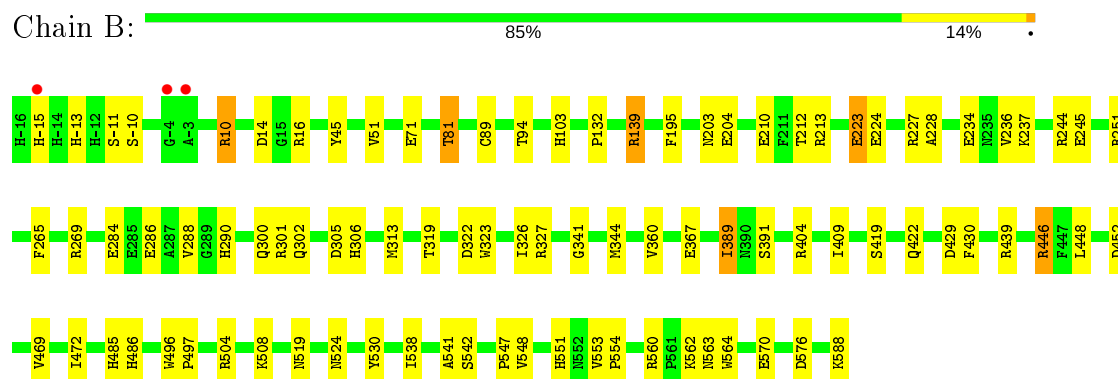
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: L-FUCOSE ISOMERASE



• Molecule 1: L-FUCOSE ISOMERASE



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	152.85Å 152.85Å 408.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.71 – 2.55 49.66 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.71-2.55) 99.4 (49.66-2.55)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.135 , 0.188 0.135 , 0.187	Depositor DCC
R_{free} test set	3022 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10132	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: MN, EDO, FOC

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	0.60	0/4732	0.74	3/6422 (0.0%)
1	B	0.61	0/4873	0.73	3/6612 (0.0%)
All	All	0.60	0/9605	0.73	6/13034 (0.0%)

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	B	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	213	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	A	560	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	B	10	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	10	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	B	446	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	159	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	326	ILE	Peptide

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	4615	0	4451	65	0
1	B	4749	0	4580	87	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	11	0	12	0	0
3	B	11	0	12	0	0
4	A	20	0	30	2	0
4	B	44	0	66	32	0
5	A	338	0	0	7	0
5	B	342	0	0	18	3
All	All	10132	0	9151	145	3

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 8.

