



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:21 PM UTC

PDB ID : 3ASJ / pdb_00003asj
Title : Crystal structure of homoisocitrate dehydrogenase in complex with a designed inhibitor
Authors : Nango, E.; Kumasaka, T.; Eguchi, T.
Deposited on : 2010-12-13
Resolution : 2.60 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

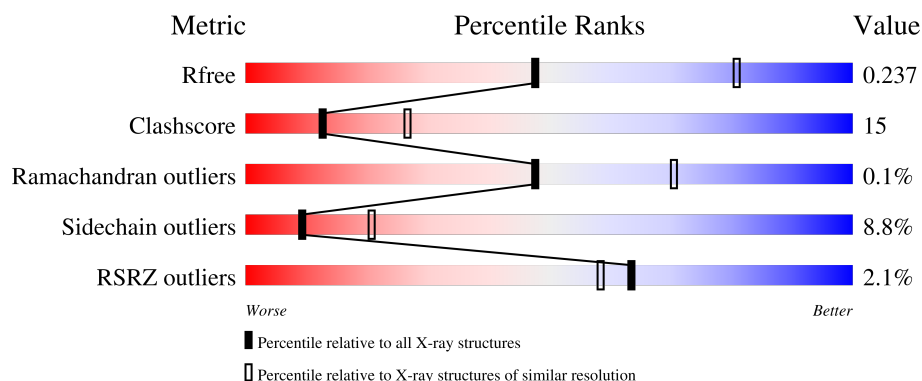
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

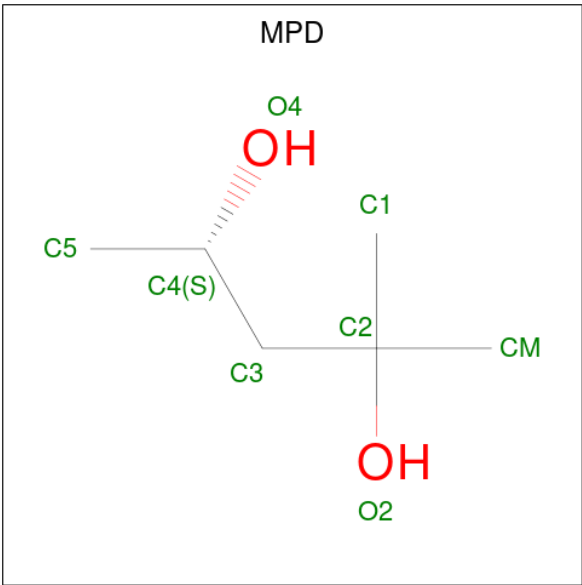
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	334	0% 77% 20% .
1	B	334	2% 75% 21% .
1	C	334	3% 76% 19% .
1	D	334	2% 78% 18% .

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
3	MPD	A	1002	-	-	X	-
3	MPD	B	1001	-	-	X	-
3	MPD	C	1000	-	-	X	-
3	MPD	C	1001	-	-	X	-
3	MPD	C	1003	-	-	X	-
3	MPD	D	1001	-	-	X	-
4	XYM	B	1000	-	X	-	-
4	XYM	D	1000	-	X	-	-



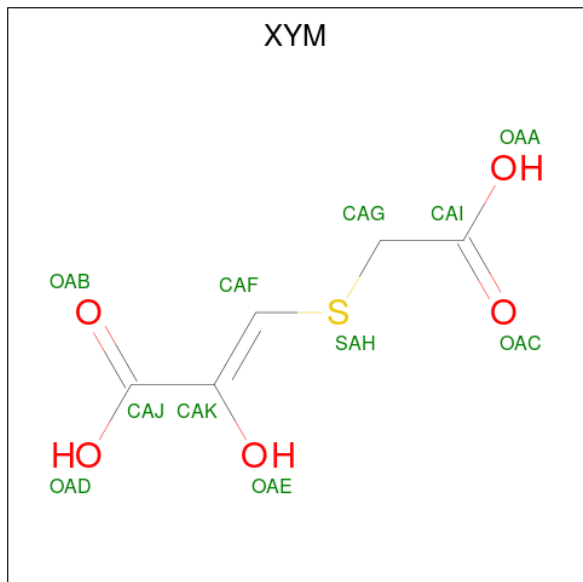
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is (2Z)-3-[(carboxymethyl)sulfanyl]-2-hydroxyprop-2-enoic acid (CCD ID: XYM) (formula: C₅H₆O₅S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	S	0	0
			11	5	5	1		
4	D	1	Total	C	O	S	0	0
			11	5	5	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	119	Total	O	0	0
			119	119		
5	B	95	Total	O	0	0
			95	95		

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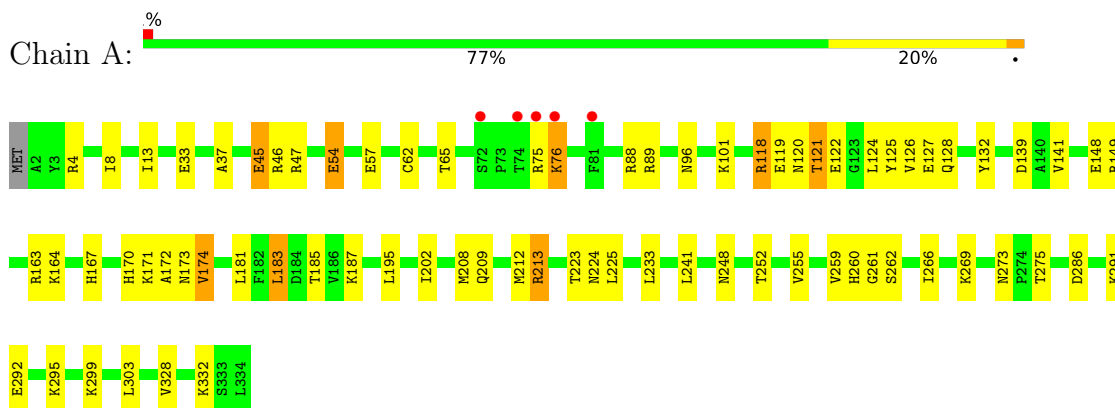
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	79	Total	O	0	0
			79	79		
5	D	95	Total	O	0	0
			95	95		

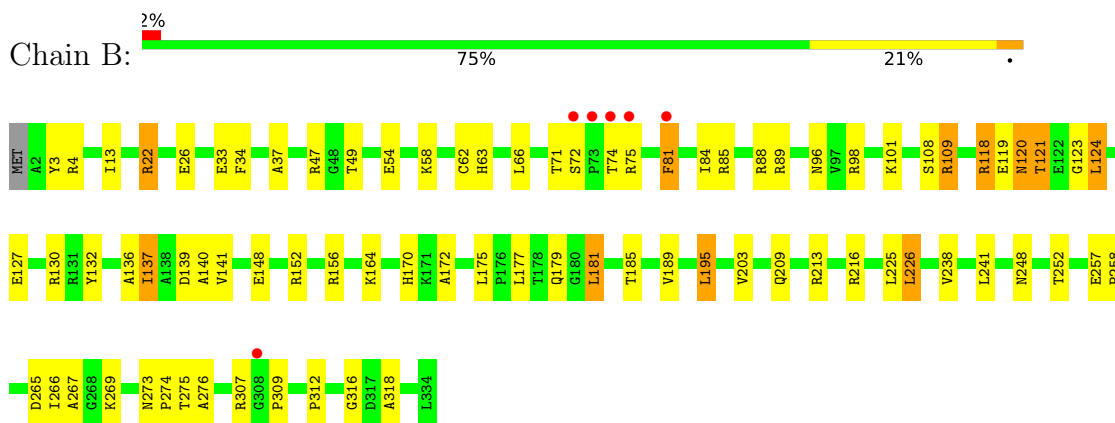
3 Residue-property plots

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.

