



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2018 – 09:12 PM EST

PDB ID : 1QJQ
Title : FERRIC HYDROXAMATE RECEPTOR FROM ESCHERICHIA COLI (FHUA)
Authors : Ferguson, A.D.; Braun, V.; Fiedler, H.-P.; Coulton, J.W.; Diederichs, K.; Welte, W.
Deposited on : 1999-06-29
Resolution : 2.95 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

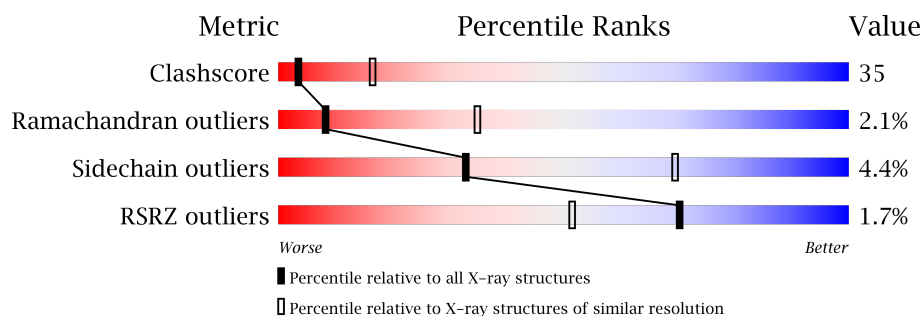
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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))
Clashscore	112137	2773 (3.00-2.92)
Ramachandran outliers	110173	2680 (3.00-2.92)
Sidechain outliers	110143	2683 (3.00-2.92)
RSRZ outliers	101464	2421 (3.00-2.92)

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. 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	725	

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	GCN	A	1001	X	-	-	-
4	GMH	A	1011	X	-	-	-
4	GMH	A	1012	X	-	-	-
5	GLC	A	1020	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	FTT	A	1002	-	-	-	X
7	FTT	A	1004	-	-	-	X
7	FTT	A	1005	-	-	-	X
7	FTT	A	1006	X	-	-	-
7	FTT	A	1007	-	-	-	X
9	PO4	A	1014	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 6218 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.

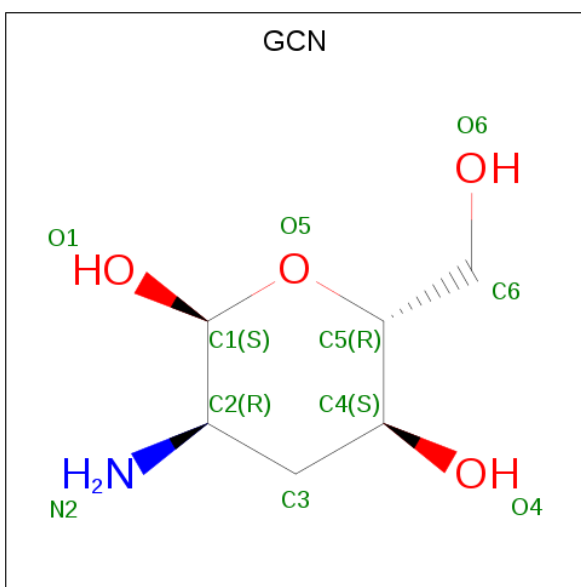
- Molecule 1 is a protein called FERRIC HYDROXAMATE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	707	Total	C	N	O	S	0	0	0
			5523	3475	944	1090	14			

There are 11 discrepancies between the modelled and reference sequences:

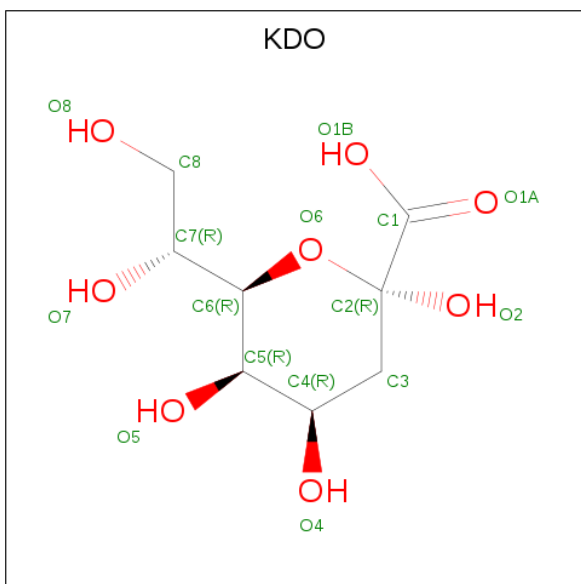
Chain	Residue	Modelled	Actual	Comment	Reference
A	406	SER	-	insertion	UNP P06971
A	407	SER	-	insertion	UNP P06971
A	408	HIS	-	insertion	UNP P06971
A	409	HIS	-	insertion	UNP P06971
A	410	HIS	-	insertion	UNP P06971
A	411	HIS	-	insertion	UNP P06971
A	412	HIS	-	insertion	UNP P06971
A	413	HIS	-	insertion	UNP P06971
A	414	GLY	-	insertion	UNP P06971
A	415	SER	-	insertion	UNP P06971
A	416	SER	-	insertion	UNP P06971

- Molecule 2 is 3-DEOXY-D-GLUCOSAMINE (three-letter code: GCN) (formula: C₆H₁₃NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	6	1	4		
2	A	1	Total	C	N	O	0	0
			10	6	1	3		

- Molecule 3 is 3-DEOXY-D-MANNO-OCT-2-ULOSONIC ACID (three-letter code: KDO) (formula: $C_8H_{14}O_8$).



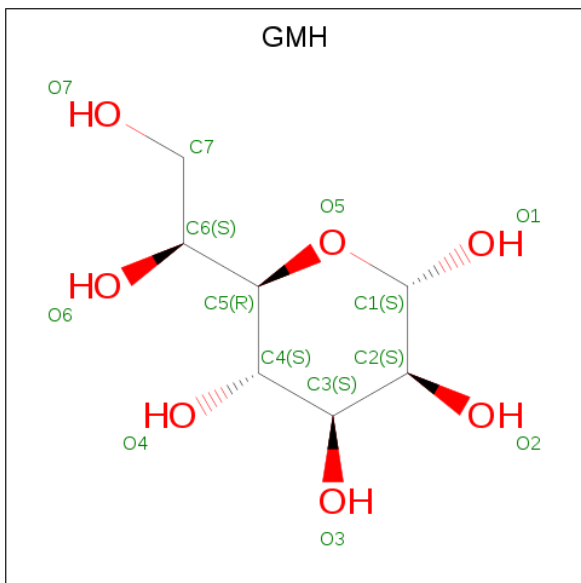
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			15	8	7		

Continued on next page...

Continued from previous page...

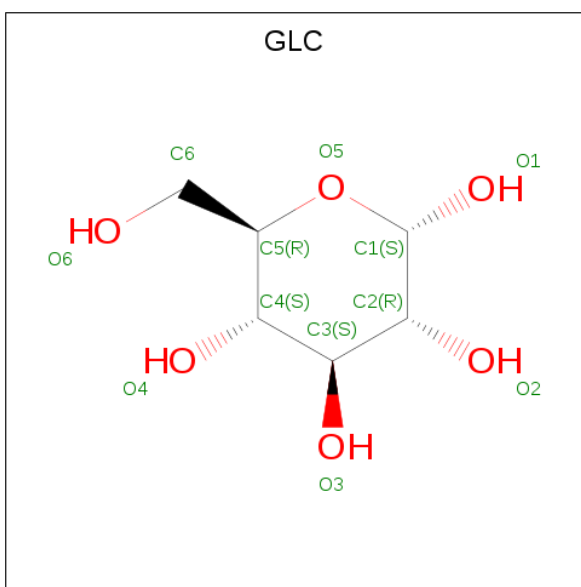
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			15	8	7		

- Molecule 4 is L-GLYCERO-D-MANNO-HEPTOPYRANOSE (three-letter code: GMH) (formula: $C_7H_{14}O_7$).



