



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:27 PM UTC

PDB ID : 2BO4 / pdb_00002bo4
Title : Dissection of mannosylglycerate synthase: an archetypal mannosyltransferase
Authors : Flint, J.; Taylor, E.; Yang, M.; Bolam, D.N.; Tailford, L.E.; Martinez-Fleites, C.; Dodson, E.J.; Davis, B.G.; Gilbert, H.J.; Davies, G.J.
Deposited on : 2005-04-07
Resolution : 1.95 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

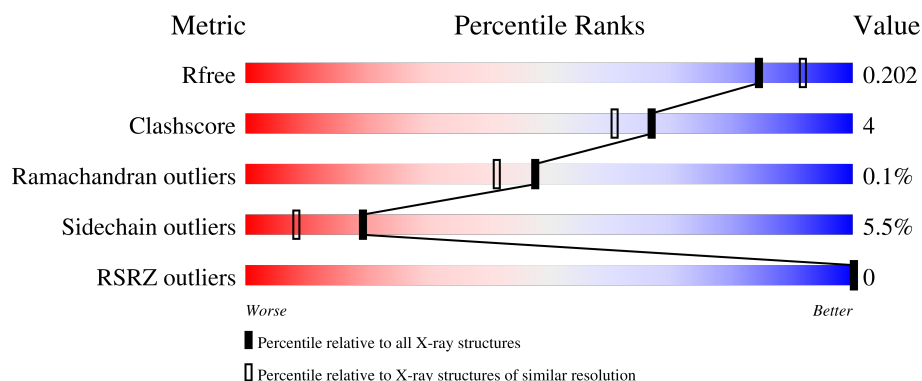
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	397	
1	B	397	
1	C	397	
1	D	397	
1	E	397	

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Mol	Chain	Length	Quality of chain
1	F	397	84% 10% . .

2 Entry composition [i](#)

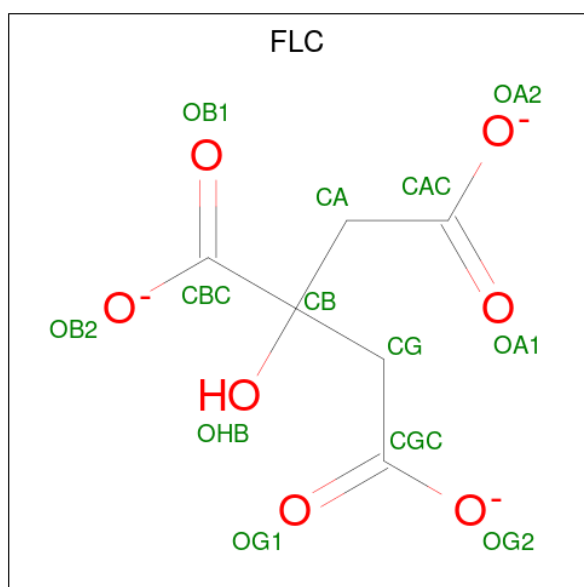
There are 3 unique types of molecules in this entry. The entry contains 20669 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MANNOSYLGLYCERATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	1
			3138	2006	558	559	15			
1	B	380	Total	C	N	O	S	0	0	0
			3137	2006	557	559	15			
1	C	381	Total	C	N	O	S	0	0	1
			3138	2006	558	559	15			
1	D	380	Total	C	N	O	S	0	0	0
			3137	2006	557	559	15			
1	E	380	Total	C	N	O	S	0	0	0
			3137	2006	557	559	15			
1	F	380	Total	C	N	O	S	0	0	0
			3137	2006	557	559	15			

- Molecule 2 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 6 7	0	0
2	B	1	Total C O 13 6 7	0	0
2	C	1	Total C O 13 6 7	0	0
2	D	1	Total C O 13 6 7	0	0
2	E	1	Total C O 13 6 7	0	0
2	F	1	Total C O 13 6 7	0	0

- Molecule 3 is water.