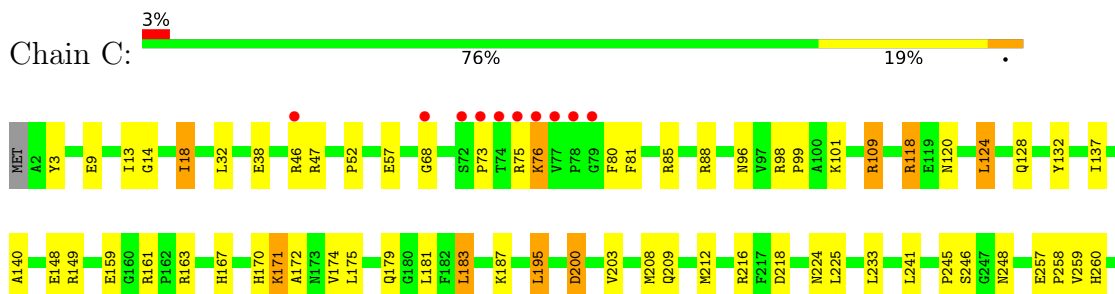
• Molecule 1: Homoisocitrate dehydrogenase

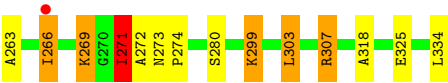


• Molecule 1: Homoisocitrate dehydrogenase

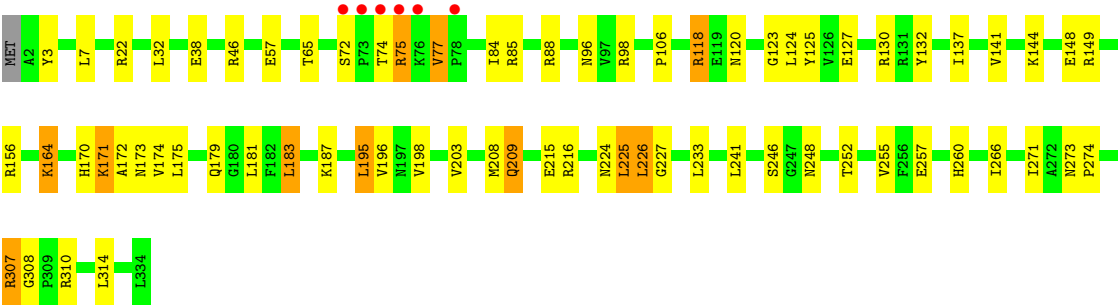
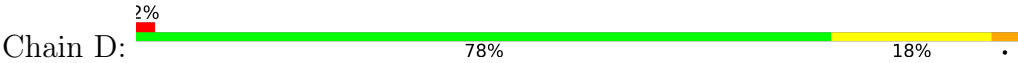


• Molecule 1: Homoisocitrate dehydrogenase





● Molecule 1: Homoiscitrate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	220.97Å 93.69Å 88.80Å 90.00° 97.68° 90.00°	Depositor
Resolution (Å)	44.02 – 2.60 44.02 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.02-2.60) 99.7 (44.02-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0063	Depositor
R, R_{free}	0.169 , 0.231 0.174 , 0.237	Depositor DCC
R_{free} test set	2799 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10657	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.40% 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: XYM, XYN, MPD

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	0.82	0/2560	0.99	0/3474
1	B	0.82	0/2560	1.03	0/3474
1	C	0.83	0/2560	0.98	2/3474 (0.1%)
1	D	0.86	0/2571	1.04	1/3488 (0.0%)
All	All	0.83	0/10251	1.01	3/13910 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	198	VAL	N-CA-C	5.50	115.51	107.37
1	C	271	ILE	N-CA-C	5.14	118.14	113.20
1	C	203	VAL	N-CA-C	5.05	116.37	110.62

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	2519	0	2582	61	0
1	B	2519	0	2582	82	0
1	C	2519	0	2582	95	0
1	D	2527	0	2595	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	11	0	4	0	0
3	A	40	0	70	21	0
3	B	56	0	98	18	0
3	C	32	0	56	38	0
3	D	24	0	42	20	0
4	B	11	0	3	1	0
4	D	11	0	3	1	0
5	A	119	0	0	6	0
5	B	95	0	0	6	0
5	C	79	0	0	10	0
5	D	95	0	0	7	0
All	All	10657	0	10617	317	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 15.

