



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:43 PM UTC

PDB ID : 2WVK / pdb_00002wvk
Title : Mannosyl-3-phosphoglycerate synthase from *Thermus thermophilus* HB27 apoprotein
Authors : Goncalves, S.; Borges, N.; Esteves, A.M.; Victor, B.; Soares, C.M.; Santos, H.; Matias, P.M.
Deposited on : 2009-10-19
Resolution : 2.97 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

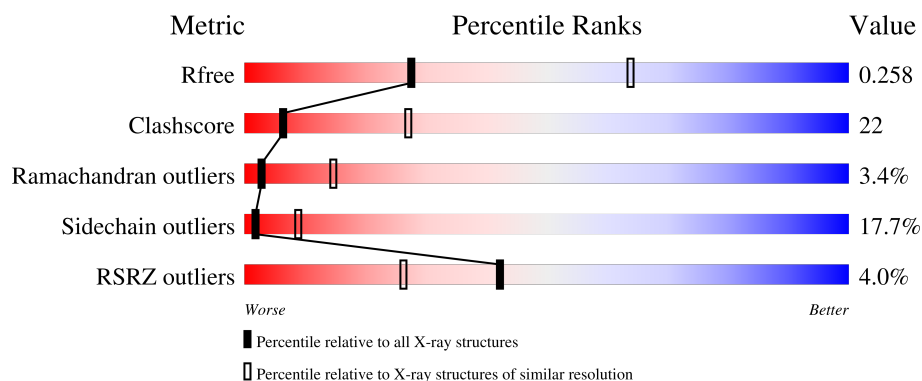
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	391	7% 51% 38% 10% .
1	B	391	% 50% 37% 10% ..

2 Entry composition [i](#)

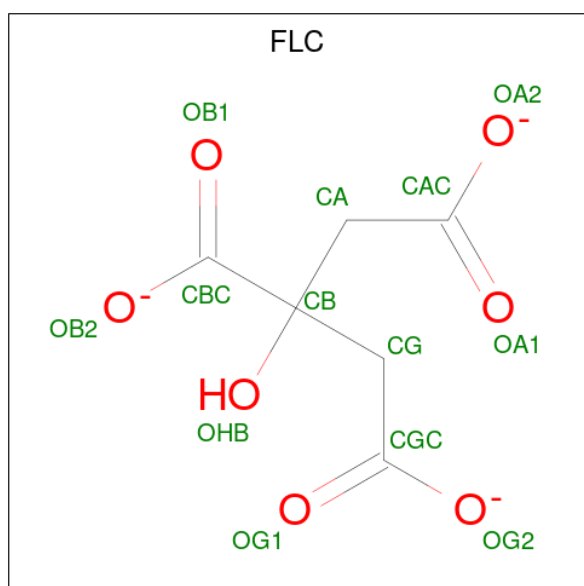
There are 4 unique types of molecules in this entry. The entry contains 6168 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MANNOSYL-3-PHOSPHOGLYCERATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			3077	1952	552	565	8			
1	B	382	Total	C	N	O	S	0	0	0
			2999	1902	541	548	8			

- 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	0	0
			13	6	7		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total 3	Zn 3	0	0

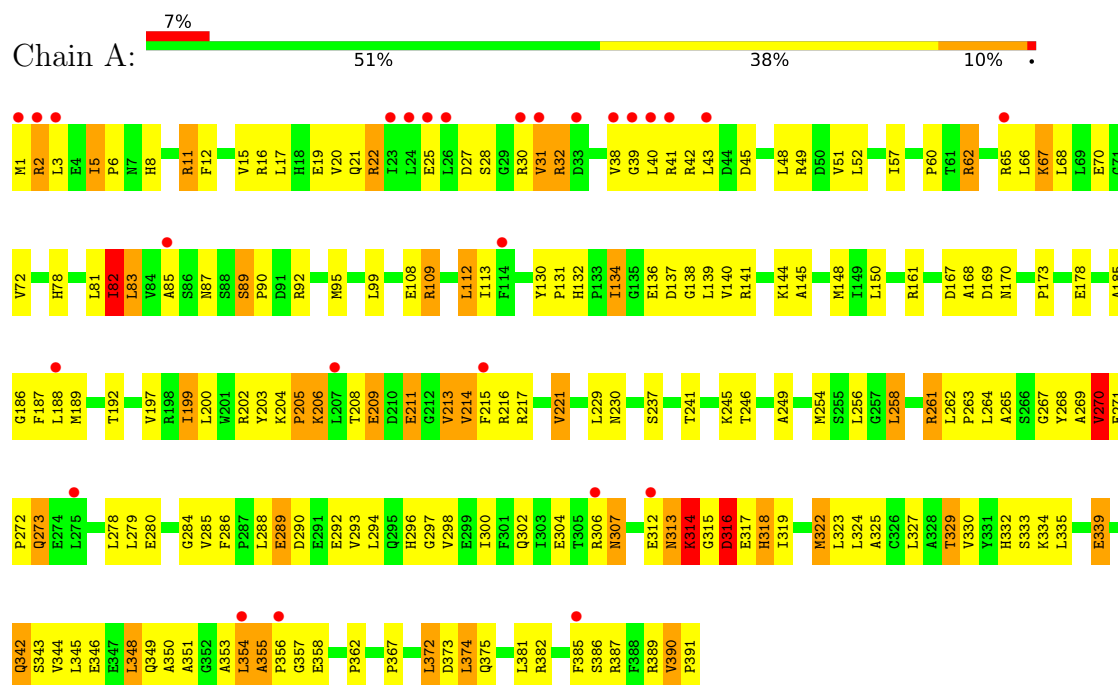
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	45	Total 45	O 45	0	0
4	B	29	Total 29	O 29	0	0