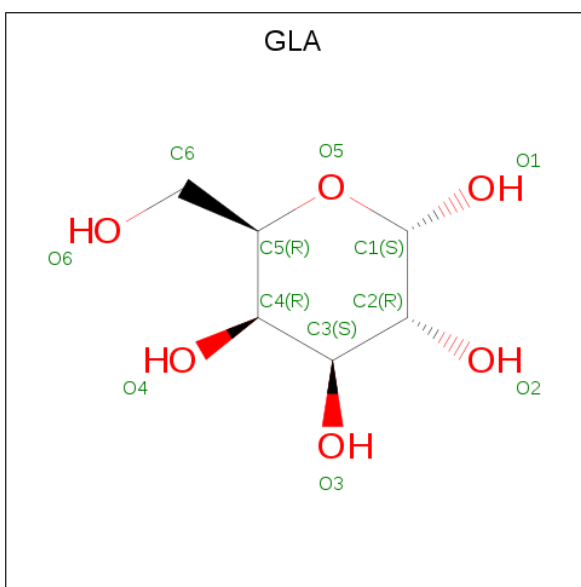
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	7	6		
4	A	1	Total	C	O	0	0
			13	7	6		
4	A	1	Total	C	O	0	0
			13	7	6		

- Molecule 5 is ALPHA-D-GLUCOSE (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



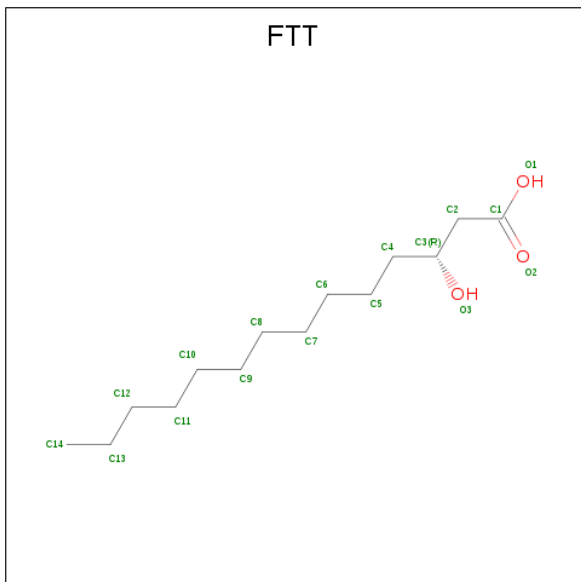
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is ALPHA D-GALACTOSE (three-letter code: GLA) (formula: $C_6H_{12}O_6$).



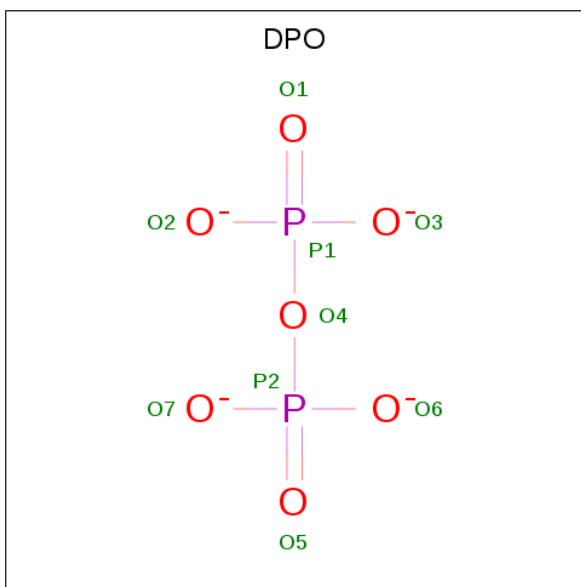
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is 3-HYDROXY-TETRADECANOIC ACID (three-letter code: FTT) (formula: $C_{14}H_{28}O_3$).



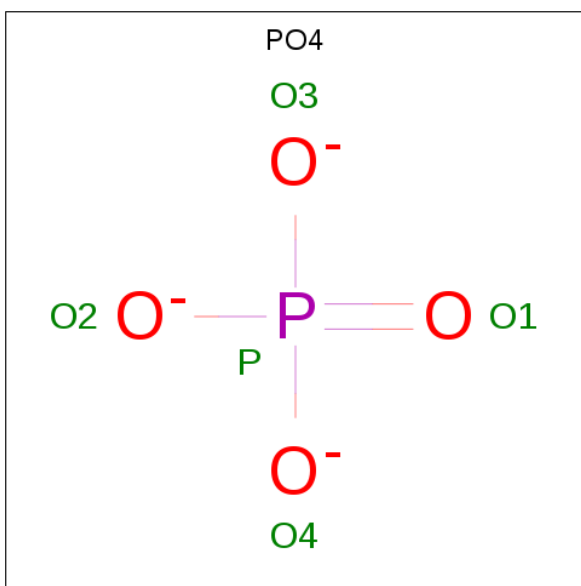
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			16	14	2		
7	A	1	Total	C	O	0	0
			8	5	3		
7	A	1	Total	C	O	0	0
			16	14	2		
7	A	1	Total	C	O	0	0
			13	12	1		
7	A	1	Total	C	O	0	0
			17	14	3		
7	A	1	Total	C	O	0	0
			15	14	1		

- Molecule 8 is DIPHOSPHATE (three-letter code: DPO) (formula: O_7P_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	P	0	0
			8	6	2		
8	A	1	Total	O	P	0	0
			8	6	2		

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

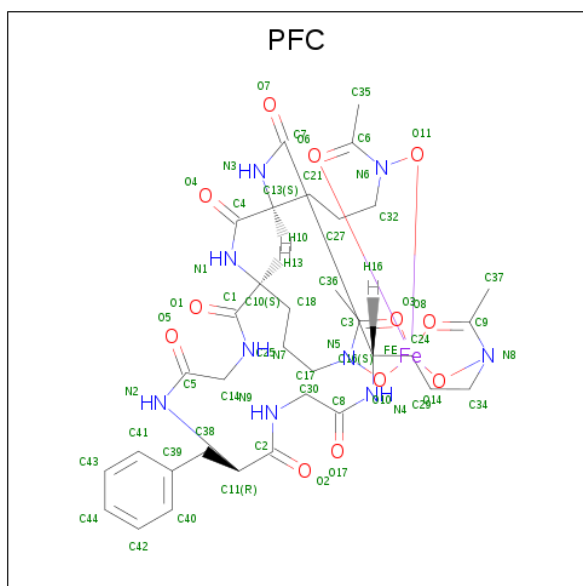


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	P	0	0
			4	3	1		
9	A	1	Total	O	P	0	0
			4	3	1		

- Molecule 10 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total Ni 1 1	0	0

- Molecule 11 is PHENYLFERRICROCIN-IRON (three-letter code: PFC) (formula: C₃₄H₄₈FeN₉O₁₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C Fe N O 56 34 1 9 12	0	0