All (317) 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)
3:D:1001:MPD:HM1	3:D:1001:MPD:C5	1.55	1.24
3:D:1001:MPD:H52	3:D:1001:MPD:CM	1.73	1.18
3:C:1003:MPD:HM2	3:C:1003:MPD:C5	1.74	1.18
1:C:124:LEU:H	3:C:1001:MPD:H11	1.01	1.15
1:C:273:ASN:H	3:C:1003:MPD:HM3	1.05	1.09
1:A:208:MET:CE	1:B:241:LEU:HG	1.81	1.09
1:A:208:MET:HE1	1:B:241:LEU:CG	1.82	1.08
1:D:124:LEU:H	3:D:1001:MPD:H11	1.15	1.07
3:C:1001:MPD:HM1	3:C:1001:MPD:O4	1.50	1.06
1:C:124:LEU:HD23	3:C:1001:MPD:HM2	1.34	1.05
1:C:208:MET:HE1	1:D:241:LEU:HG	1.39	1.04
1:B:124:LEU:H	3:B:1001:MPD:H52	1.24	1.03
1:C:124:LEU:CD2	3:C:1001:MPD:HM2	1.90	1.01
3:A:1004:MPD:H52	3:A:1004:MPD:H12	1.42	1.01
1:A:208:MET:HE1	1:B:241:LEU:HG	1.04	1.01
3:C:1003:MPD:HM2	3:C:1003:MPD:H52	1.00	0.99
3:C:1003:MPD:H52	3:C:1003:MPD:CM	1.89	0.99
1:B:273:ASN:H	3:B:1003:MPD:HM3	1.25	0.99
3:D:1001:MPD:C5	3:D:1001:MPD:CM	2.38	0.97
3:C:1003:MPD:C5	3:C:1003:MPD:CM	2.44	0.95
1:A:170:HIS:HD2	1:A:172:ALA:H	1.15	0.95
1:B:81:PHE:HD1	1:B:81:PHE:H	1.16	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ILE:HD11	1:C:68:GLY:HA2	1.51	0.93
1:C:170:HIS:HD2	1:C:172:ALA:H	1.11	0.92
1:B:124:LEU:HD22	3:B:1001:MPD:C1	2.00	0.92
3:C:1000:MPD:H52	3:C:1000:MPD:HM2	1.53	0.91
1:B:170:HIS:HD2	1:B:172:ALA:H	1.14	0.91
1:C:13:ILE:CD1	3:C:1003:MPD:H12	2.01	0.91
1:C:124:LEU:N	3:C:1001:MPD:H11	1.86	0.90
3:C:1000:MPD:HM2	3:C:1000:MPD:C5	2.00	0.90
1:A:122:GLU:HG2	3:A:1003:MPD:O2	1.70	0.90
1:C:307:ARG:HD3	5:C:1075:HOH:O	1.71	0.90
1:A:124:LEU:H	3:A:1002:MPD:HM2	1.35	0.89
1:D:170:HIS:HD2	1:D:172:ALA:H	1.14	0.88
1:D:85:ARG:NH1	1:D:127:GLU:HG3	1.87	0.88
1:D:124:LEU:HD12	3:D:1001:MPD:HM2	1.55	0.87
1:C:273:ASN:N	3:C:1003:MPD:HM3	1.89	0.87
1:B:140:ALA:HB1	3:B:1001:MPD:H13	1.57	0.84
1:C:18:ILE:CD1	1:C:68:GLY:HA2	2.09	0.83
1:C:179:GLN:HE21	3:C:1001:MPD:H4	1.43	0.82
1:B:124:LEU:HD22	3:B:1001:MPD:H12	1.63	0.81
1:D:75:ARG:HD2	1:D:77:VAL:HG22	1.63	0.81
1:A:88:ARG:HE	1:A:248:ASN:ND2	1.79	0.80
3:C:1001:MPD:O4	3:C:1001:MPD:CM	2.29	0.79
1:C:170:HIS:CD2	1:C:172:ALA:H	2.00	0.79
1:A:4:ARG:HD3	1:A:33:GLU:OE1	1.83	0.78
1:C:272:ALA:HB1	3:C:1003:MPD:H13	1.66	0.78
1:C:225:LEU:H	3:C:1001:MPD:H13	1.47	0.78
1:D:124:LEU:N	3:D:1001:MPD:H11	1.98	0.77
1:B:209:GLN:HE22	1:B:213:ARG:HE	1.33	0.77
3:D:1001:MPD:HM1	3:D:1001:MPD:H52	0.78	0.75
1:C:195:LEU:HD12	1:C:195:LEU:H	1.52	0.74
1:C:13:ILE:HD13	3:C:1003:MPD:H12	1.68	0.74
1:B:81:PHE:CD1	1:B:81:PHE:N	2.56	0.73
1:B:81:PHE:HD1	1:B:81:PHE:N	1.85	0.73
1:A:208:MET:SD	1:A:212:MET:HE2	2.29	0.73
1:D:170:HIS:CD2	1:D:172:ALA:H	2.04	0.73
1:C:124:LEU:HD23	3:C:1001:MPD:CM	2.15	0.73
1:B:54:GLU:HG2	3:B:1006:MPD:HM2	1.71	0.72
1:C:118:ARG:HH12	3:C:1000:MPD:H31	1.53	0.72
3:C:1000:MPD:C5	3:C:1000:MPD:CM	2.67	0.72
1:C:225:LEU:HB3	3:C:1001:MPD:HM3	1.70	0.71
1:C:266:ILE:HG13	1:C:271:ILE:HD11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:THR:HB	1:A:255:VAL:HG22	1.72	0.71
1:A:121:THR:HG22	1:A:122:GLU:HG3	1.72	0.71
3:A:1004:MPD:H52	3:A:1004:MPD:C1	2.20	0.71
1:C:109:ARG:HH21	1:C:109:ARG:CG	2.04	0.70
1:D:85:ARG:HH12	1:D:127:GLU:HG3	1.53	0.70
1:C:18:ILE:CD1	1:C:68:GLY:CA	2.69	0.70
1:A:119:GLU:OE2	1:A:121:THR:HB	1.91	0.69
1:B:203:VAL:HG21	1:B:226:LEU:HG	1.75	0.69
1:D:307:ARG:CD	5:D:1090:HOH:O	2.40	0.69
1:D:124:LEU:HD12	3:D:1001:MPD:CM	2.21	0.69
1:D:307:ARG:HD3	5:D:1090:HOH:O	1.91	0.69
1:C:18:ILE:HD11	1:C:68:GLY:CA	2.23	0.68
3:A:1002:MPD:O4	3:A:1002:MPD:H11	1.92	0.68
3:D:1003:MPD:H11	3:D:1003:MPD:H52	1.73	0.68
1:B:124:LEU:N	3:B:1001:MPD:H52	2.06	0.67
1:D:174:VAL:HG23	1:D:175:LEU:HG	1.76	0.67
1:C:299:LYS:HB3	1:C:334:LEU:HD11	1.77	0.67
1:B:124:LEU:H	3:B:1001:MPD:C5	2.05	0.66
3:A:1002:MPD:O4	3:A:1002:MPD:C1	2.43	0.66
3:B:1001:MPD:H52	3:B:1001:MPD:H11	1.78	0.66
1:B:273:ASN:H	3:B:1003:MPD:CM	2.04	0.66
1:D:203:VAL:HG21	1:D:226:LEU:HG	1.78	0.66
3:A:1003:MPD:H52	3:A:1003:MPD:HM1	1.77	0.65
1:C:149:ARG:HD2	5:C:1073:HOH:O	1.97	0.65
1:C:109:ARG:HH21	1:C:109:ARG:HG2	1.63	0.64
1:C:208:MET:HG2	1:C:212:MET:HE2	1.80	0.64
1:D:179:GLN:NE2	3:D:1001:MPD:H53	2.13	0.64
1:C:13:ILE:HD12	3:C:1003:MPD:H12	1.80	0.63
1:A:124:LEU:H	3:A:1002:MPD:CM	2.11	0.63
1:C:109:ARG:HH21	1:C:109:ARG:HB3	1.64	0.62
1:C:208:MET:HE1	1:D:241:LEU:CG	2.25	0.62
1:C:266:ILE:HG13	1:C:271:ILE:CD1	2.30	0.61
1:B:124:LEU:HD22	3:B:1001:MPD:H11	1.79	0.61
1:A:225:LEU:H	3:A:1002:MPD:HM3	1.63	0.61
1:C:171:LYS:NZ	4:D:1000:XYM:OAC	2.34	0.61
1:A:225:LEU:H	3:A:1002:MPD:CM	2.14	0.61
1:A:208:MET:HG2	1:A:212:MET:HE2	1.83	0.61
3:C:1001:MPD:HM1	3:C:1001:MPD:HO4	1.64	0.61
1:C:98:ARG:HD3	5:C:1042:HOH:O	2.01	0.61
1:C:183:LEU:HD22	1:C:187:LYS:HD2	1.83	0.61
1:A:328:VAL:O	1:A:332:LYS:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1001:MPD:H52	3:A:1001:MPD:O2	2.01	0.60
1:C:179:GLN:NE2	3:C:1001:MPD:H4	2.15	0.60
1:C:109:ARG:HG2	1:C:109:ARG:NH2	2.17	0.59
1:D:179:GLN:HE21	3:D:1001:MPD:H53	1.68	0.59