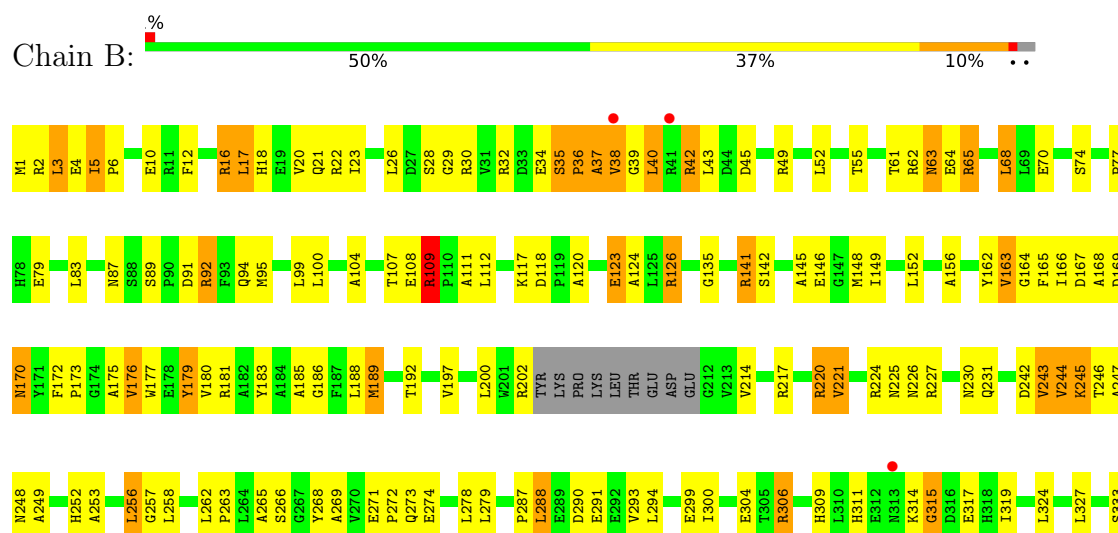
3 Residue-property plots

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: MANNOSYL-3-PHOSPHOGLYCERATE SYNTHASE



• Molecule 1: MANNOSYL-3-PHOSPHOGLYCERATE SYNTHASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	113.46Å 113.46Å 195.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.91 – 2.97 42.91 – 2.97	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.91-2.97) 98.9 (42.91-2.97)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.198 , 0.266 0.193 , 0.258	Depositor DCC
R_{free} test set	1358 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	98.3	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 99.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6168	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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: ZN, 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	0.93	0/3143	1.15	11/4261 (0.3%)
1	B	0.93	1/3062 (0.0%)	1.17	11/4150 (0.3%)
All	All	0.93	1/6205 (0.0%)	1.16	22/8411 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	38	VAL	CA-CB	6.02	1.62	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	HIS	CA-C-N	-10.56	108.27	121.04
1	A	132	HIS	C-N-CA	-10.56	108.27	121.04
1	A	199	ILE	CB-CA-C	-7.11	101.09	111.68
1	B	390	VAL	N-CA-C	6.67	114.16	107.55
1	A	270	VAL	CB-CA-C	-6.62	100.42	111.29
1	B	245	LYS	N-CA-C	-6.47	103.39	113.02
1	B	109	ARG	N-CA-C	6.34	118.51	108.23
1	B	5	ILE	CA-C-N	-6.11	113.48	119.90
1	B	5	ILE	C-N-CA	-6.11	113.48	119.90
1	B	269	ALA	N-CA-C	-5.90	107.31	114.75
1	A	82	ILE	CB-CA-C	-5.85	101.69	111.29
1	A	314	LYS	N-CA-C	5.79	115.15	108.49
1	B	231	GLN	N-CA-C	-5.51	104.91	111.69
1	B	87	ASN	N-CA-C	-5.51	104.81	112.03
1	B	35	SER	CA-C-N	5.45	126.65	119.84
1	B	35	SER	C-N-CA	5.45	126.65	119.84
1	A	353	ALA	N-CA-C	-5.30	105.09	112.03
1	A	262	LEU	CA-C-N	5.25	125.25	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	LEU	C-N-CA	5.25	125.25	120.21
1	B	189	MET	N-CA-C	-5.24	107.06	113.50
1	A	307	ASN	CA-C-N	5.11	125.02	119.76
1	A	307	ASN	C-N-CA	5.11	125.02	119.76

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3077	0	3084	140	0
1	B	2999	0	3007	134	0
2	A	13	0	5	0	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
4	A	45	0	0	8	0
4	B	29	0	0	4	0
All	All	6168	0	6096	267	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 22.