All (145) 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:439:ARG:NH2	4:B:1599:EDO:H22	1.70	1.07
1:B:486:HIS:HE1	5:B:2279:HOH:O	1.47	0.95
1:A:139:ARG:NH1	5:A:2089:HOH:O	2.00	0.95
1:A:217:ARG:HE	1:B:306:HIS:HD2	1.15	0.95
1:B:551:HIS:HD2	1:B:553:VAL:H	1.14	0.94
1:B:223:GLU:HB3	5:B:2165:HOH:O	1.64	0.94
1:B:341:GLY:HA2	1:B:344:MET:HE2	1.53	0.91
1:B:439:ARG:HH21	4:B:1599:EDO:H22	1.31	0.90
1:B:360:VAL:HB	4:B:1595:EDO:H11	1.53	0.90
1:A:471:GLN:HE22	1:A:522:GLY:H	0.91	0.89
1:A:159:ARG:HD3	1:A:536:ASP:OD1	1.73	0.88
1:B:341:GLY:HA2	1:B:344:MET:CE	2.06	0.85
1:A:471:GLN:HE22	1:A:522:GLY:N	1.75	0.82
1:A:504:ARG:HE	4:A:1592:EDO:H22	1.45	0.80
1:B:439:ARG:NH2	4:B:1599:EDO:C2	2.43	0.80
1:B:404:ARG:HH11	1:B:404:ARG:HG3	1.47	0.79
1:A:471:GLN:NE2	1:A:522:GLY:H	1.76	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:VAL:HG12	1:A:547:PRO:HG2	1.67	0.75
1:B:-13:HIS:HD2	1:B:-10:SER:H	1.35	0.72
1:B:204:GLU:OE1	1:B:290:HIS:HD2	1.73	0.71
1:B:570:GLU:O	5:B:2332:HOH:O	2.09	0.70
1:B:360:VAL:O	4:B:1595:EDO:H11	1.92	0.69
1:B:519:ASN:OD1	4:B:1593:EDO:H22	1.92	0.69
1:A:409:ILE:HG22	1:A:530:TYR:CE1	2.29	0.68
1:A:217:ARG:HE	1:B:306:HIS:CD2	2.05	0.68
1:A:209:THR:HG23	4:B:1591:EDO:H21	1.76	0.67
1:B:322:ASP:OD2	1:B:327:ARG:NH1	2.28	0.67
1:B:132:PRO:HA	1:B:563:ASN:HD21	1.60	0.66
1:B:551:HIS:CD2	1:B:553:VAL:H	2.06	0.65
1:A:496:TRP:HB3	1:A:497:PRO:HD2	1.78	0.64
1:A:404:ARG:HG3	1:A:404:ARG:HH11	1.65	0.61
1:B:300:GLN:HG2	5:B:2197:HOH:O	1.99	0.61
1:B:227:ARG:NH1	5:B:2165:HOH:O	2.32	0.61
1:B:10:ARG:NH2	1:B:94:THR:O	2.26	0.60
1:B:-13:HIS:CD2	1:B:-10:SER:H	2.17	0.60
1:A:581:GLN:HG3	5:A:2332:HOH:O	2.01	0.60
1:A:209:THR:HG23	4:B:1591:EDO:C2	2.32	0.59
1:B:588:LYS:HE3	5:B:2138:HOH:O	2.01	0.59
1:B:538:ILE:O	4:B:1589:EDO:H12	2.02	0.58
1:B:213:ARG:NH2	1:B:286:GLU:OE2	2.34	0.58
1:B:360:VAL:HB	4:B:1595:EDO:C1	2.32	0.58
1:B:496:TRP:HB3	1:B:497:PRO:CD	2.34	0.58
1:A:244:ARG:NH1	1:A:246:ASP:OD2	2.36	0.58
1:A:375:HIS:HD2	5:A:2086:HOH:O	1.86	0.57
1:B:404:ARG:HG3	1:B:404:ARG:NH1	2.15	0.57
1:A:285:GLU:OE2	1:B:301:ARG:NH2	2.38	0.57
1:A:204:GLU:OE1	1:A:290:HIS:HD2	1.87	0.57