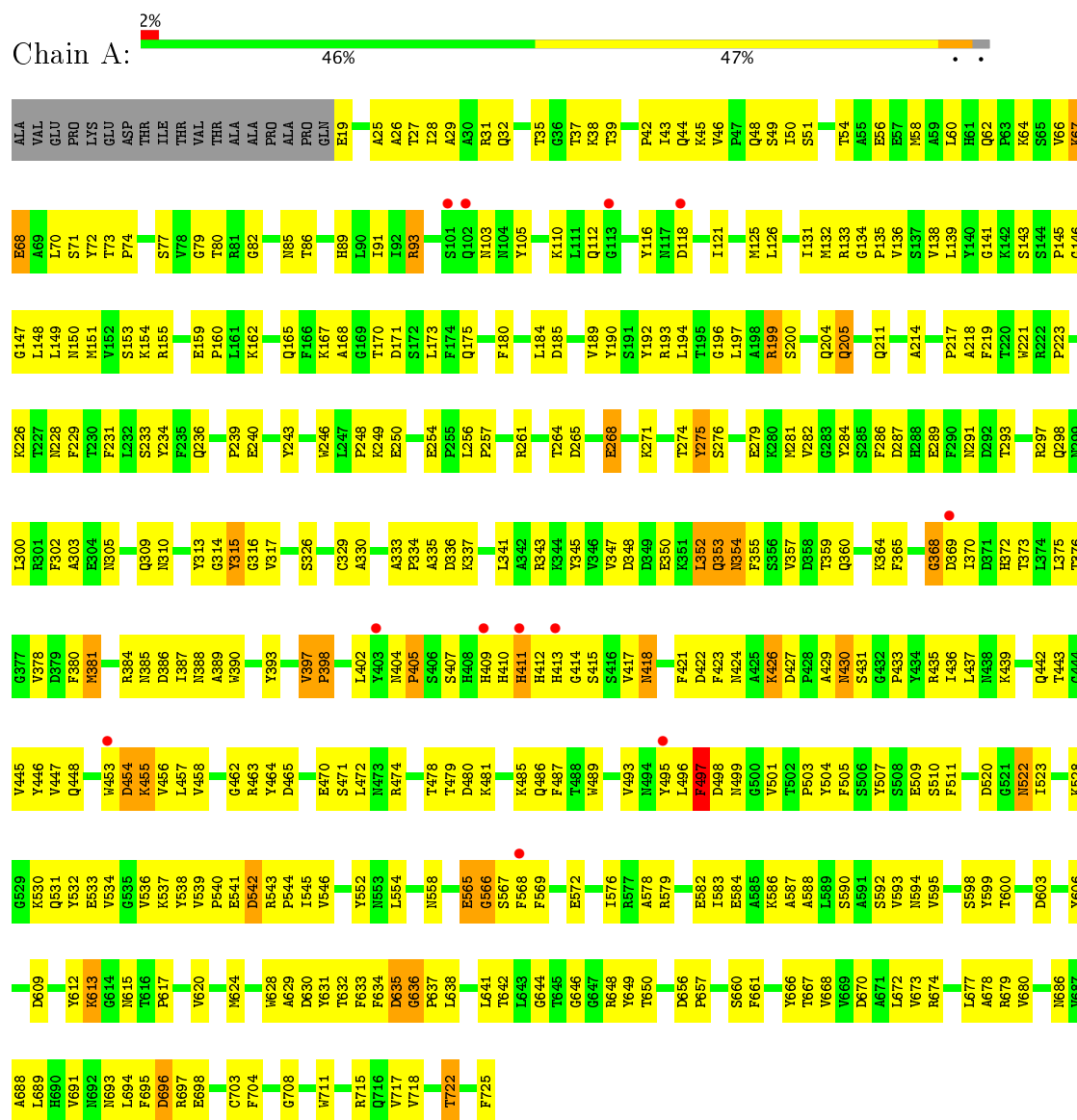
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	395	Total O 395 395	0	0

3 Residue-property plots

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: FERRIC HYDROXAMATE RECEPTOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	172.10 Å 172.10 Å 87.65 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.95 41.34 – 2.89	Depositor EDS
% Data completeness (in resolution range)	96.6 (50.00-2.95) 92.2 (41.34-2.89)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 2.90 Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.225 , 0.278 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	63.7	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.020 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6218	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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: NI, PFC, GMH, FTT, GLA, PO4, GLC, GCN, KDO, DPO

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	0.40	0/5663	0.65	0/7696

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	5523	0	5223	380	0
2	A	21	0	14	2	0
3	A	30	0	22	2	0
4	A	39	0	31	3	0
5	A	33	0	27	0	0
6	A	11	0	10	1	0
7	A	85	0	128	15	0
8	A	16	0	0	1	0
9	A	8	0	0	2	0
10	A	1	0	0	0	0
11	A	56	0	48	2	0
12	A	395	0	0	66	0
All	All	6218	0	5503	397	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 35.