All (267) 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:314:LYS:HG2	1:B:315:GLY:H	1.13	1.07
1:A:313:ASN:HB2	1:A:318:HIS:HE1	1.15	1.05
1:A:268:TYR:HA	4:A:2021:HOH:O	1.60	1.01
1:B:34:GLU:HB3	1:B:36:PRO:HD3	1.40	1.01
1:A:313:ASN:HB2	1:A:318:HIS:CE1	1.94	1.01
1:A:5:ILE:HD11	1:A:41:ARG:HD3	1.44	0.99
1:A:169:ASP:HA	4:A:2026:HOH:O	1.64	0.97
1:B:224:ARG:NH2	1:B:347:GLU:HG3	1.80	0.96
1:B:126:ARG:HH11	1:B:126:ARG:HG2	1.29	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ARG:HH21	1:B:29:GLY:HA2	1.35	0.91
1:A:22:ARG:HG2	1:A:22:ARG:HH21	1.34	0.89
1:A:65:ARG:HD3	1:A:67:LYS:HD3	1.58	0.86
1:A:49:ARG:NH2	1:B:29:GLY:HA2	1.89	0.86
1:B:226:ASN:HD21	1:B:247:ALA:H	1.25	0.84
1:B:64:GLU:O	1:B:92:ARG:NH1	2.09	0.84
1:A:214:VAL:HG13	1:A:314:LYS:HD3	1.61	0.82
1:A:356:PRO:HD2	1:A:357:GLY:HA3	1.59	0.82
1:B:126:ARG:HG2	1:B:126:ARG:NH1	1.93	0.81
1:A:81:LEU:O	1:A:82:ILE:HB	1.77	0.81
1:B:314:LYS:HG2	1:B:315:GLY:N	1.96	0.81
1:B:34:GLU:CB	1:B:36:PRO:HD3	2.12	0.80
1:A:3:LEU:HD22	1:A:189:MET:HE1	1.63	0.80
1:A:289:GLU:HA	1:A:289:GLU:OE1	1.79	0.79
1:B:224:ARG:HH21	1:B:347:GLU:HG3	1.43	0.79
1:A:214:VAL:CG1	1:A:314:LYS:HD3	2.13	0.78
1:A:271:GLU:HB2	1:A:272:PRO:HD3	1.66	0.77
1:A:6:PRO:HD3	1:A:21:GLN:NE2	1.99	0.77
1:A:11:ARG:HG2	1:A:16:ARG:CZ	2.15	0.77
1:A:11:ARG:HG2	1:A:16:ARG:NH1	2.01	0.76
1:A:148:MET:CE	1:A:264:LEU:HD22	2.15	0.76
1:B:109:ARG:HD3	4:B:2010:HOH:O	1.84	0.75
1:A:43:LEU:HD22	1:A:188:LEU:HD23	1.68	0.74
1:B:45:ASP:O	1:B:49:ARG:HG3	1.88	0.74
1:B:5:ILE:HD11	1:B:38:VAL:O	1.88	0.73
1:B:226:ASN:ND2	1:B:247:ALA:H	1.85	0.73
1:A:372:LEU:HD23	1:A:374:LEU:HD22	1.70	0.72
1:A:68:LEU:HD13	4:A:2026:HOH:O	1.90	0.71
1:B:124:ALA:HB2	1:B:381:LEU:HD13	1.73	0.70
1:A:356:PRO:CD	1:A:357:GLY:HA3	2.21	0.70
1:B:353:ALA:O	1:B:354:LEU:HB2	1.91	0.70
1:A:5:ILE:HB	1:A:39:GLY:O	1.92	0.70
1:A:245:LYS:H	1:A:302:GLN:HE22	1.38	0.70
1:B:170:ASN:HD22	1:B:172:PHE:H	1.39	0.70
1:A:22:ARG:HH21	1:A:22:ARG:CG	2.04	0.70
1:A:316:ASP:N	1:A:316:ASP:OD1	2.22	0.70
1:B:265:ALA:HB2	1:B:273:GLN:HG2	1.73	0.69
1:B:5:ILE:CD1	1:B:38:VAL:O	2.41	0.69
1:A:354:LEU:O	1:A:355:ALA:O	2.12	0.68
1:B:28:SER:O	1:B:42:ARG:NH1	2.26	0.68
1:B:164:GLY:HA2	1:B:253:ALA:HA	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:HIS:HA	1:A:109:ARG:NH1	2.09	0.67
1:B:230:ASN:ND2	1:B:243:VAL:O	2.28	0.67
1:A:372:LEU:CD2	1:A:374:LEU:HD22	2.26	0.66
1:A:168:ALA:O	4:A:2026:HOH:O	2.12	0.66
1:A:205:PRO:O	1:A:206:LYS:HB3	1.95	0.66
1:B:124:ALA:HB2	1:B:381:LEU:CD1	2.26	0.66
1:B:314:LYS:CG	1:B:315:GLY:H	1.98	0.66
1:B:352:GLY:O	1:B:354:LEU:N	2.29	0.65
1:A:81:LEU:O	1:A:82:ILE:CB	2.44	0.65
1:B:4:GLU:O	1:B:21:GLN:HG2	1.95	0.65
1:A:12:PHE:CD2	1:A:279:LEU:HD22	2.33	0.64
1:B:224:ARG:HD3	1:B:347:GLU:CD	2.23	0.64
1:B:327:LEU:HB3	1:B:344:VAL:HG13	1.78	0.64
1:A:8:HIS:HB2	1:A:19:GLU:CD	2.23	0.63
1:A:144:LYS:HD2	1:A:270:VAL:HG21	1.80	0.63
1:A:148:MET:HE1	1:A:264:LEU:HD22	1.81	0.63
