



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:46 AM UTC

PDB ID : 1EMS / pdb_00001ems
Title : CRYSTAL STRUCTURE OF THE C. ELEGANS NITFHIT PROTEIN
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Deposited on : 2000-03-17
Resolution : 2.80 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

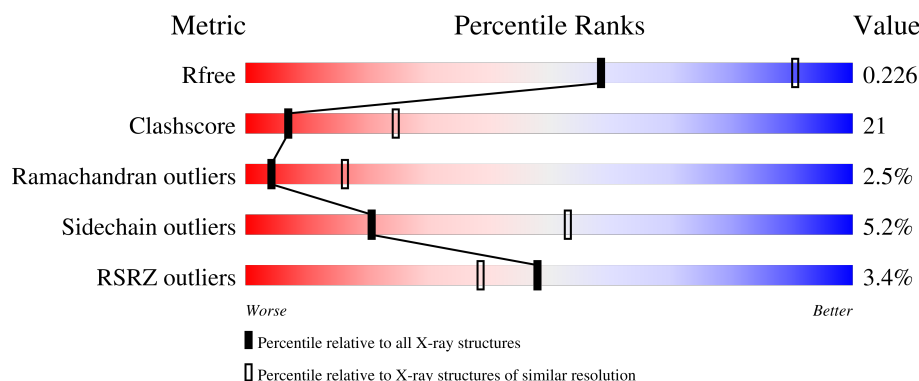
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	440	
1	B	440	

2 Entry composition [i](#)

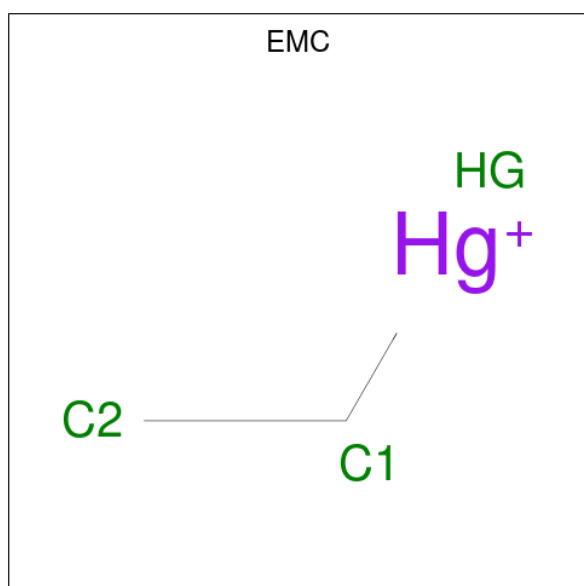
There are 5 unique types of molecules in this entry. The entry contains 6708 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NIT-FRAGILE HISTIDINE TRIAD FUSION PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	0	0
			3274	2066	581	604	23			
1	B	410	Total	C	N	O	S	0	0	0
			3246	2044	579	600	23			

- Molecule 2 is ETHYL MERCURY ION (CCD ID: EMC) (formula: C_2H_5Hg).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	Hg	0	0
			3	2	1		
2	A	1	Total	C	Hg	0	0
			3	2	1		
2	A	1	Total	C	Hg	0	0
			3	2	1		
2	B	1	Total	C	Hg	0	0
			3	2	1		

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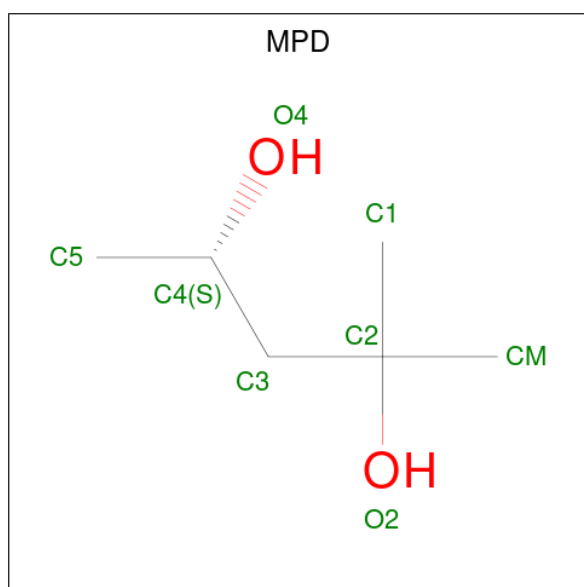
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	Hg	0	0
			3	2	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Na	0	0
			3	3		
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