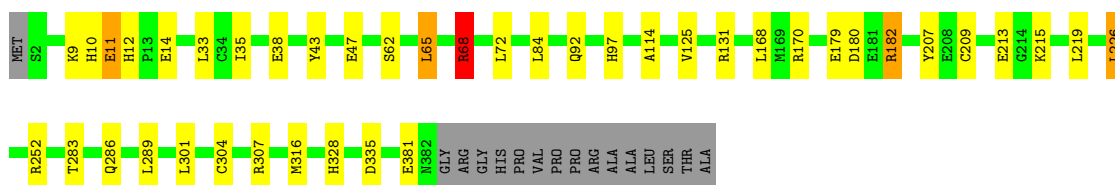
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	302	Total O 302 302	0	0
3	B	288	Total O 288 288	0	0
3	C	301	Total O 301 301	0	0
3	D	289	Total O 289 289	0	0
3	E	301	Total O 301 301	0	0
3	F	286	Total O 286 286	0	0

3 Residue-property plots

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.

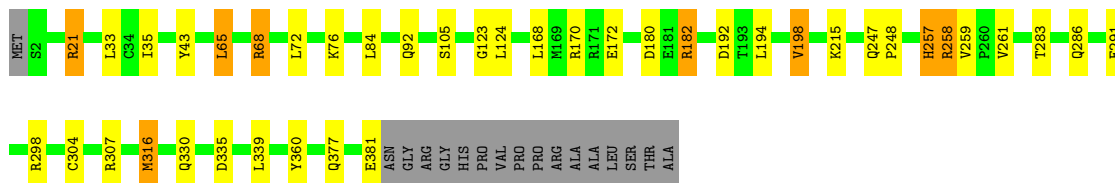
• Molecule 1: MANNOSYLGlycerate SYNTHASE

Chain A: 



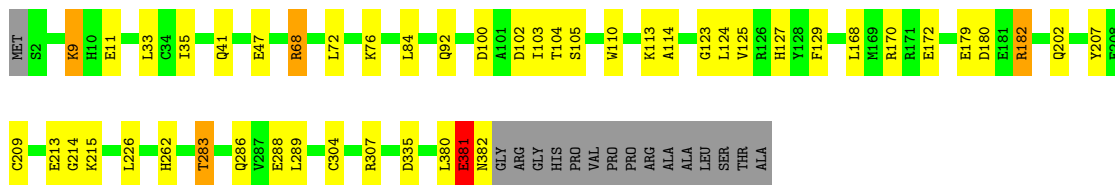
• Molecule 1: MANNOSYLGlycerate SYNTHASE

Chain B: 



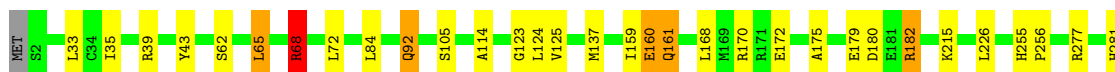
• Molecule 1: MANNOSYLGlycerate SYNTHASE

Chain C: 



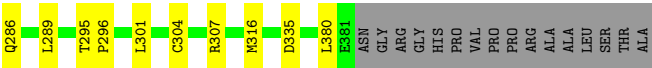
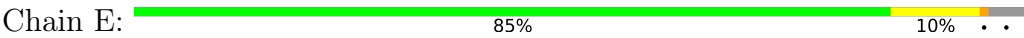
• Molecule 1: MANNOSYLGlycerate SYNTHASE

Chain D: 

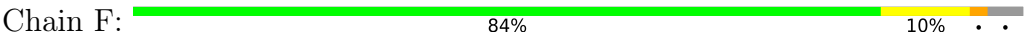




• Molecule 1: MANNOSYLGLYCERATE SYNTHASE



• Molecule 1: MANNOSYLGLYCERATE SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	261.15Å 151.29Å 153.24Å 90.00° 90.41° 90.00°	Depositor
Resolution (Å)	20.00 – 1.95 20.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	95.7 (20.00-1.95) 94.8 (20.00-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.176 , 0.192 0.187 , 0.202	Depositor DCC
R_{free} test set	20759 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.009 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.377 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.357 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.010 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	20669	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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: FLC