1:A:214:VAL:HG22	1:A:314:LYS:HG2	1.79	0.63
1:B:109:ARG:CD	4:B:2010:HOH:O	2.43	0.63
1:B:376:ALA:O	1:B:379:LYS:HB3	1.99	0.62
1:A:375:GLN:HB3	4:A:2042:HOH:O	1.99	0.62
1:B:35:SER:O	1:B:37:ALA:N	2.33	0.62
1:B:220:ARG:HD3	1:B:221:VAL:N	2.14	0.62
1:B:62:ARG:O	1:B:63:ASN:HB2	1.99	0.61
1:B:163:VAL:HG12	1:B:256:LEU:CD2	2.30	0.61
1:A:83:LEU:HD22	1:A:112:LEU:HD12	1.84	0.60
1:A:92:ARG:HA	1:A:95:MET:HE2	1.83	0.59
1:A:92:ARG:HG2	1:A:95:MET:HE2	1.84	0.59
1:B:17:LEU:HD22	1:B:300:ILE:HD12	1.85	0.59
1:B:91:ASP:O	1:B:95:MET:HG3	2.02	0.59
1:A:349:GLN:HE22	1:A:356:PRO:C	2.11	0.59
1:B:145:ALA:HB2	1:B:266:SER:HA	1.84	0.59
1:B:5:ILE:HG23	1:B:6:PRO:HD2	1.85	0.59
1:A:292:GLU:O	1:A:296:HIS:HD2	1.86	0.59
1:B:294:LEU:HD23	1:B:294:LEU:O	2.03	0.59
1:B:126:ARG:HH11	1:B:126:ARG:CG	2.09	0.58
1:B:167:ASP:OD1	1:B:169:ASP:HB2	2.04	0.58
1:B:77:PRO:HD2	1:B:180:VAL:HG11	1.85	0.58
1:A:27:ASP:OD1	1:B:49:ARG:NH2	2.36	0.58
1:B:370:SER:C	1:B:372:LEU:H	2.11	0.58
1:B:20:VAL:HG11	1:B:202:ARG:NH2	2.20	0.57
1:B:263:PRO:HB2	1:B:365:LEU:HD23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:GLU:HB2	1:A:272:PRO:CD	2.35	0.57
1:A:306:ARG:HB3	1:B:173:PRO:HG2	1.86	0.57
1:B:258:LEU:HD11	1:B:278:LEU:HD21	1.86	0.57
1:A:327:LEU:HD22	1:A:348:LEU:CD2	2.35	0.57
1:B:170:ASN:ND2	1:B:172:PHE:H	2.02	0.56
1:A:131:PRO:O	1:A:134:ILE:HG12	2.06	0.56
1:A:31:VAL:HG12	1:A:42:ARG:NE	2.21	0.55
1:A:51:VAL:HG21	1:A:188:LEU:CD1	2.36	0.55
1:A:325:ALA:O	1:A:329:THR:HG23	2.05	0.55
1:A:385:PHE:O	1:A:389:ARG:HB2	2.06	0.55
1:A:51:VAL:HG21	1:A:188:LEU:HD13	1.89	0.55
1:A:145:ALA:HB2	1:A:265:ALA:O	2.07	0.55
1:A:230:ASN:HB3	1:A:241:THR:HG23	1.89	0.54
1:A:245:LYS:H	1:A:302:GLN:NE2	2.05	0.54
1:B:186:GLY:HA3	1:B:197:VAL:HG21	1.87	0.54
1:B:355:ALA:HB3	1:B:357:GLY:O	2.08	0.54
1:B:5:ILE:CG2	1:B:6:PRO:HD2	2.38	0.54
1:A:22:ARG:CG	1:A:22:ARG:NH2	2.70	0.54
1:A:66:LEU:HD11	1:A:95:MET:HE3	1.89	0.53
1:A:178:GLU:OE1	1:A:307:ASN:ND2	2.40	0.53
1:B:167:ASP:OD1	1:B:169:ASP:CB	2.57	0.53
1:B:246:THR:HB	1:B:249:ALA:HB2	1.89	0.53
1:B:3:LEU:HB3	1:B:23:ILE:HA	1.91	0.52
1:B:165:PHE:N	1:B:165:PHE:CD2	2.78	0.52
1:B:177:TRP:CZ2	1:B:181:ARG:CD	2.93	0.52
1:B:175:ALA:O	1:B:176:VAL:C	2.52	0.52
1:A:2:ARG:HD2	1:A:25:GLU:OE1	2.10	0.52
1:A:45:ASP:O	1:A:49:ARG:HG3	2.09	0.52
1:B:104:ALA:HB1	1:B:109:ARG:O	2.10	0.52
1:B:65:ARG:HB3	1:B:68:LEU:HB2	1.92	0.52
1:B:220:ARG:HD3	1:B:220:ARG:C	2.35	0.52
1:B:177:TRP:CZ2	1:B:181:ARG:HD3	2.46	0.51
1:A:67:LYS:H	1:A:67:LYS:HD2	1.75	0.51
1:A:108:GLU:HB3	4:A:2016:HOH:O	2.10	0.51
1:A:137:ASP:OD1	1:A:137:ASP:N	2.42	0.51
1:A:323:LEU:HD22	1:A:327:LEU:HD13	1.92	0.51
1:B:186:GLY:HA3	1:B:197:VAL:CG2	2.40	0.51
1:B:179:TYR:N	1:B:179:TYR:CD2	2.79	0.50
1:A:173:PRO:HG2	1:B:306:ARG:HB3	1.93	0.50
1:B:349:GLN:HE22	1:B:357:GLY:HA2	1.75	0.50
1:A:258:LEU:HD21	1:A:278:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:PHE:CD2	1:B:279:LEU:HD22	2.46	0.50
1:A:199:ILE:HG22	1:A:200:LEU:N	2.26	0.50