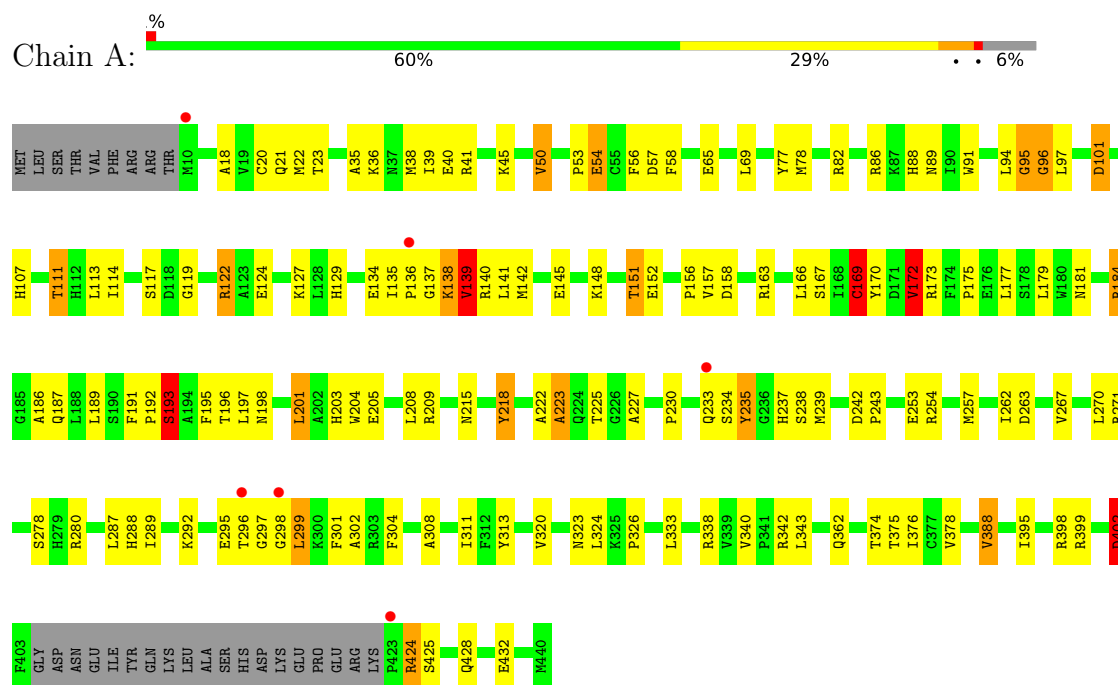
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	100	Total	O	0	0
			100	100		
5	B	61	Total	O	0	0
			61	61		