3:D:1003:MPD:H53	3:D:1003:MPD:HM2	1.84	0.59
3:A:1001:MPD:O2	3:A:1001:MPD:C5	2.50	0.59
1:C:225:LEU:H	3:C:1001:MPD:C1	2.14	0.58
1:A:183:LEU:HD22	1:A:187:LYS:HD3	1.86	0.58
1:A:208:MET:SD	1:A:212:MET:CE	2.91	0.58
1:D:225:LEU:H	3:D:1001:MPD:H13	1.67	0.58
1:C:159:GLU:OE1	1:C:195:LEU:HD13	2.03	0.58
3:D:1002:MPD:CM	5:D:1091:HOH:O	2.52	0.58
1:C:46:ARG:HD2	5:C:1026:HOH:O	2.04	0.57
3:A:1003:MPD:H13	5:A:1052:HOH:O	2.04	0.57
1:B:137:ILE:HD12	1:D:137:ILE:HD12	1.86	0.57
1:C:75:ARG:O	1:C:76:LYS:HB3	2.04	0.57
1:C:96:ASN:HB3	1:C:118:ARG:HG2	1.87	0.57
1:C:109:ARG:HH21	1:C:109:ARG:CB	2.17	0.57
1:A:124:LEU:N	3:A:1002:MPD:HM2	2.14	0.56
1:B:225:LEU:H	3:B:1001:MPD:H51	1.70	0.56
1:D:225:LEU:HB2	3:D:1001:MPD:H13	1.87	0.56
1:A:170:HIS:CD2	1:A:172:ALA:H	2.07	0.56
1:A:120:ASN:HD21	1:A:248:ASN:HD22	1.52	0.56
3:C:1000:MPD:HM2	3:C:1000:MPD:H53	1.84	0.56
3:D:1002:MPD:HM3	5:D:1091:HOH:O	2.06	0.56
1:D:183:LEU:HD22	1:D:187:LYS:HD2	1.87	0.56
1:D:310:ARG:HG3	1:D:314:LEU:HB2	1.86	0.56
1:A:96:ASN:HD22	1:A:118:ARG:HG2	1.71	0.55
1:B:123:GLY:HA3	3:B:1001:MPD:H53	1.88	0.55
1:C:18:ILE:HD13	1:C:68:GLY:CA	2.35	0.55
1:A:225:LEU:CB	3:A:1002:MPD:HM1	2.37	0.55
1:B:22:ARG:NH2	1:B:34:PHE:CD1	2.75	0.55
1:B:4:ARG:HD3	1:B:33:GLU:OE1	2.06	0.55
1:B:49:THR:HG1	1:B:81:PHE:HZ	1.53	0.55
1:C:120:ASN:HD21	1:C:248:ASN:HD22	1.53	0.55
1:B:54:GLU:HG2	3:B:1006:MPD:CM	2.35	0.55
1:D:124:LEU:CD1	3:D:1001:MPD:HM2	2.31	0.55
3:C:1000:MPD:CM	3:C:1000:MPD:H53	2.37	0.55
1:C:167:HIS:HD2	5:C:1056:HOH:O	1.90	0.55
1:C:3:TYR:HB2	1:C:32:LEU:HD23	1.89	0.55
1:D:260:HIS:HE1	5:D:1004:HOH:O	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LEU:HD11	1:B:124:LEU:HD21	1.89	0.54
1:B:170:HIS:CD2	1:B:172:ALA:H	2.07	0.54
1:D:183:LEU:HD22	1:D:187:LYS:CD	2.37	0.54
1:D:183:LEU:CD2	1:D:187:LYS:HD2	2.38	0.54
1:B:85:ARG:HH22	4:B:1000:XYM:HAG	1.72	0.54
1:B:119:GLU:OE1	1:B:121:THR:HB	2.08	0.53
1:A:225:LEU:HB3	3:A:1002:MPD:HM1	1.90	0.53
1:C:18:ILE:HD13	1:C:68:GLY:HA3	1.91	0.53
3:A:1004:MPD:C1	3:A:1004:MPD:C5	2.85	0.53
1:D:7:LEU:HD11	1:D:22[A]:ARG:HG3	1.91	0.53
1:D:88:ARG:HH21	1:D:248:ASN:HD21	1.57	0.53
1:A:208:MET:CG	1:A:212:MET:HE2	2.39	0.53
3:B:1005:MPD:H11	3:B:1005:MPD:H53	1.90	0.53
1:B:37:ALA:HB2	1:B:58:LYS:HD3	1.90	0.53
1:A:46:ARG:O	1:A:47:ARG:HG3	2.09	0.52
1:A:292:GLU:OE2	1:A:295:LYS:HE3	2.09	0.52
1:B:124:LEU:CD2	3:B:1001:MPD:H12	2.36	0.52
1:C:163:ARG:HD3	5:C:1034:HOH:O	2.09	0.52
1:D:209:GLN:HE21	1:D:216:ARG:HH21	1.57	0.52
1:D:164:LYS:HG3	1:D:196:VAL:HA	1.91	0.52
1:A:223:THR:HB	3:A:1002:MPD:C1	2.40	0.52
1:C:124:LEU:HD22	3:C:1001:MPD:HM2	1.88	0.52
1:B:216:ARG:O	1:B:216:ARG:HG3	2.09	0.51
1:B:258:PRO:HB3	1:B:276:ALA:CB	2.40	0.51
1:D:164:LYS:HG2	1:D:195:LEU:O	2.11	0.51
1:B:273:ASN:ND2	1:B:275:THR:H	2.08	0.51
1:C:118:ARG:NH2	1:C:224:ASN:OD1	2.43	0.51
1:A:273:ASN:ND2	1:A:275:THR:H	2.08	0.51
1:B:273:ASN:C	1:B:273:ASN:HD22	2.19	0.51
1:A:125:TYR:HB2	1:A:224:ASN:ND2	2.26	0.51
1:C:118:ARG:NH1	3:C:1000:MPD:H31	2.24	0.51
1:B:258:PRO:HB3	1:B:276:ALA:HB1	1.92	0.50
1:B:4:ARG:CD	1:B:33:GLU:OE1	2.59	0.50
1:A:171:LYS:HE3	1:A:174:VAL:HG13	1.92	0.50
1:C:96:ASN:HB3	1:C:118:ARG:CG	2.42	0.50
1:D:88:ARG:HE	1:D:248:ASN:ND2	2.10	0.50
1:D:144:LYS:O	1:D:148:GLU:HG3	2.11	0.50
1:D:215:GLU:CD	1:D:215:GLU:H	2.20	0.50
1:B:89:ARG:HG2	5:B:1096:HOH:O	2.10	0.50
1:B:273:ASN:HD22	1:B:274:PRO:N	2.09	0.50
1:B:309:PRO:HB2	1:B:318:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:LYS:HB3	1:C:334:LEU:CD1	2.41	0.50
1:A:45:GLU:HB2	5:A:1099:HOH:O	2.11	0.50
1:D:106:PRO:HD3	1:D:310:ARG:HH12	1.76	0.50
1:B:209:GLN:HE22	1:B:213:ARG:NE	2.08	0.49
1:C:13:ILE:HD11	1:C:260:HIS:CD2	2.47	0.49
1:C:124:LEU:HD21	1:D:124:LEU:HD11	1.94	0.49
1:D:307:ARG:HD2	5:D:1090:HOH:O	2.06	0.49
1:C:73:PRO:HD2	1:C:80:PHE:CE1	2.48	0.49
1:B:266:ILE:O	1:B:269:LYS:HB2	2.13	0.49
1:A:148:GLU:HG3	1:A:185:THR:CG2	2.43	0.49
1:B:22:ARG:NH2	1:B:26:GLU:OE2	2.46	0.49
3:A:1004:MPD:H12	3:A:1004:MPD:C5	2.25	0.48
1:D:96:ASN:HB3	1:D:118:ARG:HG2	1.95	0.48
1:C:174:VAL:HG23	1:C:175:LEU:HG	1.96	0.48
1:A:260:HIS:HD2	1:A:261:GLY:O	1.96	0.48
1:B:195:LEU:HB2	5:B:1092:HOH:O	2.12	0.48
1:C:13:ILE:CD1	3:C:1003:MPD:C1	2.85	0.48
1:C:76:LYS:CG	1:C:76:LYS:O	2.61	0.48
1:C:209:GLN:OE1	1:C:216:ARG:NH2	2.39	0.48
1:A:141:VAL:HG21	1:D:132:TYR:CZ	2.49	0.48
1:B:75:ARG:NH1	1:B:75:ARG:HB3	2.29	0.48
1:B:89:ARG:NE	5:B:1100:HOH:O	2.47	0.48
1:B:141:VAL:HG21	1:C:132:TYR:CZ	2.49	0.48
1:C:266:ILE:O	1:C:269:LYS:HB2	2.14	0.48
1:D:96:ASN:HD22	1:D:118:ARG:HG2	1.78	0.48
1:A:266:ILE:HA	1:A:269:LYS:HD2	1.95	0.47
1:B:273:ASN:HD22	1:B:274:PRO:CD	2.27	0.47
1:B:273:ASN:HD22	1:B:274:PRO:HD2	1.78	0.47
1:A:128:GLN:HE21	1:D:130:ARG:HG2	1.79	0.47
1:C:263:ALA:HB1	1:C:266:ILE:CG2	2.45	0.47
1:D:156:ARG:NE	5:D:1048:HOH:O	2.47	0.47
1:C:208:MET:CE	1:D:241:LEU:HG	2.28	0.47
1:B:13:ILE:HG22	1:B:267:ALA:HA	1.96	0.47
1:C:13:ILE:HD13	3:C:1003:MPD:C1	2.42	0.47