1:B:288:LEU:HD12	1:B:288:LEU:C	2.36	0.50
1:B:22:ARG:HD2	4:B:2001:HOH:O	2.12	0.50
1:B:372:LEU:HG	1:B:373:ASP:N	2.26	0.50
1:A:214:VAL:HG11	1:A:314:LYS:HD3	1.92	0.50
1:B:179:TYR:N	1:B:179:TYR:HD2	2.11	0.49
1:A:136:GLU:C	1:A:138:GLY:H	2.20	0.49
1:A:332:HIS:CD2	1:A:362:PRO:HA	2.47	0.49
1:A:167:ASP:OD1	1:A:169:ASP:HB3	2.12	0.49
1:A:211:GLU:O	1:A:215:PHE:HB3	2.11	0.49
1:B:34:GLU:HB3	1:B:36:PRO:CD	2.28	0.49
1:A:199:ILE:CG2	1:A:200:LEU:N	2.76	0.49
1:A:99:LEU:HD23	1:A:99:LEU:C	2.38	0.49
1:A:280:GLU:OE1	1:A:334:LYS:HD3	2.12	0.49
1:A:206:LYS:HG2	1:A:209:GLU:HB3	1.93	0.49
1:A:202:ARG:HG2	1:A:304:GLU:OE2	2.14	0.48
1:B:225:ASN:HD22	1:B:248:ASN:HD21	1.59	0.48
1:B:363:PRO:HB2	1:B:365:LEU:HD12	1.95	0.48
1:A:16:ARG:N	1:A:298:VAL:O	2.45	0.48
1:B:123:GLU:O	1:B:126:ARG:HB2	2.14	0.48
1:A:293:VAL:O	1:A:297:GLY:N	2.44	0.48
1:A:43:LEU:HD13	1:A:185:ALA:HA	1.95	0.48
1:A:221:VAL:HG11	1:A:319:ILE:HG23	1.95	0.48
1:B:52:LEU:HD23	1:B:52:LEU:HA	1.76	0.48
1:A:263:PRO:C	1:A:264:LEU:HG	2.38	0.48
1:A:51:VAL:CG2	1:A:188:LEU:CD1	2.92	0.48
1:A:246:THR:HB	1:A:249:ALA:HB2	1.95	0.48
1:B:163:VAL:HG12	1:B:256:LEU:HD23	1.94	0.48
1:A:313:ASN:CB	1:A:318:HIS:HE1	2.05	0.48
1:A:217:ARG:O	1:A:221:VAL:HG12	2.13	0.47
1:A:62:ARG:HG3	1:A:87:ASN:O	2.15	0.47
1:A:346:GLU:O	1:A:350:ALA:HB3	2.13	0.47
1:B:200:LEU:HB3	1:B:246:THR:HG22	1.96	0.47
1:B:290:ASP:HB3	1:B:293:VAL:HB	1.96	0.47
1:B:333:SER:C	1:B:335:LEU:H	2.22	0.47
1:A:45:ASP:O	1:A:48:LEU:HB2	2.14	0.47
1:A:67:LYS:H	1:A:67:LYS:CD	2.27	0.47
1:B:5:ILE:HD12	1:B:38:VAL:O	2.15	0.47
1:A:267:GLY:O	1:A:270:VAL:HG22	2.15	0.47
1:A:284:GLY:C	1:A:286:PHE:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:ARG:CD	4:B:2001:HOH:O	2.63	0.47
1:B:83:LEU:HD23	1:B:112:LEU:HB2	1.98	0.46
1:B:271:GLU:HB2	1:B:272:PRO:HD3	1.95	0.46
1:B:384:HIS:O	1:B:386:SER:N	2.48	0.46
1:A:72:VAL:HG21	1:A:168:ALA:HA	1.98	0.46
1:A:186:GLY:HA3	1:A:197:VAL:HG21	1.97	0.46
1:A:211:GLU:OE2	1:A:216:ARG:NH1	2.49	0.46
1:A:278:LEU:HD13	1:A:300:ILE:HD11	1.98	0.46
1:B:384:HIS:O	1:B:385:PHE:C	2.57	0.46
1:A:285:VAL:HG12	1:A:285:VAL:O	2.16	0.45
1:A:390:VAL:HA	1:A:391:PRO:HD2	1.70	0.45
1:B:3:LEU:N	1:B:3:LEU:HD23	2.32	0.45
1:B:37:ALA:O	1:B:39:GLY:N	2.49	0.45
1:A:322:MET:HE2	1:A:322:MET:HB3	1.80	0.45
1:A:355:ALA:HB1	1:A:356:PRO:HA	1.98	0.45
1:B:100:LEU:HD11	1:B:111:ALA:CB	2.46	0.45
1:A:205:PRO:O	1:A:206:LYS:CB	2.62	0.45
1:B:185:ALA:O	1:B:189:MET:HG3	2.17	0.45
1:A:354:LEU:C	1:A:358:GLU:HG3	2.42	0.45
1:A:292:GLU:O	1:A:296:HIS:CD2	2.67	0.44
1:B:68:LEU:HD13	1:B:168:ALA:O	2.17	0.44
1:B:243:VAL:O	1:B:244:VAL:HB	2.17	0.44
1:A:5:ILE:HD11	1:A:41:ARG:CD	2.31	0.44
1:A:199:ILE:HD13	1:A:199:ILE:HG21	1.67	0.44
1:B:242:ASP:C	1:B:242:ASP:OD1	2.58	0.44
1:B:55:THR:HA	1:B:162:TYR:O	2.18	0.44
1:A:269:ALA:HB1	1:A:329:THR:HG21	2.00	0.44
1:B:183:TYR:CG	1:B:253:ALA:HB2	2.52	0.44
1:A:333:SER:C	1:A:335:LEU:H	2.26	0.44
1:B:18:HIS:HE1	1:B:299:GLU:OE1	2.01	0.44