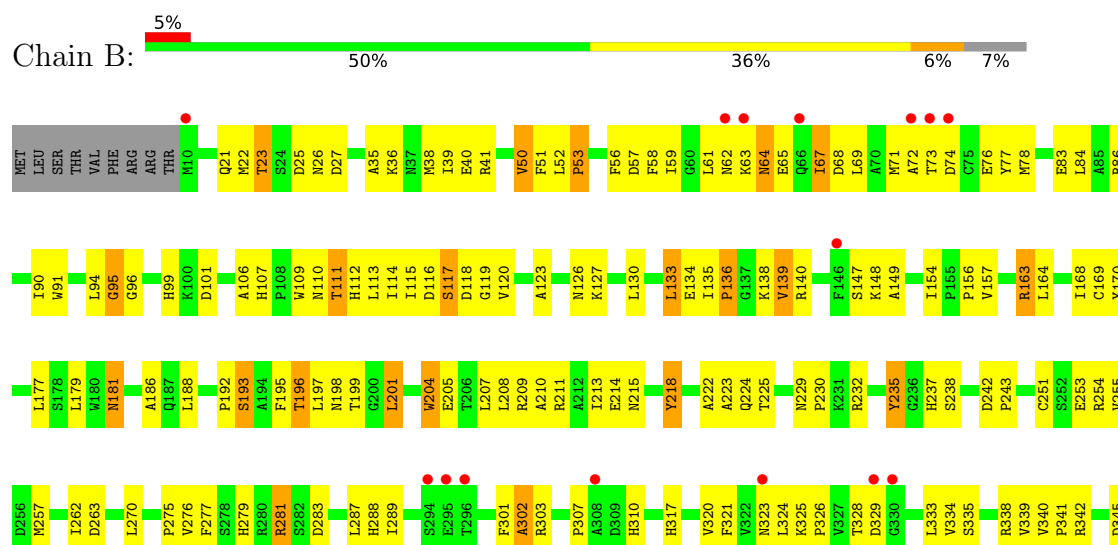
3 Residue-property plots

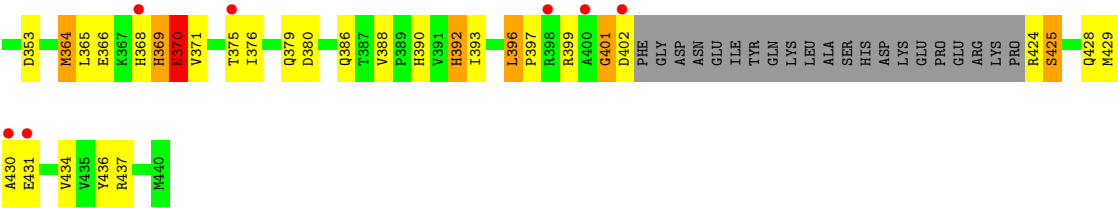
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: NIT-FRAGILE HISTIDINE TRIAD FUSION PROTEIN



• Molecule 1: NIT-FRAGILE HISTIDINE TRIAD FUSION PROTEIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	68.75Å 100.44Å 158.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.8 (30.00-2.80) 96.1 (30.00-2.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.28 (at 2.81Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.190 , 0.231 0.186 , 0.226	Depositor DCC
R_{free} test set	3344 reflections (6.70%)	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.9	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	0.92	EDS
Total number of atoms	6708	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.56% 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: MPD, NA, EMC

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	0.46	0/3351	1.01	19/4537 (0.4%)
1	B	0.41	0/3320	0.98	12/4496 (0.3%)
All	All	0.44	0/6671	1.00	31/9033 (0.3%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	SER	N-CA-C	-10.57	100.05	113.16
1	B	26	ASN	N-CA-C	-9.38	99.72	112.94
1	A	193	SER	N-CA-C	8.93	120.47	107.88
1	B	64	ASN	N-CA-C	-7.90	103.79	113.19
1	A	139	VAL	N-CA-C	7.48	119.11	108.42
1	A	138	LYS	N-CA-C	7.19	122.23	113.17
1	A	218	TYR	N-CA-C	-7.13	100.93	110.55
1	A	172	VAL	CB-CA-C	-6.39	103.52	112.14
1	B	53	PRO	N-CA-C	6.00	120.07	111.13
1	B	223	ALA	N-CA-C	5.86	117.87	109.14
1	A	187	GLN	N-CA-C	-5.74	106.63	113.97
1	A	295	GLU	N-CA-C	5.67	118.70	109.06
1	B	119	GLY	N-CA-C	-5.65	107.39	115.64
1	A	101	ASP	CA-C-N	5.64	126.89	119.84
1	A	101	ASP	C-N-CA	5.64	126.89	119.84
1	A	278	SER	N-CA-C	-5.59	106.46	113.28
1	A	223	ALA	N-CA-C	5.55	118.12	109.52
1	B	193	SER	N-CA-C	5.54	117.22	108.96
1	A	239	MET	N-CA-C	5.43	116.24	108.74
1	A	235	TYR	N-CA-C	5.39	117.24	111.36
1	B	235	TYR	N-CA-C	5.38	118.06	111.82
1	B	218	TYR	N-CA-C	-5.36	102.94	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	GLY	N-CA-C	5.34	125.84	113.18
1	A	111	THR	N-CA-C	5.31	117.90	109.24
1	B	111	THR	N-CA-C	5.30	117.16	108.52
1	A	166	LEU	N-CA-C	5.25	117.46	108.90
1	A	189	LEU	N-CA-C	-5.23	101.59	109.85
1	A	77	TYR	N-CA-C	5.16	119.67	112.90
1	A	169	CYS	N-CA-C	5.14	121.74	110.80
1	B	147	SER	N-CA-C	5.12	114.90	108.45
1	B	164	LEU	N-CA-C	5.06	116.85	108.20

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	3274	0	3210	117	0
1	B	3246	0	3184	157	0
2	A	9	0	0	0	0
2	B	6	0	0	0	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
4	A	8	0	14	0	0
5	A	100	0	0	3	0
5	B	61	0	0	1	0
All	All	6708	0	6408	272	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 21.