1:B:469:VAL:HG12	1:B:547:PRO:HG2	1.86	0.56
1:A:63:VAL:HG12	1:A:64:PRO:HD3	1.88	0.56
1:B:576:ASP:OD1	4:B:1589:EDO:H22	2.05	0.56
1:B:541:ALA:HB3	4:B:1589:EDO:H11	1.88	0.56
1:A:496:TRP:HB3	1:A:497:PRO:CD	2.36	0.55
1:B:439:ARG:HH21	4:B:1599:EDO:C2	2.10	0.54
1:A:63:VAL:CG1	1:A:64:PRO:HD3	2.37	0.54
1:A:85:THR:HG21	1:A:118:TYR:CD2	2.43	0.54
1:A:320:GLN:HE21	1:A:329:PRO:HD3	1.71	0.54
1:A:210:GLU:HB2	1:B:302:GLN:HG2	1.91	0.53
1:B:237:LYS:HG2	5:B:2169:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:PHE:HA	1:B:313:MET:HG3	1.90	0.53
4:B:1592:EDO:H12	5:B:2132:HOH:O	2.08	0.53
1:B:224:GLU:OE2	1:B:269:ARG:NH2	2.40	0.53
1:A:114:PRO:HB2	1:A:117:VAL:HB	1.91	0.53
1:A:213:ARG:HG3	1:B:306:HIS:HB2	1.90	0.52
1:B:560:ARG:HD3	1:B:564:TRP:CD1	2.44	0.52
1:B:139:ARG:NH1	5:B:2093:HOH:O	2.43	0.52
1:A:322:ASP:OD2	1:A:327:ARG:NH1	2.43	0.52
1:B:367:GLU:HG3	5:B:2231:HOH:O	2.10	0.51
1:A:315:THR:HG23	1:A:394:CYS:O	2.10	0.51
1:B:301:ARG:NH1	1:B:305:ASP:OD2	2.44	0.51
1:A:89:CYS:HB2	1:A:118:TYR:CE1	2.46	0.51
1:B:429:ASP:OD1	1:B:446:ARG:HD3	2.11	0.50
1:B:389:ILE:HG13	1:B:497:PRO:O	2.12	0.49
1:B:524:ASN:HA	4:B:1595:EDO:H21	1.94	0.49
1:A:391:SER:HA	1:A:496:TRP:CE3	2.47	0.49
1:A:327:ARG:HG2	1:A:328:LYS:O	2.12	0.49
1:A:209:THR:OG1	4:B:1591:EDO:H22	2.12	0.49
1:B:-13:HIS:CD2	1:B:-11:SER:H	2.31	0.49
1:B:360:VAL:CB	4:B:1595:EDO:H11	2.35	0.48
1:B:486:HIS:HD2	5:B:2284:HOH:O	1.96	0.48
1:B:236:VAL:HG13	1:B:430:PHE:CD1	2.48	0.48
1:B:45:TYR:CE2	1:B:51:VAL:HA	2.48	0.48
1:A:319:THR:O	1:A:327:ARG:NH2	2.47	0.48
1:A:478:LEU:HB2	1:A:500:TRP:HB2	1.96	0.48
1:A:217:ARG:HH12	4:B:1599:EDO:C1	2.26	0.48
4:B:1592:EDO:C1	5:B:2132:HOH:O	2.62	0.48
1:A:472:ILE:O	1:A:551:HIS:HA	2.14	0.47
1:B:391:SER:HA	1:B:496:TRP:CE3	2.50	0.47
1:B:319:THR:O	1:B:327:ARG:NH2	2.47	0.47
1:B:212:THR:OG1	4:B:1591:EDO:O2	2.13	0.47
1:B:-13:HIS:HE1	1:B:284:GLU:OE2	1.97	0.47
1:B:496:TRP:HB3	1:B:497:PRO:HD2	1.96	0.47
1:A:389:ILE:HD11	1:A:496:TRP:HB2	1.97	0.47
1:A:409:ILE:HG22	1:A:530:TYR:CZ	2.50	0.47
1:B:551:HIS:HD2	1:B:553:VAL:N	1.96	0.47
1:B:81:THR:CG2	5:B:2054:HOH:O	2.63	0.47
1:A:556:GLU:H	1:A:556:GLU:CD	2.18	0.47
1:B:486:HIS:CE1	5:B:2279:HOH:O	2.37	0.46