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	0.61	1/3229 (0.0%)	0.80	1/4394 (0.0%)
1	B	0.61	1/3228 (0.0%)	0.82	1/4392 (0.0%)
1	C	0.62	1/3229 (0.0%)	0.82	2/4394 (0.0%)
1	D	0.68	2/3228 (0.1%)	0.89	6/4392 (0.1%)
1	E	0.61	0/3228	0.82	1/4392 (0.0%)
1	F	0.61	1/3228 (0.0%)	0.89	6/4392 (0.1%)
All	All	0.62	6/19370 (0.0%)	0.84	17/26356 (0.1%)

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	A	1	0
1	B	1	0
1	E	1	0
1	F	1	0
All	All	4	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	137	MET	SD-CE	-17.03	1.36	1.79
1	A	381	GLU	C-N	-6.51	1.24	1.33
1	C	381	GLU	C-N	-6.14	1.24	1.33
1	B	316	MET	SD-CE	5.89	1.94	1.79
1	D	316	MET	SD-CE	5.85	1.94	1.79
1	F	160	GLU	C-N	-5.03	1.27	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	161	GLN	N-CA-CB	-16.08	90.33	111.40
1	D	160	GLU	N-CA-C	15.54	129.75	111.11
1	D	161	GLN	N-CA-CB	-14.96	91.80	111.40
1	F	160	GLU	N-CA-C	14.90	127.02	111.07
1	F	160	GLU	CA-C-N	-6.68	114.20	122.42
1	F	160	GLU	C-N-CA	-6.68	114.20	122.42
1	E	68	ARG	NE-CZ-NH2	6.42	124.98	119.20
1	F	161	GLN	N-CA-C	-6.26	94.85	108.81
1	F	68	ARG	NE-CZ-NH2	5.76	124.38	119.20
1	C	68	ARG	NE-CZ-NH2	5.69	124.32	119.20
1	D	161	GLN	N-CA-C	-5.58	96.37	108.81
1	D	68	ARG	NE-CZ-NH2	5.54	124.19	119.20
1	B	68	ARG	NE-CZ-NH2	5.46	124.11	119.20
1	A	68	ARG	NE-CZ-NH2	5.44	124.09	119.20
1	D	160	GLU	CA-C-N	-5.42	115.76	122.42
1	D	160	GLU	C-N-CA	-5.42	115.76	122.42
1	C	100	ASP	N-CA-CB	5.04	117.43	110.17

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	283	THR	CB
1	B	283	THR	CB
1	E	283	THR	CB
1	F	283	THR	CB