All (397) 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:649:TYR:HA	12:A:2340:HOH:O	1.45	1.17
1:A:66:VAL:HG21	1:A:151:MET:HE3	1.34	1.07
1:A:455:LYS:HE2	1:A:455:LYS:N	1.80	0.96
1:A:248:PRO:HB3	12:A:2217:HOH:O	1.67	0.94
1:A:219:PHE:HA	12:A:2135:HOH:O	1.67	0.93
1:A:28:ILE:HD12	1:A:28:ILE:H	1.32	0.92
1:A:274:THR:HG22	1:A:310:ASN:HB2	1.49	0.92
1:A:136:VAL:HG21	1:A:148:LEU:HD12	1.51	0.91
7:A:1003:FTT:H41	12:A:2377:HOH:O	1.74	0.87
1:A:667:THR:HA	12:A:2340:HOH:O	1.72	0.87
1:A:134:GLY:CA	1:A:146:GLY:HA2	2.05	0.87
1:A:691:VAL:HG22	1:A:717:VAL:HG22	1.57	0.87
1:A:121:ILE:HB	1:A:151:MET:CE	2.06	0.86
1:A:455:LYS:HE2	1:A:455:LYS:H	1.38	0.85
1:A:165:GLN:HE21	1:A:722:THR:HB	1.42	0.83
1:A:668:VAL:HG13	1:A:693:ASN:HA	1.58	0.82
1:A:281:MET:HB3	1:A:303:ALA:HB2	1.60	0.81
1:A:93:ARG:HD3	1:A:133:ARG:HG2	1.60	0.81
1:A:378:VAL:HG12	1:A:445:VAL:HG12	1.62	0.81
1:A:121:ILE:HB	1:A:151:MET:HE1	1.61	0.81
1:A:544:PRO:HG2	1:A:588:ALA:HB3	1.61	0.81
1:A:446:TYR:HB3	1:A:463:ARG:HB2	1.64	0.78
1:A:205:GLN:HG3	1:A:243:TYR:CG	2.19	0.78
1:A:677:LEU:HD13	1:A:686:ASN:HA	1.66	0.78
1:A:217:PRO:HD2	1:A:233:SER:OG	1.85	0.77
1:A:656:ASP:OD2	1:A:660:SER:HB3	1.84	0.77
1:A:648:ARG:NH1	1:A:670:ASP:OD2	2.19	0.76
1:A:531:GLN:HB2	1:A:554:LEU:HD13	1.68	0.75
1:A:125:MET:HG3	1:A:234:TYR:HE1	1.51	0.75
1:A:175:GLN:HG3	1:A:199:ARG:HB2	1.68	0.75
1:A:497:PHE:HB2	1:A:501:VAL:O	1.87	0.75
1:A:71:SER:HB3	1:A:648:ARG:HD2	1.69	0.73
1:A:64:LYS:HD2	1:A:85:ASN:ND2	2.04	0.73
1:A:167:LYS:HB2	1:A:175:GLN:HB3	1.71	0.73
1:A:221:TRP:CE2	1:A:223:PRO:HG3	2.25	0.72
1:A:384:ARG:HD2	12:A:2376:HOH:O	1.90	0.71
1:A:148:LEU:HD23	1:A:148:LEU:C	2.11	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ARG:HD2	12:A:2139:HOH:O	1.89	0.71
1:A:264:THR:HA	1:A:711:TRP:CD1	2.26	0.71
1:A:541:GLU:HB3	12:A:2309:HOH:O	1.92	0.70
1:A:162:LYS:HA	1:A:180:PHE:HD1	1.57	0.69
1:A:698:GLU:HB3	12:A:2363:HOH:O	1.93	0.68
1:A:693:ASN:O	1:A:715:ARG:HB2	1.93	0.68
1:A:633:PHE:HA	12:A:2336:HOH:O	1.94	0.68
1:A:390:TRP:CH2	1:A:433:PRO:HG3	2.29	0.68
1:A:51:SER:OG	1:A:133:ARG:NH2	2.27	0.67
1:A:148:LEU:HD23	1:A:149:LEU:N	2.10	0.67
1:A:211:GLN:HG2	12:A:2146:HOH:O	1.92	0.67
1:A:600:THR:HB	1:A:624:MET:HB2	1.77	0.67
1:A:126:LEU:HD11	1:A:151:MET:HE3	1.77	0.67
1:A:27:THR:HB	12:A:2007:HOH:O	1.94	0.67
1:A:594:ASN:HB2	1:A:630:ASP:OD1	1.94	0.67
1:A:642:THR:HB	1:A:674:ARG:HB3	1.76	0.67
1:A:219:PHE:CD1	12:A:2135:HOH:O	2.47	0.66
1:A:71:SER:HB3	1:A:648:ARG:CD	2.25	0.66
1:A:315:TYR:HB3	12:A:2215:HOH:O	1.96	0.66
1:A:657:PRO:HB3	12:A:2329:HOH:O	1.96	0.66
1:A:134:GLY:HA2	1:A:146:GLY:HA2	1.78	0.66
1:A:162:LYS:HA	1:A:180:PHE:CD1	2.31	0.66
1:A:228:ASN:HB3	1:A:287:ASP:OD1	1.96	0.65
1:A:633:PHE:HB2	1:A:638:LEU:O	1.97	0.65
1:A:64:LYS:HG3	1:A:199:ARG:NH2	2.12	0.65
1:A:219:PHE:HD1	12:A:2135:HOH:O	1.79	0.64
1:A:300:LEU:CG	1:A:357:VAL:HG12	2.27	0.64
1:A:613:LYS:C	1:A:615:ASN:H	2.00	0.64
1:A:390:TRP:CZ3	1:A:433:PRO:HG3	2.32	0.64
1:A:54:THR:HB	12:A:2022:HOH:O	1.96	0.64
1:A:67:LYS:HE3	12:A:2050:HOH:O	1.96	0.64
1:A:397:VAL:HG23	1:A:398:PRO:HD2	1.79	0.64
4:A:1011:GMH:O6	4:A:1012:GMH:H5	1.97	0.64
1:A:80:THR:HG21	1:A:89:HIS:CE1	2.32	0.64
1:A:121:ILE:HB	1:A:151:MET:HE2	1.80	0.64
1:A:200:SER:HA	12:A:2146:HOH:O	1.97	0.63
1:A:211:GLN:HA	12:A:2146:HOH:O	1.99	0.63
1:A:279:GLU:HA	1:A:305:ASN:OD1	1.99	0.62
1:A:540:PRO:HG3	1:A:545:ILE:CG1	2.29	0.62
1:A:132:MET:HE2	1:A:136:VAL:HG12	1.82	0.62
1:A:590:SER:HB3	1:A:593:VAL:HB	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LYS:HD3	1:A:193:ARG:NH2	2.15	0.62
1:A:457:LEU:HD22	12:A:2274:HOH:O	2.00	0.61
1:A:503:PRO:HA	1:A:536:VAL:HG12	1.82	0.61
1:A:134:GLY:C	1:A:146:GLY:HA2	2.21	0.61
1:A:354:ASN:HD22	1:A:355:PHE:N	1.98	0.61
3:A:1008:KDO:H7	4:A:1010:GMH:C1	2.31	0.61
1:A:126:LEU:HD11	1:A:151:MET:CE	2.30	0.61
1:A:35:THR:CG2	1:A:150:ASN:HD22	2.13	0.61
1:A:609:ASP:HB3	1:A:612:TYR:O	2.00	0.61
1:A:192:TYR:HA	12:A:2135:HOH:O	2.00	0.61
1:A:470:GLU:HG3	1:A:481:LYS:HG2	1.82	0.60
1:A:715:ARG:HH11	1:A:715:ARG:HG2	1.66	0.60
1:A:409:HIS:O	1:A:414:GLY:HA2	2.02	0.60
7:A:1002:FTT:H143	7:A:1005:FTT:H91	1.83	0.60
1:A:592:SER:HB2	1:A:632:THR:O	2.02	0.60
7:A:1006:FTT:H52	7:A:1007:FTT:C1	2.32	0.60
1:A:240:GLU:HA	1:A:275:TYR:O	2.01	0.59
1:A:116:TYR:OH	11:A:1022:PFC:H302	2.01	0.59
1:A:27:THR:HG23	12:A:2025:HOH:O	2.02	0.59
1:A:35:THR:HG22	1:A:150:ASN:HD22	1.65	0.59
1:A:583:ILE:HG12	1:A:599:TYR:HB3	1.83	0.59
1:A:45:LYS:HE2	1:A:496:LEU:HD22	1.84	0.59
1:A:265:ASP:HB3	12:A:2368:HOH:O	2.02	0.59
1:A:135:PRO:HB3	1:A:509:GLU:C	2.23	0.59
1:A:44:GLN:HB3	1:A:539:VAL:HG21	1.85	0.58
1:A:617:PRO:O	1:A:620:VAL:HG12	2.04	0.58
1:A:249:LYS:HG2	1:A:250:GLU:OE1	2.04	0.58
1:A:49:SER:O	1:A:50:ILE:HD12	2.04	0.58
1:A:105:TYR:CE2	1:A:110:LYS:HB2	2.38	0.58
1:A:281:MET:HB3	1:A:303:ALA:CB	2.33	0.58
1:A:370:ILE:HG22	1:A:372:HIS:CD2	2.39	0.58
1:A:352:LEU:HD12	1:A:352:LEU:C	2.24	0.58
1:A:365:PHE:HE1	1:A:372:HIS:HD1	1.52	0.57
1:A:49:SER:C	1:A:50:ILE:HD12	2.25	0.57
1:A:678:ALA:HB2	12:A:2358:HOH:O	2.05	0.57
7:A:1002:FTT:C10	7:A:1005:FTT:H71	2.35	0.57
1:A:28:ILE:H	1:A:28:ILE:CD1	2.08	0.57
1:A:291:ASN:OD1	1:A:293:THR:HG22	2.05	0.57
1:A:205:GLN:HG3	1:A:243:TYR:CB	2.35	0.57
1:A:44:GLN:HB3	1:A:539:VAL:CG2	2.35	0.57
1:A:628:TRP:CH2	1:A:630:ASP:HB3	2.40	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:VAL:O	1:A:673:VAL:HG23	2.04	0.57
1:A:249:LYS:HE2	1:A:254:GLU:OE1	2.05	0.57
1:A:545:ILE:HG22	1:A:587:ALA:HB1	1.86	0.57
1:A:376:THR:HG22	1:A:447:VAL:HG22	1.85	0.56
1:A:66:VAL:HG21	1:A:151:MET:CE	2.23	0.56
1:A:246:TRP:HZ3	1:A:315:TYR:CE1	2.24	0.56
1:A:343:ARG:O	1:A:397:VAL:HG13	2.05	0.56
1:A:79:GLY:HA2	12:A:2044:HOH:O	2.05	0.56
1:A:300:LEU:HD12	1:A:357:VAL:CG1	2.35	0.56
1:A:497:PHE:HD2	1:A:499:ASN:OD1	1.89	0.56
1:A:694:LEU:O	1:A:715:ARG:HD3	2.06	0.56
1:A:695:PHE:O	1:A:696:ASP:C	2.45	0.56