1:B:14:ASP:OD1	1:B:16:ARG:HD2	2.16	0.46
1:A:439:ARG:NH2	4:A:1593:EDO:O1	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ARG:HH12	4:B:1599:EDO:H11	1.79	0.46
1:A:318:ASN:HB3	1:A:395:THR:HB	1.97	0.46
4:B:1595:EDO:O2	5:B:2294:HOH:O	2.20	0.46
1:A:224:GLU:OE2	1:A:269:ARG:NH2	2.41	0.45
1:A:283:PHE:HB3	1:A:286:GLU:OE1	2.15	0.45
1:A:571:ASP:HB2	5:A:2326:HOH:O	2.16	0.45
1:B:504:ARG:HD3	4:B:1596:EDO:H22	1.98	0.45
1:B:195:PHE:HB2	1:B:203:ASN:HD21	1.82	0.45
1:A:209:THR:HA	4:B:1591:EDO:H22	1.98	0.45
1:B:554:PRO:HG3	4:B:1596:EDO:H21	1.98	0.45
1:B:327:ARG:HD3	5:B:2212:HOH:O	2.15	0.45
1:B:542:SER:HB3	4:B:1589:EDO:H21	1.99	0.45
1:A:562:LYS:HB3	5:A:2316:HOH:O	2.17	0.45
1:B:541:ALA:HB3	4:B:1589:EDO:C1	2.46	0.45
1:B:71:GLU:HG3	5:B:2049:HOH:O	2.18	0.44
1:B:81:THR:HB	1:B:103:HIS:ND1	2.32	0.44
1:B:548:VAL:HG23	4:B:1589:EDO:H11	2.00	0.44
1:B:542:SER:CB	4:B:1589:EDO:H21	2.48	0.44
1:A:285:GLU:OE1	1:B:301:ARG:NH2	2.41	0.44
1:A:404:ARG:NH2	1:A:415:GLU:OE1	2.51	0.44
1:B:389:ILE:HD11	1:B:496:TRP:HB2	2.00	0.44
1:A:180:SER:HB2	5:A:2120:HOH:O	2.16	0.44
1:A:214:ARG:HD2	1:A:267:ILE:HG23	1.98	0.43
1:B:504:ARG:CD	4:B:1596:EDO:H22	2.48	0.43
1:A:285:GLU:CD	1:B:301:ARG:HH22	2.20	0.43
1:A:10:ARG:O	1:A:83:THR:HA	2.18	0.43
1:A:221:ASP:HA	1:A:222:PRO:HD3	1.81	0.43
1:B:538:ILE:HG23	4:B:1589:EDO:O1	2.18	0.42
1:A:285:GLU:CD	1:B:301:ARG:NH2	2.72	0.42
1:B:448:LEU:HD13	1:B:485:HIS:CE1	2.54	0.42
1:A:434:ASN:OD1	1:A:434:ASN:C	2.57	0.42
1:B:360:VAL:O	4:B:1595:EDO:C1	2.63	0.41
1:B:472:ILE:O	1:B:551:HIS:HA	2.20	0.41
1:A:180:SER:HB3	1:A:181:VAL:H	1.11	0.41
1:A:302:GLN:HG2	1:B:210:GLU:HB2	2.02	0.41
1:B:409:ILE:HG22	1:B:530:TYR:CE1	2.55	0.41
1:B:228:ALA:HB2	1:B:323:TRP:CE2	2.55	0.41
1:A:390:ASN:C	1:A:392:GLY:H	2.24	0.41
1:A:306:HIS:HB2	1:B:213:ARG:HG3	2.02	0.41
1:B:341:GLY:CA	1:B:344:MET:HE2	2.35	0.41
1:A:560:ARG:HD3	1:A:564:TRP:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:ARG:CG	1:B:404:ARG:NH1	2.84	0.40
1:B:10:ARG:HD2	5:B:2011:HOH:O	2.20	0.40
1:A:219:ILE:HG12	1:A:283:PHE:CE1	2.57	0.40
1:A:404:ARG:NH1	5:A:2248:HOH:O	2.54	0.40
1:A:460:LEU:HD13	1:A:470:LEU:HD13	2.04	0.40