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	3138	0	3037	24	0
1	B	3137	0	3037	26	0
1	C	3138	0	3037	25	0
1	D	3137	0	3037	23	0
1	E	3137	0	3037	20	0
1	F	3137	0	3037	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	13	0	5	2	0
2	B	13	0	5	0	0
2	C	13	0	5	0	0
2	D	13	0	5	0	0
2	E	13	0	5	0	0
2	F	13	0	5	0	0
3	A	302	0	0	5	0
3	B	288	0	0	6	0
3	C	301	0	0	5	0
3	D	289	0	0	4	0
3	E	301	0	0	3	0
3	F	286	0	0	4	0
All	All	20669	0	18252	137	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (137) 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:D:283:THR:HG22	1:D:286:GLN:H	1.36	0.88
1:E:283:THR:HG21	1:E:335:ASP:OD2	1.81	0.81
1:F:316:MET:HE3	3:F:2236:HOH:O	1.82	0.79
1:E:316:MET:HA	1:E:316:MET:HE2	1.64	0.79
1:B:316:MET:HE3	3:B:2241:HOH:O	1.83	0.79
1:A:283:THR:HG21	1:A:335:ASP:OD2	1.84	0.78
1:B:283:THR:HG21	1:B:335:ASP:OD2	1.85	0.76
1:A:68:ARG:HD3	3:D:2160:HOH:O	1.85	0.75
1:D:316:MET:HE3	3:D:2242:HOH:O	1.89	0.72
1:D:283:THR:HG21	1:D:335:ASP:OD2	1.91	0.69
1:B:316:MET:HA	1:B:316:MET:HE2	1.75	0.69
1:B:283:THR:HG23	1:B:286:GLN:H	1.59	0.68
1:F:316:MET:HA	1:F:316:MET:HE2	1.74	0.68
1:F:76:LYS:NZ	1:F:192:ASP:OD2	2.27	0.68
1:C:283:THR:HG22	1:C:286:GLN:H	1.59	0.68
1:F:283:THR:HG21	1:F:335:ASP:OD2	1.95	0.67
1:D:175:ALA:O	1:D:179:GLU:HG2	1.94	0.66
1:D:316:MET:HA	1:D:316:MET:HE2	1.75	0.66
1:D:180:ASP:OD1	1:D:182:ARG:HD3	1.95	0.66
1:A:180:ASP:OD1	1:A:182:ARG:HD3	1.96	0.65
1:A:283:THR:HG23	1:A:286:GLN:H	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:GLU:CG	1:C:102:ASP:HB3	2.28	0.64
1:C:180:ASP:OD1	1:C:182:ARG:HD3	1.97	0.64
1:E:283:THR:HG23	1:E:286:GLN:H	1.63	0.63
1:E:180:ASP:OD1	1:E:182:ARG:HD3	1.97	0.63
1:B:123:GLY:HA2	1:B:170:ARG:CD	2.29	0.63
1:F:283:THR:HG23	1:F:286:GLN:H	1.64	0.63
1:B:180:ASP:OD1	1:B:182:ARG:HD3	1.99	0.63
1:C:11:GLU:HG2	1:C:102:ASP:HB3	1.81	0.62
1:F:123:GLY:HA2	1:F:170:ARG:CD	2.29	0.62
1:D:123:GLY:HA2	1:D:170:ARG:CD	2.29	0.62
1:D:43:TYR:CE2	1:D:65:LEU:HD13	2.34	0.62
1:F:123:GLY:HA2	1:F:170:ARG:HD3	1.82	0.61
1:B:123:GLY:HA2	1:B:170:ARG:HD3	1.83	0.60
1:A:226:LEU:HD11	2:A:1382:FLC:OA2	2.01	0.60
1:D:33:LEU:HD21	1:D:35:ILE:HD11	1.84	0.60
1:B:258:ARG:HG2	3:B:2188:HOH:O	2.03	0.58
1:A:38:GLU:HB2	1:D:68:ARG:HD2	1.86	0.58
1:F:180:ASP:OD1	1:F:182:ARG:HD3	2.04	0.58
1:C:283:THR:HG21	1:C:335:ASP:OD2	2.04	0.56
1:E:316:MET:HE3	3:E:2254:HOH:O	2.05	0.55
1:F:33:LEU:HD21	1:F:35:ILE:HD11	1.89	0.55
1:B:259:VAL:HG21	1:B:360:TYR:CE1	2.42	0.55
1:C:113:LYS:NZ	3:C:2087:HOH:O	2.37	0.54
1:B:43:TYR:CE2	1:B:65:LEU:HD13	2.43	0.54
1:F:43:TYR:CE2	1:F:65:LEU:HD13	2.43	0.54
1:B:330:GLN:NE2	3:B:2250:HOH:O	2.41	0.53
1:C:33:LEU:HD21	1:C:35:ILE:HD11	1.89	0.53
1:C:123:GLY:HA2	1:C:170:ARG:CD	2.39	0.53
1:C:283:THR:HG23	3:C:2231:HOH:O	2.08	0.53
1:E:316:MET:HA	1:E:316:MET:CE	2.36	0.53
1:E:9:LYS:HB2	3:E:2004:HOH:O	2.10	0.51
1:F:9:LYS:HE3	3:F:2006:HOH:O	2.09	0.51
1:D:123:GLY:HA2	1:D:170:ARG:HD3	1.92	0.51
1:F:194:LEU:O	1:F:198:VAL:HG13	2.11	0.51
1:B:76:LYS:NZ	1:B:192:ASP:OD2	2.42	0.50
1:A:43:TYR:CE2	1:A:65:LEU:HD13	2.46	0.50
1:C:381:GLU:HG2	1:C:382:ASN:N	2.26	0.50
1:D:168:LEU:C	1:D:168:LEU:HD23	2.37	0.50
3:B:2189:HOH:O	1:F:261:VAL:HG21	2.11	0.49
1:A:170:ARG:HD2	3:A:2088:HOH:O	2.11	0.49
1:A:304:CYS:HA	1:A:307:ARG:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:316:MET:HE1	1:F:377:GLN:NE2	2.27	0.49
1:B:168:LEU:C	1:B:168:LEU:HD23	2.37	0.49
1:B:33:LEU:HD21	1:B:35:ILE:HD11	1.94	0.48
1:B:194:LEU:O	1:B:198:VAL:HG13	2.13	0.48
1:C:207:TYR:HE2	1:C:209:CYS:HB3	1.78	0.48