1:A:49:ARG:HD3	1:B:30:ARG:HD3	2.00	0.44
1:B:10:GLU:HB3	1:B:17:LEU:HB2	1.99	0.44
1:B:146:GLU:HA	1:B:149:ILE:HD12	1.99	0.44
1:B:64:GLU:O	1:B:65:ARG:C	2.59	0.43
1:B:135:GLY:HA2	1:B:141:ARG:NH1	2.32	0.43
1:B:177:TRP:CH2	1:B:181:ARG:HD3	2.52	0.43
1:B:243:VAL:HG13	1:B:244:VAL:HG23	2.00	0.43
1:A:60:PRO:HA	1:A:85:ALA:O	2.18	0.43
1:A:134:ILE:HG12	1:A:134:ILE:H	1.69	0.43
1:A:1:MET:H2	1:A:28:SER:HG	1.61	0.43
1:A:261:ARG:HD3	1:A:290:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:HIS:HB3	1:B:311:HIS:CD2	2.53	0.43
1:A:256:LEU:HD12	1:A:256:LEU:HA	1.83	0.43
1:B:16:ARG:HD2	1:B:16:ARG:N	2.34	0.43
1:A:89:SER:O	1:A:90:PRO:C	2.62	0.43
1:A:314:LYS:HB3	1:A:315:GLY:H	1.68	0.43
1:A:349:GLN:NE2	1:A:356:PRO:O	2.51	0.43
1:B:1:MET:N	1:B:28:SER:H	2.15	0.43
1:A:5:ILE:O	1:A:5:ILE:HG22	2.19	0.43
1:B:252:HIS:NE2	1:B:274:GLU:OE2	2.51	0.43
1:A:187:PHE:HZ	1:A:254:MET:N	2.17	0.43
1:A:342:GLN:HE21	1:A:343:SER:N	2.17	0.42
1:A:30:ARG:O	1:A:32:ARG:HD2	2.20	0.42
1:B:363:PRO:HB2	1:B:365:LEU:CD1	2.50	0.42
1:A:20:VAL:HA	1:A:302:GLN:O	2.18	0.42
1:B:148:MET:O	1:B:152:LEU:HG	2.19	0.42
1:B:20:VAL:HG23	1:B:245:LYS:HG3	2.01	0.42
1:B:390:VAL:HA	1:B:391:PRO:HD2	1.87	0.42
1:B:120:ALA:CB	1:B:387:ARG:HH22	2.32	0.42
1:B:141:ARG:H	1:B:141:ARG:HG2	1.66	0.42
1:A:2:ARG:HD3	1:B:107:THR:HA	2.01	0.42
1:B:271:GLU:N	1:B:272:PRO:CD	2.83	0.42
1:B:359:GLU:HA	1:B:360:PRO:HD2	1.81	0.42
1:A:20:VAL:HG11	1:A:202:ARG:HH21	1.84	0.42
1:A:339:GLU:CD	1:A:339:GLU:H	2.26	0.42
1:B:118:ASP:C	1:B:118:ASP:OD1	2.62	0.42
1:B:2:ARG:HG2	1:B:40:LEU:HD13	2.02	0.42
1:B:266:SER:OG	1:B:364:VAL:HG23	2.19	0.41
1:A:11:ARG:CG	1:A:16:ARG:CZ	2.94	0.41
1:A:208:THR:HG22	1:A:208:THR:O	2.20	0.41
1:B:1:MET:HG2	1:B:3:LEU:HD22	2.02	0.41
1:B:202:ARG:HB2	1:B:304:GLU:OE1	2.21	0.41
1:A:161:ARG:HE	1:A:161:ARG:HB3	1.47	0.41
1:A:265:ALA:HB2	1:A:273:GLN:HG3	2.01	0.41
1:B:148:MET:HG2	1:B:165:PHE:CE1	2.56	0.41
1:B:120:ALA:HB3	1:B:387:ARG:HH22	1.85	0.41
1:B:271:GLU:N	1:B:271:GLU:OE1	2.39	0.41
1:A:43:LEU:HD23	1:A:43:LEU:HA	1.65	0.41
1:A:327:LEU:HD22	1:A:348:LEU:HD21	2.01	0.41
1:B:124:ALA:HB1	1:B:377:VAL:HG13	2.03	0.41
1:A:170:ASN:ND2	4:A:2027:HOH:O	2.48	0.41
1:A:30:ARG:HG2	4:A:2009:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LEU:HD23	1:A:150:LEU:HA	1.87	0.41
1:B:256:LEU:HD22	1:B:256:LEU:HA	1.76	0.41
1:B:256:LEU:O	1:B:257:GLY:C	2.64	0.40
1:A:15:VAL:O	1:A:16:ARG:HD2	2.22	0.40
1:A:130:TYR:OH	1:A:367:PRO:O	2.33	0.40
1:A:52:LEU:HD23	1:A:52:LEU:HA	1.95	0.40
1:A:136:GLU:C	1:A:138:GLY:N	2.79	0.40
1:B:156:ALA:HB1	1:B:374:LEU:HD21	2.03	0.40
1:B:163:VAL:CG1	1:B:256:LEU:CD2	2.99	0.40
1:B:290:ASP:O	1:B:291:GLU:C	2.64	0.40
1:B:370:SER:O	1:B:372:LEU:N	2.52	0.40
1:B:342:GLN:HA	1:B:342:GLN:HE21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	389/391 (100%)	334 (86%)	41 (10%)	14 (4%)	2	14
1	B	378/391 (97%)	320 (85%)	46 (12%)	12 (3%)	3	16
All	All	767/782 (98%)	654 (85%)	87 (11%)	26 (3%)	3	15