All (3) 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)
5:B:2314:HOH:O	5:B:2328:HOH:O[3_455]	1.44	0.76
5:B:2081:HOH:O	5:B:2265:HOH:O[2_565]	1.47	0.73
5:B:2039:HOH:O	5:B:2267:HOH:O[2_565]	1.95	0.25

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	585/605 (97%)	558 (95%)	26 (4%)	1 (0%)	47	60
1	B	603/605 (100%)	578 (96%)	24 (4%)	1 (0%)	47	60
All	All	1188/1210 (98%)	1136 (96%)	50 (4%)	2 (0%)	47	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	GLY
1	B	389	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	490/507 (97%)	473 (96%)	17 (4%)	36	49
1	B	503/507 (99%)	488 (97%)	15 (3%)	41	55
All	All	993/1014 (98%)	961 (97%)	32 (3%)	39	53

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	34	SER
1	A	54	VAL
1	A	139	ARG
1	A	147	THR
1	A	180	SER
1	A	223	GLU
1	A	246	ASP
1	A	284	GLU
1	A	327	ARG
1	A	370	LYS
1	A	389	ILE
1	A	460	LEU
1	A	482	GLU
1	A	493	ASP
1	A	556	GLU
1	A	562	LYS
1	B	-15	HIS
1	B	81	THR
1	B	89	CYS
1	B	139	ARG
1	B	223	GLU
1	B	234	GLU
1	B	244	ARG
1	B	245	GLU
1	B	251	ARG
1	B	288	VAL

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Mol	Chain	Res	Type
1	B	419	SER
1	B	422	GLN
1	B	452	ASP
1	B	508	LYS
1	B	562	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	30	ASN
1	A	70	HIS
1	A	203	ASN
1	A	290	HIS
1	A	300	GLN
1	A	320	GLN
1	A	352	ASN
1	A	461	ASN
1	A	471	GLN
1	B	-16	HIS
1	B	-15	HIS
1	B	-13	HIS
1	B	70	HIS
1	B	126	HIS
1	B	196	GLN
1	B	203	ASN
1	B	290	HIS
1	B	306	HIS
1	B	486	HIS
1	B	490	ASN
1	B	551	HIS
1	B	563	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 2 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	$\# Z > 2$
4	EDO	A	1591	-	3,3,3	0.48	0	2,2,2	0.62	0
4	EDO	B	1597	-	3,3,3	0.63	0	2,2,2	0.05	0
3	FOC	B	601	2	9,10,10	0.24	0	10,13,13	0.93	0
3	FOC	A	601	2	9,10,10	0.36	0	10,13,13	1.38	3 (30%)
4	EDO	A	1592	-	3,3,3	0.31	0	2,2,2	1.27	0
4	EDO	B	1592	-	3,3,3	0.38	0	2,2,2	0.57	0
4	EDO	A	1593	-	3,3,3	0.31	0	2,2,2	1.95	1 (50%)
4	EDO	B	1596	-	3,3,3	0.80	0	2,2,2	0.30	0
4	EDO	B	1591	-	3,3,3	0.40	0	2,2,2	0.39	0
4	EDO	B	1590	-	3,3,3	0.37	0	2,2,2	0.92	0
4	EDO	B	1595	-	3,3,3	0.60	0	2,2,2	0.34	0
4	EDO	A	1590	-	3,3,3	0.46	0	2,2,2	0.36	0
4	EDO	B	1594	-	3,3,3	0.60	0	2,2,2	0.25	0
4	EDO	B	1599	-	3,3,3	0.25	0	2,2,2	1.18	0
4	EDO	B	1598	-	3,3,3	0.60	0	2,2,2	0.41	0
4	EDO	A	1589	-	3,3,3	0.35	0	2,2,2	0.64	0
4	EDO	B	1589	-	3,3,3	0.39	0	2,2,2	0.42	0
4	EDO	B	1593	-	3,3,3	0.37	0	2,2,2	0.48	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	A	1591	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	1597	-	-	0/1/1/1	-
3	FOC	B	601	2	-	0/14/14/14	-
3	FOC	A	601	2	-	5/14/14/14	-
4	EDO	A	1592	-	-	0/1/1/1	-
4	EDO	B	1592	-	-	0/1/1/1	-
4	EDO	A	1593	-	-	1/1/1/1	-
4	EDO	B	1596	-	-	0/1/1/1	-
4	EDO	B	1591	-	-	1/1/1/1	-
4	EDO	B	1590	-	-	0/1/1/1	-
4	EDO	B	1595	-	-	1/1/1/1	-
4	EDO	A	1590	-	-	0/1/1/1	-
4	EDO	B	1594	-	-	0/1/1/1	-
4	EDO	B	1599	-	-	0/1/1/1	-
4	EDO	B	1598	-	-	1/1/1/1	-
4	EDO	A	1589	-	-	1/1/1/1	-
4	EDO	B	1589	-	-	1/1/1/1	-
4	EDO	B	1593	-	-	1/1/1/1	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	FOC	C2-C3-C4	-2.43	108.66	112.47
3	A	601	FOC	O1-C1-C2	-2.40	105.85	111.07
3	A	601	FOC	O3-C3-C4	-2.08	104.63	109.47
4	A	1593	EDO	O2-C2-C1	-2.00	97.51	111.91