1:C:11:GLU:HG3	1:C:102:ASP:HB3	1.95	0.48
1:E:170:ARG:HD2	3:E:2100:HOH:O	2.14	0.48
1:B:21:ARG:HD2	3:B:2029:HOH:O	2.14	0.47
1:D:316:MET:HE1	1:D:377:GLN:NE2	2.29	0.47
1:C:207:TYR:CE2	1:C:209:CYS:HB3	2.49	0.47
1:F:168:LEU:C	1:F:168:LEU:HD23	2.39	0.47
1:A:131:ARG:NH2	2:A:1382:FLC:OHB	2.48	0.47
1:C:123:GLY:HA2	1:C:170:ARG:HD3	1.96	0.47
1:B:259:VAL:HG21	1:B:360:TYR:HE1	1.78	0.47
1:A:97:HIS:CE1	1:A:168:LEU:HD12	2.50	0.47
1:B:247:GLN:N	1:B:248:PRO:CD	2.78	0.47
1:C:168:LEU:C	1:C:168:LEU:HD23	2.41	0.46
1:D:328:HIS:HD2	3:D:2079:HOH:O	1.98	0.46
1:E:210:TYR:CE2	1:E:212:PRO:HA	2.51	0.46
1:F:281:HIS:CD2	3:F:2207:HOH:O	2.68	0.46
1:C:213:GLU:OE2	1:C:262:HIS:CE1	2.69	0.46
1:D:255:HIS:HD2	1:D:256:PRO:O	1.99	0.46
1:A:62:SER:OG	3:A:2032:HOH:O	2.21	0.45
1:E:123:GLY:HA2	1:E:170:ARG:HD3	1.98	0.45
1:F:304:CYS:HA	1:F:307:ARG:O	2.15	0.45
1:A:33:LEU:HD21	1:A:35:ILE:HD11	1.98	0.45
1:C:129:PHE:CD1	1:C:214:GLY:HA3	2.51	0.45
1:F:255:HIS:HD2	1:F:256:PRO:O	1.99	0.45
1:A:207:TYR:HE2	1:A:209:CYS:HB3	1.81	0.44
1:B:283:THR:HG22	1:B:286:GLN:NE2	2.32	0.44
1:B:316:MET:HA	1:B:316:MET:CE	2.45	0.44
1:E:43:TYR:CE2	1:E:65:LEU:HD13	2.53	0.44
1:E:304:CYS:HA	1:E:307:ARG:O	2.18	0.44
1:C:182:ARG:HD2	3:C:2130:HOH:O	2.18	0.44
1:A:11:GLU:O	1:A:12:HIS:C	2.61	0.43
1:A:316:MET:HG2	3:A:2077:HOH:O	2.17	0.43
1:E:114:ALA:HA	1:E:125:VAL:HG11	1.99	0.43
1:A:252:ARG:HD3	3:F:2100:HOH:O	2.17	0.43
1:D:92:GLN:HG2	3:D:2055:HOH:O	2.18	0.43
1:D:304:CYS:HA	1:D:307:ARG:O	2.17	0.43
1:F:172:GLU:H	1:F:172:GLU:CD	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:THR:HG22	1:A:286:GLN:NE2	2.34	0.43
1:C:304:CYS:HA	1:C:307:ARG:O	2.18	0.43
1:F:247:GLN:N	1:F:248:PRO:CD	2.80	0.43
1:B:316:MET:HE1	1:B:377:GLN:NE2	2.33	0.43
1:D:114:ALA:HA	1:D:125:VAL:HG11	2.01	0.43
1:E:168:LEU:HD23	1:E:168:LEU:C	2.44	0.43
1:B:257:HIS:HD2	3:B:2188:HOH:O	2.02	0.43
1:E:103:ILE:HG21	1:E:110:TRP:CH2	2.54	0.43
1:C:213:GLU:OE2	1:C:262:HIS:NE2	2.52	0.42
1:A:328:HIS:HD2	3:A:2083:HOH:O	2.02	0.42
1:B:291:GLU:HA	1:B:298:ARG:HD3	2.00	0.42
1:C:103:ILE:HG21	1:C:110:TRP:CH2	2.55	0.42
1:A:207:TYR:CE2	1:A:209:CYS:HB3	2.55	0.42
1:B:283:THR:CG2	1:B:335:ASP:OD2	2.63	0.42
1:C:110:TRP:O	1:C:127:HIS:HE1	2.03	0.42
1:B:258:ARG:HD2	1:F:261:VAL:HG13	2.01	0.42
1:B:304:CYS:HA	1:B:307:ARG:O	2.19	0.42
1:F:316:MET:HA	1:F:316:MET:CE	2.47	0.41
1:A:114:ALA:HA	1:A:125:VAL:HG11	2.01	0.41
1:E:207:TYR:HE2	1:E:209:CYS:HB3	1.85	0.41
1:C:114:ALA:HA	1:C:125:VAL:HG11	2.03	0.41
1:D:362:TYR:O	1:D:365:GLN:HG3	2.20	0.41
1:A:38:GLU:OE1	1:D:68:ARG:HD3	2.20	0.41
1:A:38:GLU:OE1	1:D:68:ARG:CD	2.68	0.41
1:D:160:GLU:O	1:D:161:GLN:HG3	2.21	0.41
1:E:14:GLU:CD	1:E:14:GLU:H	2.29	0.41
1:E:182:ARG:HH21	1:E:243:GLU:CD	2.29	0.41
1:F:295:THR:HB	1:F:296:PRO:HD3	2.02	0.41
1:D:277:ARG:CZ	1:D:281:HIS:HD2	2.34	0.41
1:E:97:HIS:CE1	1:E:168:LEU:HD12	2.56	0.41
1:C:213:GLU:HG3	3:C:2158:HOH:O	2.21	0.40
1:C:76:LYS:NZ	3:C:2056:HOH:O	2.53	0.40
1:A:215:LYS:NZ	3:A:2301:HOH:O	2.54	0.40
1:E:295:THR:HB	1:E:296:PRO:HD3	2.04	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	379/397 (96%)	368 (97%)	9 (2%)	2 (0%)	24	16
1	B	378/397 (95%)	371 (98%)	7 (2%)	0	100	100
1	C	379/397 (96%)	366 (97%)	12 (3%)	1 (0%)	36	28
1	D	378/397 (95%)	370 (98%)	8 (2%)	0	100	100
1	E	378/397 (95%)	369 (98%)	9 (2%)	0	100	100
1	F	378/397 (95%)	369 (98%)	9 (2%)	0	100	100
All	All	2270/2382 (95%)	2213 (98%)	54 (2%)	3 (0%)	48	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	11	GLU
1	C	9	LYS