1:C:260:HIS:HE1	5:C:1069:HOH:O	1.98	0.47
3:C:1003:MPD:CM	3:C:1003:MPD:H53	2.41	0.47
3:D:1002:MPD:H52	3:D:1002:MPD:O2	2.14	0.47
1:A:167:HIS:HD2	5:A:1009:HOH:O	1.97	0.47
1:A:76:LYS:HE3	1:A:76:LYS:O	2.15	0.47
1:B:123:GLY:HA3	3:B:1001:MPD:C5	2.45	0.46
1:B:98:ARG:HD3	5:B:1088:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:LEU:O	1:C:307:ARG:HD2	2.14	0.46
1:C:98:ARG:HD2	1:C:246:SER:HB3	1.98	0.46
1:A:139:ASP:OD2	1:D:130:ARG:HD2	2.16	0.46
1:D:118:ARG:HB2	1:D:227:GLY:HA3	1.97	0.46
1:A:273:ASN:C	1:A:273:ASN:HD22	2.23	0.46
1:C:273:ASN:HD22	1:C:274:PRO:HD2	1.81	0.46
1:D:125:TYR:HB2	1:D:224:ASN:ND2	2.31	0.46
1:A:13:ILE:HG12	1:A:262:SER:O	2.16	0.45
1:B:152:ARG:O	1:B:156:ARG:HG3	2.17	0.45
1:B:312:PRO:HA	1:B:316:GLY:O	2.16	0.45
1:C:183:LEU:HD22	1:C:187:LYS:CD	2.46	0.45
1:A:4:ARG:HG2	1:A:62:CYS:SG	2.56	0.45
1:A:260:HIS:HE1	5:A:1007:HOH:O	2.00	0.45
1:B:96:ASN:HB3	1:B:118:ARG:HG2	1.98	0.45
1:B:136:ALA:C	1:B:137:ILE:HG12	2.41	0.45
1:C:88:ARG:HE	1:C:248:ASN:ND2	2.15	0.45
1:C:257:GLU:HG2	1:C:258:PRO:O	2.17	0.45
1:D:106:PRO:HD3	1:D:310:ARG:NH1	2.30	0.45
1:D:233:LEU:C	1:D:233:LEU:HD23	2.42	0.45
1:D:170:HIS:HD2	1:D:172:ALA:N	1.97	0.45
1:A:208:MET:CE	1:B:241:LEU:CG	2.65	0.44
1:B:156:ARG:HD2	5:B:1077:HOH:O	2.16	0.44
1:D:98:ARG:HD2	1:D:246:SER:HB3	1.98	0.44
1:A:223:THR:HB	3:A:1002:MPD:H13	2.00	0.44
1:D:65:THR:HB	1:D:255:VAL:HG22	2.00	0.44
1:A:209:GLN:HE22	1:A:213:ARG:HH21	1.66	0.44
1:B:120:ASN:ND2	5:B:1056:HOH:O	2.50	0.44
1:B:130:ARG:HG2	1:C:128:GLN:NE2	2.33	0.44
3:B:1005:MPD:H53	3:B:1005:MPD:C1	2.47	0.44
1:C:318:ALA:HA	5:C:1080:HOH:O	2.17	0.44
1:B:54:GLU:H	1:B:54:GLU:CD	2.26	0.44
1:A:132:TYR:CZ	1:D:141:VAL:HG21	2.52	0.43
1:D:225:LEU:HB3	3:D:1001:MPD:HM3	2.00	0.43
1:C:241:LEU:HG	1:D:208:MET:SD	2.58	0.43
1:C:9:GLU:O	1:C:14:GLY:HA3	2.18	0.43
1:A:208:MET:HE1	1:B:241:LEU:CD2	2.47	0.43
1:C:170:HIS:CD2	1:C:170:HIS:C	2.96	0.43
1:A:173:ASN:ND2	1:A:202:ILE:HD13	2.34	0.43
1:C:47:ARG:HH11	1:C:52:PRO:HB3	1.84	0.43
1:C:109:ARG:CG	1:C:109:ARG:NH2	2.70	0.43
1:B:132:TYR:OH	1:C:128:GLN:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:ARG:NH1	1:D:127:GLU:CG	2.69	0.43
1:A:88:ARG:HE	1:A:248:ASN:HD21	1.59	0.43
1:A:171:LYS:HE3	1:A:174:VAL:CG1	2.48	0.43
1:B:137:ILE:HD12	1:D:137:ILE:CD1	2.48	0.43
1:C:140:ALA:HB1	3:C:1001:MPD:H53	2.01	0.43
1:B:88:ARG:HH21	1:B:248:ASN:HD21	1.66	0.42
1:D:171:LYS:HD2	1:D:203:VAL:HG12	2.01	0.42
1:B:273:ASN:ND2	1:B:273:ASN:C	2.74	0.42
1:C:85:ARG:HG2	5:C:1083:HOH:O	2.19	0.42
1:B:175:LEU:O	1:B:179:GLN:HB2	2.19	0.42
1:C:118:ARG:HH12	3:C:1000:MPD:C3	2.25	0.42
1:C:161:ARG:NH2	1:C:218:ASP:OD1	2.52	0.42
1:A:8:ILE:HG12	1:A:37:ALA:HB3	2.02	0.42
1:A:259:VAL:HG12	1:A:259:VAL:O	2.20	0.42
1:B:130:ARG:HG2	1:C:128:GLN:HE21	1.84	0.42
1:A:208:MET:CE	1:B:241:LEU:CD2	2.98	0.42
1:D:96:ASN:HB3	1:D:118:ARG:CG	2.50	0.42
1:C:149:ARG:CD	5:C:1073:HOH:O	2.62	0.42
1:D:171:LYS:HE2	1:D:173:ASN:OD1	2.20	0.42
1:D:273:ASN:HD22	1:D:274:PRO:HD2	1.85	0.42
1:A:88:ARG:HH21	1:A:248:ASN:HD21	1.68	0.42
1:B:85:ARG:HD3	1:B:127:GLU:OE1	2.19	0.42
1:C:299:LYS:HD3	1:C:299:LYS:HA	1.87	0.42
1:B:118:ARG:O	1:B:118:ARG:HG3	2.19	0.42
1:B:3:TYR:HA	1:B:63:HIS:CE1	2.55	0.41
1:C:98:ARG:CZ	1:C:259:VAL:HG21	2.50	0.41
1:B:238:VAL:O	1:B:238:VAL:HG23	2.19	0.41
3:C:1000:MPD:O4	1:D:171:LYS:NZ	2.52	0.41
1:C:76:LYS:O	1:C:76:LYS:HG2	2.19	0.41
1:B:109:ARG:HE	1:B:109:ARG:HB3	1.37	0.41
1:B:4:ARG:O	1:B:62:CYS:HB3	2.20	0.41
1:B:88:ARG:HE	1:B:248:ASN:ND2	2.18	0.41
1:B:148:GLU:HG3	1:B:185:THR:HG21	2.02	0.41
1:C:170:HIS:HE1	1:C:200:ASP:OD1	2.03	0.41
1:D:3:TYR:HB2	1:D:32:LEU:HD23	2.02	0.41
1:A:286:ASP:HB2	3:A:1001:MPD:H11	2.03	0.41
1:B:120:ASN:HD22	1:B:120:ASN:HA	1.74	0.41
1:C:81:PHE:CD1	1:C:81:PHE:N	2.89	0.41
1:B:49:THR:OG1	1:B:81:PHE:HZ	2.03	0.41
1:C:99:PRO:HG2	1:C:245:PRO:HG2	2.03	0.41
1:D:266:ILE:HD12	1:D:271:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:ARG:HH12	3:C:1000:MPD:H32	1.86	0.40
1:A:149:ARG:HD2	5:A:1015:HOH:O	2.20	0.40
1:A:54:GLU:HB3	5:A:1074:HOH:O	2.22	0.40
1:B:177:LEU:O	1:B:181:LEU:HB2	2.22	0.40
1:B:130:ARG:NH2	1:B:139:ASP:OD1	2.54	0.40
1:D:38:GLU:OE2	1:D:46:ARG:NH2	2.54	0.40
1:D:85:ARG:HH11	1:D:127:GLU:HG3	1.79	0.40
1:D:123:GLY:HA3	3:D:1001:MPD:C1	2.51	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	331/334 (99%)	312 (94%)	19 (6%)	0	100	100
1	B	331/334 (99%)	313 (95%)	18 (5%)	0	100	100
1	C	331/334 (99%)	311 (94%)	20 (6%)	0	100	100
1	D	332/334 (99%)	317 (96%)	14 (4%)	1 (0%)	36	58
All	All	1325/1336 (99%)	1253 (95%)	71 (5%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	308	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	263/264 (100%)	239 (91%)	24 (9%)	9	19
1	B	263/264 (100%)	238 (90%)	25 (10%)	8	18
1	C	263/264 (100%)	239 (91%)	24 (9%)	9	19
1	D	264/264 (100%)	244 (92%)	20 (8%)	12	27
All	All	1053/1056 (100%)	960 (91%)	93 (9%)	9	21