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	FOC	O3-C3-C4-O4
4	A	1593	EDO	O1-C1-C2-O2
4	B	1598	EDO	O1-C1-C2-O2
3	A	601	FOC	C2-C3-C4-O4
3	A	601	FOC	O3-C3-C4-C5
4	B	1591	EDO	O1-C1-C2-O2
4	B	1595	EDO	O1-C1-C2-O2
4	B	1589	EDO	O1-C1-C2-O2
4	A	1591	EDO	O1-C1-C2-O2
4	A	1589	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	601	FOC	O1-C1-C2-O2
4	B	1593	EDO	O1-C1-C2-O2
3	A	601	FOC	C2-C3-C4-C5

There are no ring outliers.

9 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1592	EDO	1	0
4	B	1592	EDO	2	0
4	A	1593	EDO	1	0
4	B	1596	EDO	3	0
4	B	1591	EDO	5	0
4	B	1595	EDO	7	0
4	B	1599	EDO	6	0
4	B	1589	EDO	8	0
4	B	1593	EDO	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	587/605 (97%)	-0.71	1 (0%) 95 97	21, 31, 50, 66	0
1	B	605/605 (100%)	-0.65	3 (0%) 91 94	17, 30, 53, 107	0
All	All	1192/1210 (98%)	-0.68	4 (0%) 94 96	17, 31, 52, 107	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-4	GLY	3.7
1	B	-3	ALA	2.7
1	A	406	GLY	2.6
1	B	-15	HIS	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 carbohydrates 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	EDO	B	1596	4/4	0.74	0.44	52,59,64,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	B	1598	4/4	0.88	0.23	61,66,80,80	0
4	EDO	B	1597	4/4	0.93	0.14	43,47,52,53	0
4	EDO	B	1599	4/4	0.94	0.11	47,48,51,58	0
4	EDO	A	1592	4/4	0.94	0.12	55,56,62,67	0
4	EDO	A	1593	4/4	0.95	0.17	41,46,50,51	0
4	EDO	B	1592	4/4	0.96	0.19	34,38,42,44	0
4	EDO	A	1591	4/4	0.96	0.11	41,44,48,48	0
4	EDO	B	1594	4/4	0.97	0.11	30,38,40,42	0
4	EDO	B	1593	4/4	0.97	0.15	32,36,36,40	0
4	EDO	B	1595	4/4	0.98	0.20	41,46,49,51	0
3	FOC	A	601	11/11	0.98	0.12	34,44,48,51	0
3	FOC	B	601	11/11	0.98	0.13	34,42,46,51	0
4	EDO	B	1591	4/4	0.98	0.22	48,49,49,51	0
2	MN	A	600	1/1	0.98	0.09	55,55,55,55	0
4	EDO	B	1589	4/4	0.98	0.20	35,36,37,42	0
4	EDO	B	1590	4/4	0.98	0.13	36,37,40,41	0
4	EDO	A	1589	4/4	0.99	0.15	34,35,38,45	0
2	MN	B	600	1/1	0.99	0.08	47,47,47,47	0
4	EDO	A	1590	4/4	0.99	0.10	34,35,36,40	0

6.5 Other polymers

There are no such residues in this entry.