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	326/338 (96%)	311 (95%)	15 (5%)	24	13
1	B	326/338 (96%)	309 (95%)	17 (5%)	21	9
1	C	326/338 (96%)	305 (94%)	21 (6%)	16	6
1	D	326/338 (96%)	307 (94%)	19 (6%)	18	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	326/338 (96%)	310 (95%)	16 (5%)	22	11
1	F	326/338 (96%)	307 (94%)	19 (6%)	18	7
All	All	1956/2028 (96%)	1849 (94%)	107 (6%)	19	8

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	14	GLU
1	A	47	GLU
1	A	65	LEU
1	A	68	ARG
1	A	72	LEU
1	A	84	LEU
1	A	92	GLN
1	A	179	GLU
1	A	182	ARG
1	A	213	GLU
1	A	219	LEU
1	A	226	LEU
1	A	289	LEU
1	A	301	LEU
1	B	21	ARG
1	B	65	LEU
1	B	68	ARG
1	B	72	LEU
1	B	84	LEU
1	B	92	GLN
1	B	105	SER
1	B	124	LEU
1	B	172	GLU
1	B	182	ARG
1	B	198	VAL
1	B	215	LYS
1	B	257	HIS
1	B	258	ARG
1	B	261	VAL
1	B	339	LEU
1	B	381	GLU
1	C	9	LYS
1	C	41	GLN