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLU
1	A	54	GLU
1	A	57	GLU
1	A	75	ARG
1	A	76	LYS
1	A	89	ARG
1	A	101	LYS
1	A	118	ARG
1	A	121	THR
1	A	126	VAL
1	A	127	GLU
1	A	163	ARG
1	A	164	LYS
1	A	174	VAL
1	A	181	LEU
1	A	183	LEU
1	A	195	LEU
1	A	213	ARG
1	A	233	LEU
1	A	241	LEU
1	A	252	THR
1	A	291	LYS
1	A	299	LYS
1	A	303	LEU
1	B	22	ARG
1	B	47	ARG
1	B	66	LEU
1	B	71	THR
1	B	72	SER
1	B	74	THR

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Mol	Chain	Res	Type
1	B	81	PHE
1	B	84	ILE
1	B	101	LYS
1	B	108	SER
1	B	109	ARG
1	B	118	ARG
1	B	120	ASN
1	B	121	THR
1	B	124	LEU
1	B	137	ILE
1	B	164	LYS
1	B	181	LEU
1	B	189	VAL
1	B	195	LEU
1	B	226	LEU
1	B	252	THR
1	B	257	GLU
1	B	265	ASP
1	B	307	ARG
1	C	18	ILE
1	C	38	GLU
1	C	57	GLU
1	C	76	LYS
1	C	101	LYS
1	C	109	ARG
1	C	118	ARG
1	C	124	LEU
1	C	137	ILE
1	C	148	GLU
1	C	171	LYS
1	C	181	LEU
1	C	183	LEU
1	C	195	LEU
1	C	200	ASP
1	C	233	LEU
1	C	266	ILE
1	C	269	LYS
1	C	271	ILE
1	C	280	SER
1	C	299	LYS
1	C	303	LEU
1	C	307	ARG