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	ASP
1	A	355	ALA
1	B	351	ALA
1	B	353	ALA
1	A	206	LYS
1	A	213	VAL

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Mol	Chain	Res	Type
1	B	36	PRO
1	B	37	ALA
1	B	315	GLY
1	B	354	LEU
1	B	371	SER
1	A	270	VAL
1	A	317	GLU
1	A	318	HIS
1	A	82	ILE
1	A	140	VAL
1	A	205	PRO
1	B	287	PRO
1	A	351	ALA
1	A	382	ARG
1	B	176	VAL
1	B	244	VAL
1	A	373	ASP
1	B	63	ASN
1	B	355	ALA
1	A	214	VAL

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	323/323 (100%)	266 (82%)	57 (18%)	2	9
1	B	314/323 (97%)	258 (82%)	56 (18%)	2	9
All	All	637/646 (99%)	524 (82%)	113 (18%)	2	9

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	5	ILE
1	A	11	ARG

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Mol	Chain	Res	Type
1	A	17	LEU
1	A	22	ARG
1	A	31	VAL
1	A	32	ARG
1	A	38	VAL
1	A	40	LEU
1	A	57	ILE
1	A	62	ARG
1	A	67	LYS
1	A	70	GLU
1	A	83	LEU
1	A	89	SER
1	A	109	ARG
1	A	112	LEU
1	A	113	ILE
1	A	134	ILE
1	A	139	LEU
1	A	141	ARG
1	A	192	THR
1	A	203	TYR
1	A	204	LYS
1	A	209	GLU
1	A	211	GLU
1	A	213	VAL
1	A	221	VAL
1	A	229	LEU
1	A	237	SER
1	A	258	LEU
1	A	261	ARG
1	A	270	VAL
1	A	273	GLN
1	A	288	LEU
1	A	289	GLU
1	A	294	LEU
1	A	312	GLU
1	A	313	ASN
1	A	314	LYS
1	A	316	ASP
1	A	322	MET
1	A	324	LEU
1	A	329	THR
1	A	330	VAL