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Mol	Chain	Res	Type
1	C	47	GLU
1	C	68	ARG
1	C	72	LEU
1	C	84	LEU
1	C	92	GLN
1	C	104	THR
1	C	105	SER
1	C	124	LEU
1	C	172	GLU
1	C	179	GLU
1	C	182	ARG
1	C	202	GLN
1	C	215	LYS
1	C	226	LEU
1	C	283	THR
1	C	288	GLU
1	C	289	LEU
1	C	380	LEU
1	C	381	GLU
1	D	39	ARG
1	D	62	SER
1	D	65	LEU
1	D	68	ARG
1	D	72	LEU
1	D	84	LEU
1	D	92	GLN
1	D	105	SER
1	D	124	LEU
1	D	159	ILE
1	D	172	GLU
1	D	182	ARG
1	D	215	LYS
1	D	226	LEU
1	D	283	THR
1	D	289	LEU
1	D	301	LEU
1	D	316	MET
1	D	339	LEU
1	E	47	GLU
1	E	65	LEU
1	E	68	ARG
1	E	84	LEU

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Mol	Chain	Res	Type
1	E	92	GLN
1	E	105	SER
1	E	109	ASP
1	E	124	LEU
1	E	179	GLU
1	E	182	ARG
1	E	202	GLN
1	E	219	LEU
1	E	258	ARG
1	E	289	LEU
1	E	301	LEU
1	E	380	LEU
1	F	9	LYS
1	F	21	ARG
1	F	62	SER
1	F	65	LEU
1	F	68	ARG
1	F	72	LEU
1	F	84	LEU
1	F	92	GLN
1	F	105	SER
1	F	109	ASP
1	F	124	LEU
1	F	172	GLU
1	F	179	GLU
1	F	182	ARG
1	F	198	VAL
1	F	215	LYS
1	F	257	HIS
1	F	301	LEU
1	F	339	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	66	GLN
1	A	81	ASN
1	A	153	HIS
1	A	202	GLN
1	A	257	HIS
1	A	377	GLN

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Mol	Chain	Res	Type
1	B	66	GLN
1	B	81	ASN
1	B	202	GLN
1	B	217	HIS
1	B	238	GLN
1	B	262	HIS
1	B	281	HIS
1	B	330	GLN
1	C	81	ASN
1	C	127	HIS
1	C	153	HIS
1	C	257	HIS
1	C	330	GLN
1	C	377	GLN
1	D	81	ASN
1	D	253	GLN
1	D	255	HIS
1	D	330	GLN
1	D	377	GLN
1	E	66	GLN
1	E	81	ASN
1	E	127	HIS
1	E	257	HIS
1	E	330	GLN
1	E	377	GLN
1	F	18	HIS
1	F	81	ASN
1	F	92	GLN
1	F	161	GLN
1	F	217	HIS
1	F	255	HIS
1	F	377	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FLC	E	1382	-	12,12,12	1.23	1 (8%)	17,17,17	1.20	3 (17%)
2	FLC	C	1382	-	12,12,12	1.09	1 (8%)	17,17,17	1.26	3 (17%)
2	FLC	A	1382	-	12,12,12	1.06	0	17,17,17	1.34	2 (11%)
2	FLC	B	1382	-	12,12,12	1.16	0	17,17,17	1.01	1 (5%)
2	FLC	D	1382	-	12,12,12	1.18	0	17,17,17	1.01	0
2	FLC	F	1382	-	12,12,12	1.12	0	17,17,17	1.04	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
2	FLC	E	1382	-	-	8/16/16/16	-
2	FLC	C	1382	-	-	2/16/16/16	-
2	FLC	A	1382	-	-	12/16/16/16	-
2	FLC	B	1382	-	-	2/16/16/16	-
2	FLC	D	1382	-	-	4/16/16/16	-
2	FLC	F	1382	-	-	4/16/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1382	FLC	OG2-CGC	-2.17	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1382	FLC	OG2-CGC	-2.12	1.23	1.30