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Mol	Chain	Res	Type
1	C	325	GLU
1	D	57	GLU
1	D	72	SER
1	D	74	THR
1	D	75	ARG
1	D	77	VAL
1	D	84	ILE
1	D	118	ARG
1	D	120	ASN
1	D	149	ARG
1	D	164	LYS
1	D	171	LYS
1	D	181	LEU
1	D	183	LEU
1	D	195	LEU
1	D	209	GLN
1	D	225	LEU
1	D	226	LEU
1	D	252	THR
1	D	257	GLU
1	D	307	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	128	GLN
1	A	167	HIS
1	A	170	HIS
1	A	205	ASN
1	A	248	ASN
1	A	260	HIS
1	A	273	ASN
1	B	96	ASN
1	B	120	ASN
1	B	167	HIS
1	B	170	HIS
1	B	197	ASN
1	B	199	GLN
1	B	209	GLN
1	B	248	ASN
1	B	273	ASN

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Mol	Chain	Res	Type
1	C	128	GLN
1	C	170	HIS
1	C	248	ASN
1	C	260	HIS
1	C	273	ASN
1	D	96	ASN
1	D	120	ASN
1	D	170	HIS
1	D	199	GLN
1	D	205	ASN
1	D	209	GLN
1	D	248	ASN
1	D	260	HIS
1	D	273	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

22 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
3	MPD	D	1003	-	7,7,7	0.44	0	9,10,10	1.08	0
2	XYN	A	1000	-	9,10,10	1.03	0	11,12,12	2.10	4 (36%)
3	MPD	B	1004	-	7,7,7	0.34	0	9,10,10	0.99	1 (11%)
3	MPD	C	1001	-	7,7,7	0.48	0	9,10,10	1.38	2 (22%)
4	XYM	B	1000	-	9,10,10	1.58	2 (22%)	11,12,12	4.21	6 (54%)
3	MPD	A	1005	-	7,7,7	0.31	0	9,10,10	0.55	0
3	MPD	C	1003	-	7,7,7	0.33	0	9,10,10	0.54	0
3	MPD	C	1002	-	7,7,7	0.31	0	9,10,10	0.86	0
3	MPD	B	1005	-	7,7,7	0.39	0	9,10,10	0.53	0
3	MPD	B	1002	-	7,7,7	0.33	0	9,10,10	0.49	0
3	MPD	B	1006	-	7,7,7	0.37	0	9,10,10	0.75	0
3	MPD	A	1002	-	7,7,7	0.38	0	9,10,10	1.47	1 (11%)
3	MPD	A	1003	-	7,7,7	0.40	0	9,10,10	0.99	1 (11%)
3	MPD	D	1001	-	7,7,7	0.39	0	9,10,10	1.97	4 (44%)
3	MPD	C	1000	-	7,7,7	0.45	0	9,10,10	0.84	0
3	MPD	B	1007	-	7,7,7	0.47	0	9,10,10	0.94	0
3	MPD	B	1001	-	7,7,7	0.55	0	9,10,10	1.21	2 (22%)
3	MPD	A	1004	-	7,7,7	0.28	0	9,10,10	0.69	0
4	XYM	D	1000	-	9,10,10	1.86	1 (11%)	11,12,12	3.69	6 (54%)
3	MPD	A	1001	-	7,7,7	0.27	0	9,10,10	0.56	0
3	MPD	B	1003	-	7,7,7	0.37	0	9,10,10	0.65	0
3	MPD	D	1002	-	7,7,7	0.36	0	9,10,10	0.75	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
3	MPD	D	1003	-	-	3/5/5/5	-
2	XYN	A	1000	-	-	5/9/10/10	-
3	MPD	B	1004	-	-	0/5/5/5	-
3	MPD	C	1001	-	-	2/5/5/5	-
4	XYM	B	1000	-	-	7/8/10/10	-
3	MPD	A	1005	-	-	4/5/5/5	-
3	MPD	C	1003	-	-	3/5/5/5	-
3	MPD	C	1002	-	-	2/5/5/5	-
3	MPD	B	1005	-	-	2/5/5/5	-
3	MPD	B	1002	-	-	3/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	B	1006	-	-	1/5/5/5	-
3	MPD	A	1002	-	-	3/5/5/5	-
3	MPD	A	1003	-	-	3/5/5/5	-
3	MPD	D	1001	-	-	3/5/5/5	-
3	MPD	C	1000	-	-	3/5/5/5	-
3	MPD	B	1007	-	-	2/5/5/5	-
3	MPD	B	1001	-	-	3/5/5/5	-
3	MPD	A	1004	-	-	1/5/5/5	-
4	XYM	D	1000	-	-	8/8/10/10	-
3	MPD	A	1001	-	-	2/5/5/5	-
3	MPD	B	1003	-	-	1/5/5/5	-
3	MPD	D	1002	-	-	3/5/5/5	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1000	XYM	CAK-CAJ	4.50	1.55	1.48
4	B	1000	XYM	CAF-SAH	-2.83	1.69	1.73
4	B	1000	XYM	CAK-CAJ	2.45	1.52	1.48

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1000	XYM	OAE-CAK-CAJ	11.02	124.61	114.17
4	D	1000	XYM	OAE-CAK-CAJ	10.12	123.76	114.17
4	B	1000	XYM	CAF-CAK-CAJ	-5.36	114.83	122.54
2	A	1000	XYN	OBB-CBJ-CBK	-4.04	116.78	121.81
4	B	1000	XYM	OAB-CAJ-CAK	-3.87	115.68	120.12
3	A	1002	MPD	CM-C2-C1	-3.36	103.09	110.63
4	D	1000	XYM	CAF-CAK-CAJ	-3.28	117.82	122.54
3	D	1001	MPD	O2-C2-C3	3.16	121.09	109.27
4	D	1000	XYM	OAD-CAJ-CAK	3.05	119.17	115.78
4	B	1000	XYM	CAG-SAH-CAF	-3.01	95.03	100.38
2	A	1000	XYN	CBK-CBG-SBH	-2.94	101.84	111.38
4	D	1000	XYM	OAC-CAI-CAG	-2.90	115.02	122.85
3	D	1001	MPD	O2-C2-C1	-2.75	99.40	107.99
3	C	1001	MPD	O2-C2-CM	-2.74	99.44	107.99
4	B	1000	XYM	OAC-CAI-CAG	-2.72	115.50	122.85
4	D	1000	XYM	OAB-CAJ-CAK	-2.70	117.02	120.12
2	A	1000	XYN	OBC-CBK-CBJ	2.61	123.39	119.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	MPD	C5-C4-C3	2.49	123.26	111.67
3	C	1001	MPD	O2-C2-C3	2.40	118.26	109.27
3	D	1001	MPD	CM-C2-C1	2.36	115.91	110.63
2	A	1000	XYN	OBA-CBI-CBF	-2.25	116.78	122.85
4	B	1000	XYM	CAI-CAG-SAH	-2.20	106.65	113.52
4	D	1000	XYM	OAE-CAK-CAF	-2.18	118.42	122.60
3	B	1001	MPD	O4-C4-C3	-2.15	102.81	111.35
3	D	1001	MPD	CM-C2-C3	-2.10	101.15	110.20
3	A	1003	MPD	CM-C2-C3	2.06	119.07	110.20
3	B	1004	MPD	O2-C2-C1	2.01	114.24	107.99