1:A:435:ARG:O	1:A:436:ILE:HD13	2.06	0.55
1:A:693:ASN:HB2	12:A:2365:HOH:O	2.05	0.55
1:A:462:GLY:HA2	1:A:489:TRP:HA	1.88	0.55
1:A:192:TYR:CA	12:A:2135:HOH:O	2.55	0.55
1:A:185:ASP:CG	1:A:189:VAL:HG12	2.27	0.55
1:A:234:TYR:HB3	1:A:281:MET:HG3	1.88	0.55
1:A:486:GLN:OE1	1:A:528:LYS:HE2	2.07	0.55
1:A:268:GLU:OE1	1:A:314:GLY:N	2.39	0.55
1:A:493:VAL:HB	1:A:505:PHE:CE2	2.42	0.55
1:A:350:GLU:HG2	1:A:387:ILE:HA	1.88	0.54
1:A:472:LEU:HD12	1:A:478:THR:O	2.08	0.54
1:A:317:VAL:N	12:A:2217:HOH:O	2.40	0.54
1:A:62:GLN:OE1	1:A:167:LYS:NZ	2.39	0.54
1:A:352:LEU:HB2	1:A:384:ARG:O	2.08	0.54
1:A:165:GLN:NE2	1:A:722:THR:HB	2.17	0.54
4:A:1010:GMH:H6	8:A:1015:DPO:O6	2.08	0.54
1:A:520:ASP:OD2	1:A:522:ASN:HB2	2.08	0.54
7:A:1002:FTT:H102	7:A:1005:FTT:H71	1.90	0.54
1:A:297:ARG:HH11	1:A:360:GLN:HE21	1.56	0.54
1:A:704:PHE:CE2	1:A:708:GLY:HA3	2.44	0.53
1:A:390:TRP:CZ2	1:A:426:LYS:HB2	2.43	0.53
1:A:504:TYR:CE2	1:A:537:LYS:HE3	2.43	0.53
1:A:93:ARG:HD2	1:A:582:GLU:OE2	2.08	0.53
1:A:214:ALA:HB1	12:A:2166:HOH:O	2.07	0.53
1:A:38:LYS:HE3	1:A:139:LEU:O	2.08	0.53
1:A:567:SER:O	1:A:568:PHE:HB2	2.07	0.53
1:A:427:ASP:C	1:A:429:ALA:H	2.12	0.53
1:A:72:TYR:CE2	1:A:628:TRP:HB2	2.43	0.53
1:A:595:VAL:HG12	1:A:629:ALA:HB2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LYS:HG3	1:A:139:LEU:HD22	1.90	0.53
1:A:300:LEU:HG	1:A:357:VAL:HG12	1.90	0.53
1:A:509:GLU:HB3	12:A:2305:HOH:O	2.09	0.53
1:A:67:LYS:HZ2	1:A:67:LYS:CB	2.22	0.53
1:A:189:VAL:HG13	1:A:190:TYR:CD2	2.44	0.53
1:A:143:SER:HB2	12:A:2092:HOH:O	2.08	0.53
1:A:404:ASN:HB3	1:A:405:PRO:HD3	1.90	0.52
1:A:261:ARG:O	1:A:410:HIS:HE1	1.92	0.52
1:A:544:PRO:CG	1:A:588:ALA:HB3	2.38	0.52
7:A:1002:FTT:C14	7:A:1005:FTT:H91	2.40	0.52
1:A:28:ILE:HG13	1:A:56:GLU:OE1	2.09	0.52
1:A:126:LEU:HD22	1:A:151:MET:HB3	1.91	0.52
1:A:341:LEU:HB2	1:A:402:LEU:HD21	1.91	0.52
1:A:592:SER:HB3	1:A:634:PHE:HE1	1.74	0.52
1:A:433:PRO:HD2	12:A:2264:HOH:O	2.10	0.52
1:A:505:PHE:HB2	1:A:534:VAL:HG12	1.92	0.52
1:A:353:GLN:HG3	12:A:2376:HOH:O	2.09	0.51
1:A:703:CYS:HA	1:A:708:GLY:O	2.10	0.51
1:A:45:LYS:HB3	1:A:457:LEU:CD2	2.40	0.51
1:A:496:LEU:HD21	12:A:2011:HOH:O	2.10	0.51
1:A:300:LEU:C	1:A:300:LEU:HD23	2.31	0.51
1:A:347:VAL:O	1:A:389:ALA:HB1	2.10	0.51
1:A:58:MET:C	1:A:60:LEU:H	2.14	0.51
1:A:45:LYS:HD3	12:A:2274:HOH:O	2.11	0.51
1:A:192:TYR:CB	12:A:2135:HOH:O	2.58	0.51
1:A:538:TYR:CD2	1:A:540:PRO:HD3	2.45	0.51
1:A:628:TRP:CD1	1:A:646:GLY:HA3	2.45	0.51
1:A:205:GLN:HG3	1:A:243:TYR:HB2	1.93	0.51
1:A:133:ARG:HD2	1:A:582:GLU:OE1	2.11	0.51
1:A:148:LEU:CD2	1:A:148:LEU:C	2.79	0.51
1:A:300:LEU:CB	1:A:357:VAL:HG12	2.40	0.51
1:A:297:ARG:HH11	1:A:360:GLN:NE2	2.09	0.51
1:A:231:PHE:CD1	7:A:1004:FTT:H143	2.46	0.50
1:A:300:LEU:HD12	1:A:357:VAL:HG11	1.92	0.50
1:A:316:GLY:C	12:A:2217:HOH:O	2.50	0.50
1:A:390:TRP:HE1	1:A:431:SER:HB2	1.75	0.50
1:A:542:ASP:OD2	1:A:543:ARG:HG3	2.11	0.50
1:A:313:TYR:HA	12:A:2211:HOH:O	2.11	0.50
1:A:422:ASP:O	1:A:423:PHE:HB2	2.11	0.50
1:A:370:ILE:HG22	1:A:372:HIS:NE2	2.27	0.50
1:A:25:ALA:O	1:A:26:ALA:HB3	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:THR:HG23	1:A:375:LEU:HD22	1.93	0.50
1:A:650:THR:HB	1:A:666:TYR:CE1	2.47	0.50
1:A:60:LEU:HD21	1:A:628:TRP:CZ3	2.47	0.50
1:A:159:GLU:HA	12:A:2109:HOH:O	2.12	0.50
1:A:31:ARG:O	1:A:43:ILE:HG12	2.12	0.50
1:A:422:ASP:O	1:A:424:ASN:N	2.40	0.50
1:A:540:PRO:HD2	1:A:545:ILE:O	2.12	0.49
1:A:45:LYS:HE2	1:A:496:LEU:CD2	2.42	0.49
1:A:364:LYS:HG2	12:A:2231:HOH:O	2.12	0.49
1:A:386:ASP:OD2	1:A:437:LEU:HD13	2.13	0.49
1:A:628:TRP:HD1	1:A:646:GLY:HA3	1.78	0.49
1:A:86:THR:HA	12:A:2047:HOH:O	2.12	0.49
1:A:333:ALA:O	1:A:335:ALA:N	2.46	0.49
1:A:424:ASN:HA	12:A:2258:HOH:O	2.12	0.49
1:A:93:ARG:HG3	1:A:552:TYR:OH	2.13	0.49
1:A:637:PRO:HA	12:A:2359:HOH:O	2.13	0.49
1:A:693:ASN:HD22	1:A:715:ARG:N	2.11	0.49
1:A:540:PRO:HG3	1:A:545:ILE:HG13	1.95	0.49
1:A:67:LYS:CE	12:A:2050:HOH:O	2.57	0.49
1:A:402:LEU:O	1:A:405:PRO:HD2	2.13	0.49
1:A:455:LYS:CE	1:A:455:LYS:N	2.66	0.49
1:A:93:ARG:HG3	1:A:552:TYR:CZ	2.47	0.49
1:A:134:GLY:N	1:A:146:GLY:HA2	2.27	0.49
1:A:387:ILE:O	1:A:435:ARG:HA	2.12	0.49
1:A:422:ASP:C	1:A:424:ASN:H	2.17	0.49
1:A:680:VAL:HG12	1:A:680:VAL:O	2.12	0.48
1:A:330:ALA:HA	1:A:337:LYS:NZ	2.28	0.48
1:A:165:GLN:NE2	12:A:2115:HOH:O	2.46	0.48
1:A:693:ASN:HB3	1:A:715:ARG:HA	1.95	0.48
1:A:192:TYR:HB3	12:A:2135:HOH:O	2.13	0.48
1:A:19:GLU:HG2	12:A:2087:HOH:O	2.14	0.48
1:A:82:GLY:HA2	12:A:2044:HOH:O	2.12	0.48
1:A:454:ASP:C	1:A:456:VAL:H	2.16	0.48
1:A:29:ALA:HB1	1:A:546:VAL:HG23	1.94	0.48
1:A:600:THR:HG23	12:A:2036:HOH:O	2.14	0.48
1:A:674:ARG:HG3	1:A:688:ALA:HB2	1.96	0.48
1:A:167:LYS:HD2	1:A:175:GLN:CD	2.33	0.48
1:A:264:THR:HA	1:A:711:TRP:CG	2.49	0.48
1:A:393:TYR:HB3	12:A:2247:HOH:O	2.12	0.47
1:A:412:HIS:H	1:A:412:HIS:CD2	2.32	0.47
1:A:153:SER:HB3	12:A:2106:HOH:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ARG:NH2	1:A:533:GLU:OE1	2.27	0.47
1:A:337:LYS:HD3	12:A:2222:HOH:O	2.13	0.47
1:A:384:ARG:NH2	3:A:1009:KDO:O1B	2.47	0.47
1:A:410:HIS:O	1:A:411:HIS:C	2.53	0.47
1:A:631:TYR:HE2	1:A:633:PHE:CE1	2.32	0.47
1:A:381:MET:HG3	1:A:442:GLN:HB3	1.94	0.47
1:A:594:ASN:O	1:A:629:ALA:HA	2.15	0.47
1:A:480:ASP:HB3	1:A:523:ILE:HD11	1.96	0.47
1:A:204:GLN:HB2	12:A:2141:HOH:O	2.14	0.47
1:A:430:ASN:HD22	1:A:430:ASN:C	2.16	0.47
1:A:184:LEU:HD12	1:A:190:TYR:HB3	1.97	0.46
1:A:218:ALA:HA	1:A:231:PHE:O	2.14	0.46
1:A:567:SER:O	1:A:569:PHE:N	2.41	0.46
1:A:155:ARG:O	1:A:193:ARG:HD2	2.15	0.46
7:A:1004:FTT:H42	7:A:1006:FTT:H22	1.97	0.46
1:A:486:GLN:HG2	1:A:511:PHE:CG	2.51	0.46
1:A:505:PHE:HA	1:A:534:VAL:HA	1.96	0.46
6:A:1019:GLA:H3	12:A:2389:HOH:O	2.15	0.46
1:A:185:ASP:OD2	1:A:189:VAL:HG12	2.15	0.46
1:A:309:GLN:HG2	1:A:348:ASP:HB3	1.97	0.46
1:A:298:GLN:HG3	1:A:359:THR:OG1	2.16	0.46
1:A:465:ASP:O	1:A:485:LYS:HA	2.16	0.46