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Mol	Chain	Res	Type
1	A	339	GLU
1	A	342	GLN
1	A	344	VAL
1	A	345	LEU
1	A	348	LEU
1	A	354	LEU
1	A	372	LEU
1	A	374	LEU
1	A	381	LEU
1	A	386	SER
1	A	387	ARG
1	A	390	VAL
1	B	3	LEU
1	B	16	ARG
1	B	17	LEU
1	B	26	LEU
1	B	32	ARG
1	B	40	LEU
1	B	42	ARG
1	B	43	LEU
1	B	61	THR
1	B	65	ARG
1	B	68	LEU
1	B	70	GLU
1	B	74	SER
1	B	79	GLU
1	B	89	SER
1	B	92	ARG
1	B	94	GLN
1	B	99	LEU
1	B	108	GLU
1	B	109	ARG
1	B	117	LYS
1	B	123	GLU
1	B	126	ARG
1	B	141	ARG
1	B	142	SER
1	B	163	VAL
1	B	166	ILE
1	B	170	ASN
1	B	179	TYR
1	B	188	LEU

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Mol	Chain	Res	Type
1	B	192	THR
1	B	214	VAL
1	B	217	ARG
1	B	220	ARG
1	B	221	VAL
1	B	227	ARG
1	B	243	VAL
1	B	256	LEU
1	B	262	LEU
1	B	268	TYR
1	B	288	LEU
1	B	306	ARG
1	B	317	GLU
1	B	319	ILE
1	B	324	LEU
1	B	339	GLU
1	B	341	ARG
1	B	342	GLN
1	B	343	SER
1	B	344	VAL
1	B	345	LEU
1	B	372	LEU
1	B	374	LEU
1	B	381	LEU
1	B	387	ARG
1	B	390	VAL

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

Mol	Chain	Res	Type
1	A	21	GLN
1	A	54	GLN
1	A	116	GLN
1	A	132	HIS
1	A	225	ASN
1	A	248	ASN
1	A	273	GLN
1	A	296	HIS
1	A	302	GLN
1	A	318	HIS
1	A	332	HIS
1	A	342	GLN

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Mol	Chain	Res	Type
1	A	349	GLN
1	A	384	HIS
1	B	18	HIS
1	B	116	GLN
1	B	132	HIS
1	B	170	ASN
1	B	225	ASN
1	B	226	ASN
1	B	273	GLN
1	B	342	GLN
1	B	349	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 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	FLC	A	1392	-	12,12,12	1.28	1 (8%)	17,17,17	1.54	2 (11%)

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	A	1392	-	-	9/16/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1392	FLC	OHB-CB	2.46	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1392	FLC	CB-CG-CGC	-3.76	103.65	113.92
2	A	1392	FLC	OB2-CBC-CB	3.40	119.67	113.14

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1392	FLC	CG-CB-CBC-OB1
2	A	1392	FLC	CG-CB-CBC-OB2
2	A	1392	FLC	OHB-CB-CBC-OB1
2	A	1392	FLC	OHB-CB-CBC-OB2
2	A	1392	FLC	CA-CB-CG-CGC
2	A	1392	FLC	CBC-CB-CG-CGC
2	A	1392	FLC	OHB-CB-CG-CGC
2	A	1392	FLC	CA-CB-CBC-OB1
2	A	1392	FLC	CA-CB-CBC-OB2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	391/391 (100%)	0.47	27 (6%) 23 14	45, 71, 74, 82	3 (0%)
1	B	382/391 (97%)	-0.08	4 (1%) 79 63	46, 71, 74, 77	2 (0%)
All	All	773/782 (98%)	0.20	31 (4%) 42 26	45, 71, 74, 82	5 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	41	ARG	6.1
1	B	41	ARG	5.3
1	A	23	ILE	3.5
1	A	65	ARG	3.3
1	A	24	LEU	3.2
1	A	3	LEU	3.1
1	A	385	PHE	3.0
1	A	43	LEU	3.0
1	A	2	ARG	2.9
1	A	38	VAL	2.9
1	A	207	LEU	2.8
1	B	38	VAL	2.8
1	A	25	GLU	2.7
1	A	40	LEU	2.7
1	A	356	PRO	2.7
1	A	1	MET	2.6
1	A	354	LEU	2.6
1	B	313	ASN	2.5
1	A	114	PHE	2.4
1	A	30	ARG	2.4
1	A	215	PHE	2.2
1	B	391	PRO	2.2
1	A	188	LEU	2.2
1	A	33	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	26	LEU	2.2
1	A	275	LEU	2.2
1	A	31	VAL	2.2
1	A	39	GLY	2.1
1	A	312	GLU	2.1
1	A	85	ALA	2.0
1	A	306	ARG	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 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($\text{\AA}^2$)	Q<0.9
2	FLC	A	1392	13/13	0.74	0.11	87,95,103,105	0
3	ZN	B	1392	1/1	0.97	0.06	90,90,90,90	0
3	ZN	B	1393	1/1	0.97	0.05	94,94,94,94	0
3	ZN	A	1393	1/1	0.98	0.06	90,90,90,90	0
3	ZN	A	1394	1/1	0.98	0.04	92,92,92,92	0
3	ZN	B	1394	1/1	0.98	0.04	91,91,91,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.