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1000	XYN	SBH-CBG-CBK-OBC
2	A	1000	XYN	SBH-CBG-CBK-CBJ
3	A	1001	MPD	C2-C3-C4-O4
3	A	1001	MPD	C2-C3-C4-C5
3	A	1003	MPD	O2-C2-C3-C4
3	A	1003	MPD	CM-C2-C3-C4
3	B	1001	MPD	C1-C2-C3-C4
3	B	1005	MPD	C2-C3-C4-C5
3	C	1000	MPD	C2-C3-C4-O4
3	C	1000	MPD	C2-C3-C4-C5
3	C	1003	MPD	C2-C3-C4-O4
3	D	1001	MPD	O2-C2-C3-C4
3	D	1001	MPD	CM-C2-C3-C4
3	D	1003	MPD	C2-C3-C4-C5
4	B	1000	XYM	OAB-CAJ-CAK-OAE
4	B	1000	XYM	OAB-CAJ-CAK-CAF
4	B	1000	XYM	OAD-CAJ-CAK-OAE
4	D	1000	XYM	CAK-CAF-SAH-CAG
4	D	1000	XYM	OAB-CAJ-CAK-OAE
4	D	1000	XYM	OAB-CAJ-CAK-CAF
4	D	1000	XYM	OAD-CAJ-CAK-OAE
4	D	1000	XYM	CAI-CAG-SAH-CAF
2	A	1000	XYN	CBI-CBF-SBH-CBG
3	B	1005	MPD	O2-C2-C3-C4
3	D	1003	MPD	O2-C2-C3-C4
3	B	1001	MPD	C2-C3-C4-O4
3	C	1001	MPD	C2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
3	C	1002	MPD	C2-C3-C4-O4
3	A	1002	MPD	C1-C2-C3-C4
3	A	1003	MPD	C1-C2-C3-C4
3	A	1005	MPD	C1-C2-C3-C4
3	A	1005	MPD	CM-C2-C3-C4
3	D	1001	MPD	C1-C2-C3-C4
3	D	1002	MPD	C1-C2-C3-C4
3	D	1002	MPD	CM-C2-C3-C4
3	A	1004	MPD	C2-C3-C4-C5
3	B	1003	MPD	C2-C3-C4-C5
3	C	1003	MPD	C2-C3-C4-C5
4	D	1000	XYM	SAH-CAG-CAI-OAA
4	B	1000	XYM	OAD-CAJ-CAK-CAF
4	D	1000	XYM	OAD-CAJ-CAK-CAF
2	A	1000	XYN	SBH-CBF-CBI-OBA
4	D	1000	XYM	SAH-CAG-CAI-OAC
2	A	1000	XYN	SBH-CBF-CBI-OB
3	A	1005	MPD	O2-C2-C3-C4
3	B	1007	MPD	O2-C2-C3-C4
3	C	1000	MPD	O2-C2-C3-C4
3	C	1002	MPD	O2-C2-C3-C4
3	C	1003	MPD	O2-C2-C3-C4
3	D	1002	MPD	O2-C2-C3-C4
4	B	1000	XYM	SAH-CAG-CAI-OAC
3	A	1002	MPD	C2-C3-C4-O4
3	A	1005	MPD	C2-C3-C4-O4
3	B	1002	MPD	C2-C3-C4-O4
3	D	1003	MPD	C2-C3-C4-O4
3	A	1002	MPD	CM-C2-C3-C4
3	B	1001	MPD	CM-C2-C3-C4
3	B	1002	MPD	C1-C2-C3-C4
3	B	1002	MPD	CM-C2-C3-C4
3	B	1006	MPD	C1-C2-C3-C4
3	B	1007	MPD	CM-C2-C3-C4
3	C	1001	MPD	CM-C2-C3-C4
4	B	1000	XYM	CAK-CAF-SAH-CAG
4	B	1000	XYM	SAH-CAG-CAI-OAA

There are no ring outliers.

16 monomers are involved in 99 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1003	MPD	2	0
3	C	1001	MPD	15	0
4	B	1000	XYM	1	0
3	C	1003	MPD	13	0
3	B	1005	MPD	2	0
3	B	1006	MPD	2	0
3	A	1002	MPD	11	0
3	A	1003	MPD	3	0
3	D	1001	MPD	15	0
3	C	1000	MPD	10	0
3	B	1001	MPD	12	0
3	A	1004	MPD	4	0
4	D	1000	XYM	1	0
3	A	1001	MPD	3	0
3	B	1003	MPD	2	0
3	D	1002	MPD	3	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

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	333/334 (99%)	-0.38	5 (1%) 72 68	20, 29, 49, 78	0
1	B	333/334 (99%)	-0.24	6 (1%) 67 63	20, 31, 52, 76	0
1	C	333/334 (99%)	-0.11	11 (3%) 49 43	21, 32, 55, 80	0
1	D	333/334 (99%)	-0.29	6 (1%) 67 63	15, 30, 48, 74	1 (0%)
All	All	1332/1336 (99%)	-0.26	28 (2%) 63 58	15, 30, 53, 80	1 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	73	PRO	4.6
1	C	74	THR	4.1
1	B	75	ARG	3.9
1	C	73	PRO	3.6
1	B	308	GLY	3.6
1	C	77	VAL	3.2
1	C	79	GLY	3.2
1	B	72	SER	3.1
1	B	74	THR	3.0
1	D	74	THR	3.0
1	C	78	PRO	3.0
1	A	75	ARG	2.9
1	A	74	THR	2.9
1	D	72	SER	2.6
1	A	76	LYS	2.6
1	B	81	PHE	2.6
1	D	73	PRO	2.5
1	A	81	PHE	2.5
1	C	76	LYS	2.4
1	C	72	SER	2.4
1	D	78	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	72	SER	2.3
1	C	46	ARG	2.2
1	D	75	ARG	2.2
1	C	75	ARG	2.2
1	C	266	ILE	2.1
1	D	76	LYS	2.0
1	C	68	GLY	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(Å ²)	Q<0.9
3	MPD	A	1003	8/8	0.75	0.24	34,37,37,37	8
4	XYM	D	1000	11/11	0.76	0.25	48,54,58,58	11
3	MPD	C	1003	8/8	0.77	0.23	36,36,38,40	8
2	XYN	A	1000	11/11	0.80	0.21	29,40,45,46	11
3	MPD	B	1003	8/8	0.80	0.27	37,39,40,41	8
3	MPD	D	1002	8/8	0.81	0.27	28,29,29,32	8
3	MPD	B	1006	8/8	0.82	0.22	38,39,40,41	8
3	MPD	A	1004	8/8	0.82	0.23	25,30,36,39	8
3	MPD	C	1000	8/8	0.83	0.23	30,31,32,32	8
4	XYM	B	1000	11/11	0.84	0.19	41,45,50,52	11
3	MPD	C	1002	8/8	0.84	0.21	34,36,37,38	8
3	MPD	C	1001	8/8	0.87	0.14	23,25,27,27	0
3	MPD	B	1001	8/8	0.87	0.17	21,26,30,36	0
3	MPD	B	1005	8/8	0.87	0.20	46,47,48,49	8
3	MPD	D	1003	8/8	0.88	0.15	34,35,37,38	0
3	MPD	B	1007	8/8	0.90	0.14	36,39,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MPD	A	1001	8/8	0.90	0.18	33,35,36,37	8
3	MPD	A	1005	8/8	0.90	0.20	31,32,35,36	8
3	MPD	A	1002	8/8	0.91	0.13	21,27,29,29	0
3	MPD	D	1001	8/8	0.91	0.12	17,20,22,22	0
3	MPD	B	1004	8/8	0.91	0.17	31,33,36,37	8
3	MPD	B	1002	8/8	0.92	0.12	38,39,40,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.