1:A:495:TYR:HD1	1:A:497:PHE:HD1	1.63	0.46
1:A:644:GLY:O	1:A:672:LEU:N	2.49	0.46
1:A:578:ALA:HA	1:A:603:ASP:O	2.15	0.46
1:A:326:SER:HB3	1:A:329:CYS:HB2	1.96	0.46
1:A:74:PRO:HG3	1:A:584:GLU:HB2	1.97	0.46
1:A:436:ILE:HG22	1:A:437:LEU:N	2.31	0.46
1:A:474:ARG:HH11	1:A:474:ARG:HG2	1.80	0.46
1:A:628:TRP:CZ3	1:A:630:ASP:OD1	2.69	0.46
1:A:345:TYR:C	1:A:345:TYR:CD1	2.89	0.46
1:A:368:GLY:O	1:A:369:ASP:HB2	2.15	0.46
1:A:583:ILE:O	1:A:598:SER:HA	2.16	0.46
1:A:427:ASP:C	1:A:429:ALA:N	2.69	0.46
1:A:199:ARG:HG3	1:A:199:ARG:HH11	1.81	0.45
1:A:631:TYR:O	1:A:642:THR:HA	2.17	0.45
1:A:673:VAL:CG2	1:A:689:LEU:HB3	2.46	0.45
1:A:352:LEU:HB3	1:A:385:ASN:OD1	2.16	0.45
1:A:635:ASP:O	1:A:636:GLY:O	2.34	0.45
1:A:390:TRP:HE1	1:A:431:SER:CB	2.28	0.45
1:A:446:TYR:CB	1:A:463:ARG:HB2	2.41	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:678:ALA:C	1:A:680:VAL:H	2.20	0.45
1:A:80:THR:HG21	1:A:89:HIS:ND1	2.30	0.45
1:A:80:THR:OG1	1:A:91:ILE:HG13	2.16	0.45
1:A:167:LYS:HD2	1:A:175:GLN:HB3	1.99	0.45
1:A:236:GLN:HB2	12:A:2166:HOH:O	2.17	0.45
1:A:522:ASN:HD22	1:A:522:ASN:HA	1.58	0.45
1:A:725:PHE:CD1	1:A:725:PHE:N	2.85	0.45
2:A:1001:GCN:C6	9:A:1014:PO4:O3	2.64	0.45
1:A:412:HIS:N	1:A:412:HIS:CD2	2.83	0.45
1:A:586:LYS:HA	1:A:595:VAL:O	2.16	0.45
1:A:576:ILE:HD11	1:A:606:TYR:CE1	2.52	0.45
1:A:126:LEU:CD2	1:A:151:MET:HB3	2.47	0.45
1:A:246:TRP:CZ3	1:A:315:TYR:CE1	3.04	0.45
1:A:390:TRP:CE2	1:A:426:LYS:CB	3.00	0.45
1:A:390:TRP:CE2	1:A:426:LYS:HB2	2.52	0.45
1:A:42:PRO:CG	1:A:45:LYS:HD2	2.48	0.45
1:A:592:SER:O	1:A:631:TYR:HA	2.16	0.45
1:A:302:PHE:CE2	7:A:1006:FTT:H3	2.53	0.44
1:A:486:GLN:HG2	1:A:511:PHE:CB	2.48	0.44
1:A:583:ILE:HG13	1:A:583:ILE:O	2.15	0.44
1:A:93:ARG:HH11	1:A:133:ARG:HD2	1.82	0.44
1:A:390:TRP:NE1	1:A:431:SER:HB2	2.32	0.44
1:A:507:TYR:HD1	1:A:532:TYR:CE1	2.35	0.44
1:A:612:TYR:O	1:A:613:LYS:HB2	2.18	0.44
1:A:82:GLY:CA	12:A:2044:HOH:O	2.64	0.44
1:A:28:ILE:HD12	12:A:2025:HOH:O	2.18	0.44
1:A:407:SER:HA	12:A:2250:HOH:O	2.17	0.44
1:A:397:VAL:HB	1:A:421:PHE:CE1	2.52	0.44
1:A:595:VAL:HG12	1:A:629:ALA:CB	2.47	0.44
1:A:234:TYR:HB3	1:A:281:MET:CG	2.48	0.43
1:A:370:ILE:HG12	1:A:453:TRP:CD1	2.52	0.43
1:A:470:GLU:HG3	1:A:481:LYS:CG	2.47	0.43
1:A:636:GLY:HA3	1:A:637:PRO:HD2	1.90	0.43
1:A:384:ARG:NH1	1:A:439:LYS:HE2	2.33	0.43
1:A:418:ASN:HB3	12:A:2256:HOH:O	2.18	0.43
1:A:507:TYR:OH	1:A:530:LYS:HD2	2.18	0.43
1:A:565:GLU:O	1:A:566:GLY:O	2.35	0.43
1:A:695:PHE:O	1:A:697:ARG:N	2.50	0.43
1:A:722:THR:HG21	12:A:2115:HOH:O	2.17	0.43
1:A:471:SER:O	1:A:479:THR:HA	2.18	0.43
1:A:558:ASN:OD1	1:A:572:GLU:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:PHE:HD2	1:A:641:LEU:HB3	1.82	0.43
1:A:284:TYR:HD2	7:A:1004:FTT:H131	1.84	0.43
1:A:365:PHE:HE1	1:A:372:HIS:ND1	2.15	0.43
1:A:631:TYR:CE2	1:A:633:PHE:CE1	3.06	0.43
1:A:612:TYR:CZ	1:A:657:PRO:HB2	2.54	0.43
1:A:413:HIS:HD2	12:A:2252:HOH:O	2.01	0.43
1:A:427:ASP:O	1:A:429:ALA:N	2.52	0.43
1:A:430:ASN:HD22	1:A:431:SER:N	2.17	0.43
1:A:196:GLY:HA2	1:A:214:ALA:O	2.19	0.43
1:A:135:PRO:HB3	1:A:510:SER:HB3	2.01	0.43
1:A:197:LEU:HD12	1:A:197:LEU:C	2.40	0.42
1:A:44:GLN:HG2	1:A:45:LYS:N	2.34	0.42
1:A:80:THR:HB	12:A:2055:HOH:O	2.18	0.42
1:A:93:ARG:NH1	1:A:582:GLU:OE1	2.52	0.42
1:A:300:LEU:HB2	1:A:357:VAL:HG12	2.00	0.42
1:A:134:GLY:O	1:A:136:VAL:HG13	2.20	0.42
1:A:264:THR:HG21	1:A:698:GLU:HG2	2.00	0.42
1:A:495:TYR:HD1	1:A:497:PHE:CD1	2.38	0.42
1:A:64:LYS:HG3	1:A:199:ARG:HH22	1.82	0.42
7:A:1002:FTT:C10	7:A:1005:FTT:H51	2.50	0.42
1:A:103:ASN:ND2	1:A:147:GLY:O	2.52	0.42
1:A:229:PHE:HB2	1:A:286:PHE:HD1	1.84	0.42
1:A:357:VAL:O	1:A:357:VAL:HG23	2.20	0.42
1:A:364:LYS:CD	1:A:373:THR:HG23	2.49	0.42
1:A:282:VAL:HG11	7:A:1007:FTT:H72	2.02	0.42
1:A:300:LEU:HD12	1:A:357:VAL:HG12	2.00	0.42
1:A:661:PHE:N	1:A:661:PHE:CD1	2.87	0.42
1:A:138:VAL:HG23	1:A:462:GLY:HA2	2.01	0.42
1:A:28:ILE:HD12	1:A:28:ILE:N	2.16	0.42
1:A:173:LEU:HD23	1:A:718:VAL:HG22	2.02	0.42
11:A:1022:PFC:O11	11:A:1022:PFC:N3	2.46	0.42
1:A:199:ARG:HG3	1:A:199:ARG:NH1	2.35	0.42
1:A:465:ASP:N	1:A:486:GLN:O	2.48	0.42
1:A:46:VAL:HG12	1:A:48:GLN:H	1.85	0.42
1:A:155:ARG:O	1:A:193:ARG:CD	2.68	0.42
1:A:194:LEU:HA	1:A:194:LEU:HD12	1.88	0.42
1:A:410:HIS:HB3	1:A:411:HIS:H	1.71	0.42
1:A:271:LYS:HG3	1:A:417:VAL:HG21	2.02	0.42
1:A:160:PRO:HG3	12:A:2126:HOH:O	2.20	0.42
1:A:226:LYS:HB3	1:A:289:GLU:HB3	2.01	0.42
1:A:388:ASN:HD22	1:A:435:ARG:HG2	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:TRP:HZ3	1:A:630:ASP:OD1	2.02	0.42
1:A:715:ARG:NH1	1:A:715:ARG:HG2	2.33	0.42
1:A:633:PHE:CE2	1:A:641:LEU:HD23	2.55	0.41
7:A:1002:FTT:O2	7:A:1005:FTT:H22	2.21	0.41
1:A:458:VAL:HG13	1:A:458:VAL:O	2.20	0.41
1:A:131:ILE:HD13	1:A:149:LEU:HA	2.02	0.41
1:A:145:PRO:HD2	12:A:2057:HOH:O	2.19	0.41
1:A:590:SER:HB3	1:A:593:VAL:CB	2.50	0.41
1:A:497:PHE:HB3	1:A:498:ASP:H	1.61	0.41
1:A:673:VAL:HG22	1:A:689:LEU:HB3	2.02	0.41
1:A:184:LEU:HB2	1:A:190:TYR:HB2	2.01	0.41
1:A:256:LEU:O	1:A:257:PRO:C	2.59	0.41
1:A:613:LYS:C	1:A:615:ASN:N	2.67	0.41
1:A:422:ASP:C	1:A:424:ASN:N	2.74	0.41
1:A:170:THR:HG22	1:A:171:ASP:N	2.36	0.41
1:A:62:GLN:HB3	1:A:167:LYS:HZ1	1.86	0.41
1:A:507:TYR:CD1	1:A:532:TYR:CE1	3.09	0.41
1:A:446:TYR:HB3	1:A:463:ARG:CB	2.44	0.41
7:A:1002:FTT:H101	7:A:1005:FTT:H51	2.02	0.41
1:A:141:GLY:HA3	1:A:442:GLN:HE22	1.86	0.41
1:A:32:GLN:HB2	12:A:2087:HOH:O	2.21	0.41
1:A:68:GLU:C	1:A:70:LEU:H	2.24	0.41
2:A:1001:GCN:H61	9:A:1014:PO4:O3	2.21	0.40
1:A:579:ARG:HG3	1:A:579:ARG:HH11	1.86	0.40
1:A:138:VAL:HG13	1:A:139:LEU:HG	2.02	0.40
1:A:168:ALA:HA	1:A:173:LEU:O	2.22	0.40
1:A:67:LYS:HB3	1:A:67:LYS:HZ2	1.86	0.40
1:A:217:PRO:CB	7:A:1007:FTT:H143	2.51	0.40
1:A:37:THR:HB	1:A:448:GLN:HE22	1.86	0.40
1:A:239:PRO:O	1:A:276:SER:HB3	2.22	0.40
1:A:380:PHE:HD1	1:A:443:THR:OG1	2.05	0.40
1:A:464:TYR:HD1	1:A:487:PHE:HB2	1.85	0.40