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1382	FLC	OHB-CB-CA	-3.07	102.38	109.38
2	E	1382	FLC	OHB-CB-CBC	-2.40	105.56	108.96
2	E	1382	FLC	OA1-CAC-CA	-2.35	116.30	122.95
2	C	1382	FLC	OA1-CAC-CA	-2.28	116.50	122.95
2	C	1382	FLC	CA-CB-CBC	2.23	114.96	110.03
2	B	1382	FLC	OA1-CAC-CA	-2.12	116.94	122.95
2	E	1382	FLC	OA2-CAC-CA	2.03	120.77	114.35
2	A	1382	FLC	OG2-CGC-CG	2.02	120.75	114.35
2	C	1382	FLC	OA2-CAC-CA	2.01	120.72	114.35

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1382	FLC	CAC-CA-CB-CG
2	A	1382	FLC	CAC-CA-CB-OHB
2	A	1382	FLC	CG-CB-CBC-OB1
2	A	1382	FLC	CG-CB-CBC-OB2
2	A	1382	FLC	OHB-CB-CBC-OB1
2	A	1382	FLC	OHB-CB-CBC-OB2
2	A	1382	FLC	CAC-CA-CB-CBC
2	E	1382	FLC	CB-CA-CAC-OA2
2	E	1382	FLC	CB-CA-CAC-OA1
2	A	1382	FLC	CA-CB-CG-CGC
2	C	1382	FLC	CB-CA-CAC-OA2
2	E	1382	FLC	CG-CB-CBC-OB1
2	C	1382	FLC	CB-CA-CAC-OA1
2	A	1382	FLC	CBC-CB-CG-CGC
2	A	1382	FLC	OHB-CB-CG-CGC
2	B	1382	FLC	CB-CA-CAC-OA2
2	E	1382	FLC	CA-CB-CBC-OB1
2	E	1382	FLC	CA-CB-CBC-OB2
2	E	1382	FLC	CG-CB-CBC-OB2
2	F	1382	FLC	CG-CB-CBC-OB1
2	F	1382	FLC	CG-CB-CBC-OB2
2	B	1382	FLC	CB-CA-CAC-OA1
2	F	1382	FLC	CB-CA-CAC-OA2

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Mol	Chain	Res	Type	Atoms
2	D	1382	FLC	CG-CB-CBC-OB1
2	D	1382	FLC	CG-CB-CBC-OB2
2	D	1382	FLC	CB-CA-CAC-OA2
2	F	1382	FLC	CB-CA-CAC-OA1
2	D	1382	FLC	CB-CA-CAC-OA1
2	E	1382	FLC	OHB-CB-CBC-OB1
2	E	1382	FLC	OHB-CB-CBC-OB2
2	A	1382	FLC	CB-CG-CGC-OG1
2	A	1382	FLC	CB-CG-CGC-OG2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1382	FLC	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	381/397 (95%)	-1.38	0 100 100	14, 19, 28, 42	0
1	B	380/397 (95%)	-1.39	0 100 100	14, 19, 27, 39	0
1	C	381/397 (95%)	-1.38	0 100 100	14, 19, 28, 42	0
1	D	380/397 (95%)	-1.40	0 100 100	14, 19, 27, 39	0
1	E	380/397 (95%)	-1.40	0 100 100	14, 19, 28, 44	0
1	F	380/397 (95%)	-1.42	0 100 100	14, 18, 27, 39	0
All	All	2282/2382 (95%)	-1.39	0 100 100	14, 19, 28, 44	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FLC	B	1382	13/13	0.98	0.05	30,37,41,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FLC	A	1382	13/13	0.99	0.04	29,38,47,51	0
2	FLC	C	1382	13/13	0.99	0.04	26,34,40,41	0
2	FLC	D	1382	13/13	0.99	0.04	29,35,40,41	0
2	FLC	E	1382	13/13	0.99	0.04	26,34,41,42	0
2	FLC	F	1382	13/13	0.99	0.04	30,36,40,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.