There are no symmetry-related clashes.

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	705/725 (97%)	618 (88%)	72 (10%)	15 (2%)	8	35

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	411	HIS
1	A	636	GLY
1	A	368	GLY
1	A	418	ASN
1	A	454	ASP
1	A	497	PHE
1	A	566	GLY
1	A	613	LYS
1	A	696	ASP
1	A	334	PRO
1	A	415	SER
1	A	679	ARG
1	A	635	ASP
1	A	405	PRO
1	A	398	PRO

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	587/601 (98%)	561 (96%)	26 (4%)	33	69

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LYS
1	A	68	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	73	THR
1	A	77	SER
1	A	93	ARG
1	A	112	GLN
1	A	118	ASP
1	A	199	ARG
1	A	205	GLN
1	A	268	GLU
1	A	275	TYR
1	A	315	TYR
1	A	336	ASP
1	A	352	LEU
1	A	353	GLN
1	A	354	ASN
1	A	381	MET
1	A	397	VAL
1	A	426	LYS
1	A	430	ASN
1	A	455	LYS
1	A	497	PHE
1	A	522	ASN
1	A	542	ASP
1	A	565	GLU
1	A	722	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	112	GLN
1	A	165	GLN
1	A	202	ASN
1	A	205	GLN
1	A	310	ASN
1	A	328	GLN
1	A	354	ASN
1	A	360	GLN
1	A	388	ASN
1	A	404	ASN
1	A	410	HIS
1	A	412	HIS
1	A	430	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	438	ASN
1	A	522	ASN
1	A	594	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 1 is monoatomic - leaving 22 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
2	GCN	A	1000	8,2,7	11,11,11	1.12	1 (9%)	12,15,15	1.28	3 (25%)
2	GCN	A	1001	9,3,2,7	10,10,11	1.36	1 (10%)	9,13,15	2.74	5 (55%)
7	FTT	A	1002	2	15,15,16	0.41	0	15,15,17	0.74	1 (6%)
7	FTT	A	1003	2	4,7,16	1.04	0	4,8,17	0.80	0
7	FTT	A	1004	2,7	15,15,16	0.95	1 (6%)	15,15,17	1.80	3 (20%)
7	FTT	A	1005	7	12,12,16	0.53	0	11,11,17	0.68	0
7	FTT	A	1006	2,7	13,16,16	0.23	0	13,17,17	0.71	0
7	FTT	A	1007	7	14,14,16	0.33	0	13,13,17	0.80	0
3	KDO	A	1008	3,2,4	12,15,16	0.76	0	13,21,24	0.94	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	KDO	A	1009	3	12,15,16	0.57	0	13,21,24	0.81	1 (7%)
4	GMH	A	1010	8,3,4	13,13,14	0.76	0	16,18,20	0.73	0
4	GMH	A	1011	9,5,4	13,13,14	0.94	1 (7%)	16,18,20	1.04	2 (12%)
4	GMH	A	1012	4	13,13,14	0.77	0	16,18,20	1.70	3 (18%)
8	DPO	A	1013	2	4,7,8	2.88	1 (25%)	4,10,13	0.46	0
9	PO4	A	1014	2	0,3,4	0.00	-	0,3,6	0.00	-
8	DPO	A	1015	4	4,7,8	2.39	1 (25%)	4,10,13	0.45	0
9	PO4	A	1016	10,4	0,3,4	0.00	-	0,3,6	0.00	-
5	GLC	A	1017	5,4,6	11,11,12	1.08	0	13,15,17	1.72	4 (30%)
5	GLC	A	1018	5	11,11,12	1.04	1 (9%)	13,15,17	1.88	3 (23%)
6	GLA	A	1019	5	11,11,12	0.69	0	13,15,17	1.05	1 (7%)
5	GLC	A	1020	5	11,11,12	1.48	2 (18%)	13,15,17	1.01	1 (7%)
11	PFC	A	1022	-	62,62,62	0.65	0	71,95,95	0.87	3 (4%)

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
2	GCN	A	1000	8,2,7	-	0/2/18/18	0/1/1/1
2	GCN	A	1001	9,3,2,7	1/1/3/4	0/2/15/18	0/1/1/1
7	FTT	A	1002	2	-	0/14/14/15	0/0/0/0
7	FTT	A	1003	2	-	0/4/6/15	0/0/0/0
7	FTT	A	1004	2,7	-	0/14/14/15	0/0/0/0
7	FTT	A	1005	7	-	0/9/10/15	0/0/0/0
7	FTT	A	1006	2,7	1/1/2/2	0/13/15/15	0/0/0/0
7	FTT	A	1007	7	-	0/11/12/15	0/0/0/0
3	KDO	A	1008	3,2,4	-	0/6/26/30	0/1/1/1
3	KDO	A	1009	3	-	0/6/26/30	0/1/1/1
4	GMH	A	1010	8,3,4	-	0/6/23/26	0/1/1/1
4	GMH	A	1011	9,5,4	1/1/5/6	0/6/23/26	1/1/1/1
4	GMH	A	1012	4	1/1/5/6	0/6/23/26	0/1/1/1
8	DPO	A	1013	2	-	0/2/5/6	0/0/0/0
9	PO4	A	1014	2	-	0/0/0/0	0/0/0/0
8	DPO	A	1015	4	-	0/2/5/6	0/0/0/0
9	PO4	A	1016	10,4	-	0/0/0/0	0/0/0/0
5	GLC	A	1017	5,4,6	-	0/2/19/22	0/1/1/1
5	GLC	A	1018	5	-	0/2/19/22	0/1/1/1
6	GLA	A	1019	5	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GLC	A	1020	5	1/1/4/5	0/2/19/22	0/1/1/1
11	PFC	A	1022	-	-	0/64/118/118	0/1/7/7

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1013	DPO	P2-O4	-5.31	1.50	1.59
8	A	1015	DPO	P2-O4	-4.40	1.52	1.59
2	A	1000	GCN	C3-C4	-2.54	1.48	1.52
4	A	1011	GMH	O5-C5	2.14	1.46	1.43
2	A	1001	GCN	O5-C5	2.32	1.48	1.43
5	A	1018	GLC	C4-C3	2.46	1.58	1.52
5	A	1020	GLC	C1-C2	2.47	1.58	1.52
7	A	1004	FTT	C10-C9	3.09	1.69	1.51
5	A	1020	GLC	C2-C3	3.47	1.57	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	GCN	O5-C1-C2	-4.66	104.75	111.59
5	A	1018	GLC	C1-C2-C3	-4.29	104.22	109.65
5	A	1017	GLC	C6-C5-C4	-3.53	104.73	113.00
5	A	1020	GLC	C1-C2-C3	-2.57	106.39	109.65
7	A	1004	FTT	O2-C1-C2	-2.57	117.15	125.48
11	A	1022	PFC	O17-C8-N4	-2.54	118.58	122.97
5	A	1018	GLC	C3-C4-C5	-2.16	106.41	110.22
2	A	1000	GCN	C3-C2-N2	-2.14	103.16	110.94
7	A	1002	FTT	O2-C1-C2	-2.13	118.60	125.48
3	A	1008	KDO	C3-C4-C5	-2.11	107.83	110.59
2	A	1000	GCN	O4-C4-C3	-2.07	105.01	110.02
3	A	1009	KDO	C3-C4-C5	-2.06	107.90	110.59
5	A	1017	GLC	O3-C3-C4	-2.00	106.00	110.36
11	A	1022	PFC	C17-N9-C2	2.09	125.84	121.29
2	A	1001	GCN	O5-C5-C4	2.16	113.27	109.64
11	A	1022	PFC	C17-C8-N4	2.29	121.76	116.12
6	A	1019	GLA	C1-O5-C5	2.47	115.56	112.17
2	A	1000	GCN	C1-C2-N2	2.47	115.01	110.49
7	A	1004	FTT	C11-C10-C9	2.59	127.78	114.45
5	A	1017	GLC	O3-C3-C2	2.65	114.85	110.02
2	A	1001	GCN	C1-O5-C5	2.69	115.87	112.17
4	A	1011	GMH	C7-C6-C5	2.76	117.88	112.17
4	A	1011	GMH	C1-O5-C5	2.80	115.88	111.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	GCN	C1-C2-N2	2.85	117.86	111.32
5	A	1017	GLC	C1-O5-C5	3.30	116.71	112.17
4	A	1012	GMH	C1-C2-C3	3.34	113.88	109.65
4	A	1012	GMH	O5-C1-C2	3.46	116.21	110.79
5	A	1018	GLC	C6-C5-C4	3.47	121.12	113.00
4	A	1012	GMH	C1-O5-C5	4.07	117.86	111.56
2	A	1001	GCN	C3-C4-C5	4.75	117.06	110.82
7	A	1004	FTT	C12-C11-C10	5.43	142.43	114.45

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	1006	FTT	C3
4	A	1011	GMH	C6
2	A	1001	GCN	C1
5	A	1020	GLC	C1
4	A	1012	GMH	C6

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1011	GMH	C1-C2-C3-C4-C5-O5

16 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	GCN	2	0
7	A	1002	FTT	7	0
7	A	1003	FTT	1	0
7	A	1004	FTT	3	0
7	A	1005	FTT	7	0
7	A	1006	FTT	3	0
7	A	1007	FTT	3	0
3	A	1008	KDO	1	0
3	A	1009	KDO	1	0
4	A	1010	GMH	2	0
4	A	1011	GMH	1	0
4	A	1012	GMH	1	0
9	A	1014	PO4	2	0
8	A	1015	DPO	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1019	GLA	1	0
11	A	1022	PFC	2	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	707/725 (97%)	-0.28	12 (1%)	70 51	37, 68, 106, 121	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	413	HIS	5.1
1	A	411	HIS	4.6
1	A	495	TYR	3.3
1	A	403	TYR	3.0
1	A	118	ASP	2.3
1	A	101	SER	2.2
1	A	409	HIS	2.2
1	A	568	PHE	2.2
1	A	102	GLN	2.1
1	A	369	ASP	2.1
1	A	113	GLY	2.0
1	A	453	TRP	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 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
7	FTT	A	1007	15/17	0.89	0.69	29.89	76,91,104,107	0
7	FTT	A	1005	13/17	0.92	0.37	8.66	58,65,69,69	0
7	FTT	A	1002	16/17	0.89	0.33	5.81	63,68,77,81	0
7	FTT	A	1004	16/17	0.93	0.27	4.49	46,60,65,66	0
11	PFC	A	1022	56/56	0.96	0.22	0.09	43,57,96,99	0
3	KDO	A	1008	15/16	0.97	0.09	-2.52	64,67,75,78	0
7	FTT	A	1006	17/17	0.92	0.25	-	67,77,82,82	0
2	GCN	A	1000	11/11	0.95	0.11	-	51,63,74,80	0
5	GLC	A	1020	11/12	0.60	0.52	-	116,120,120,120	0
6	GLA	A	1019	11/12	0.77	0.27	-	120,120,120,120	0
4	GMH	A	1012	13/14	0.81	0.22	-	115,119,120,120	0
5	GLC	A	1018	11/12	0.86	0.36	-	120,120,120,120	0
9	PO4	A	1014	4/5	0.94	0.14	-	70,71,72,73	0
4	GMH	A	1010	13/14	0.96	0.12	-	71,76,84,85	0
4	GMH	A	1011	13/14	0.88	0.12	-	93,104,117,118	0
10	NI	A	1021	1/1	0.90	0.07	-	120,120,120,120	0
9	PO4	A	1016	4/5	0.86	0.09	-	116,117,120,120	0
3	KDO	A	1009	15/16	0.90	0.18	-	84,88,91,93	0
5	GLC	A	1017	11/12	0.82	0.19	-	108,112,119,120	0
8	DPO	A	1013	8/9	0.97	0.12	-	64,71,81,82	4
8	DPO	A	1015	8/9	0.94	0.11	-	84,99,111,113	0
7	FTT	A	1003	8/17	0.90	0.19	-	81,89,91,97	0
2	GCN	A	1001	10/11	0.89	0.13	-	35,49,58,61	0

6.5 Other polymers ⓘ

There are no such residues in this entry.