All (272) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:CYS:HB3	1:A:193:SER:CB	1.67	1.23
1:A:169:CYS:HB3	1:A:193:SER:HB3	1.30	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ASP:HB2	1:B:399:ARG:HH22	1.20	1.05
1:A:54:GLU:HB2	1:A:193:SER:HA	1.40	1.03
1:B:67:ILE:HD11	1:B:106:ALA:HA	1.43	0.98
1:B:329:ASP:HB2	1:B:399:ARG:NH2	1.82	0.94
1:A:169:CYS:HB3	1:A:193:SER:HB2	1.50	0.93
1:B:364:MET:HE2	1:B:365:LEU:HD23	1.56	0.88
1:A:41:ARG:HB2	1:A:257:MET:HE1	1.55	0.87
1:B:135:ILE:HG21	1:B:138:LYS:HD2	1.54	0.87
1:A:156:PRO:HD3	1:A:181:ASN:HD22	1.39	0.86
1:A:169:CYS:CB	1:A:193:SER:HB3	2.05	0.86
1:A:243:PRO:HB2	1:A:270:LEU:HD12	1.58	0.85
1:B:41:ARG:HB2	1:B:257:MET:HE1	1.57	0.85
1:B:116:ASP:HB3	1:B:118:ASP:H	1.44	0.83
1:B:323:ASN:HD22	1:B:324:LEU:H	1.27	0.83
1:B:41:ARG:CZ	1:B:257:MET:HE3	2.14	0.77
1:A:135:ILE:HB	1:A:139:VAL:HG23	1.67	0.76
1:B:99:HIS:HB3	1:B:109:TRP:HB2	1.66	0.76
1:A:169:CYS:O	1:A:172:VAL:HG22	1.87	0.75
1:B:23:THR:HB	1:B:225:THR:O	1.87	0.75
1:B:57:ASP:HB2	1:B:71:MET:HE1	1.70	0.73
1:B:324:LEU:HD22	1:B:424:ARG:HB2	1.71	0.72
1:B:25:ASP:HB3	1:B:27:ASP:H	1.56	0.71
1:A:21:GLN:NE2	1:A:238:SER:H	1.89	0.71
1:B:243:PRO:HB2	1:B:270:LEU:HD12	1.73	0.71
1:A:184:ARG:HH11	1:A:184:ARG:HB3	1.57	0.70
1:B:72:ALA:O	1:B:73:THR:HB	1.93	0.69
1:B:116:ASP:HB2	1:B:120:VAL:H	1.55	0.68
1:B:134:GLU:HG3	1:B:140:ARG:HG3	1.73	0.68
1:B:329:ASP:CB	1:B:399:ARG:HH22	2.02	0.68
1:B:430:ALA:O	1:B:434:VAL:HG13	1.93	0.68
1:B:323:ASN:ND2	1:B:324:LEU:H	1.90	0.68
1:A:172:VAL:HG13	1:A:191:PHE:CD2	2.29	0.68
1:A:184:ARG:HB3	1:A:184:ARG:NH1	2.09	0.67
1:B:112:HIS:HB2	1:B:168:ILE:HD11	1.75	0.67
1:A:36:LYS:O	1:A:40:GLU:HG3	1.95	0.67
1:B:425:SER:OG	1:B:428:GLN:HB3	1.94	0.66
1:B:71:MET:SD	1:B:77:TYR:HD2	2.19	0.65
1:A:288:HIS:C	1:A:289:ILE:HD12	2.20	0.65
1:B:323:ASN:HD22	1:B:324:LEU:N	1.93	0.64
1:B:287:LEU:HG	1:B:289:ILE:CD1	2.27	0.64
1:B:364:MET:HG3	1:B:365:LEU:N	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:HIS:C	1:B:289:ILE:HD12	2.23	0.63
1:A:41:ARG:CZ	1:A:257:MET:HE3	2.29	0.63
1:B:201:LEU:C	1:B:201:LEU:HD23	2.24	0.63
1:A:399:ARG:O	1:A:402:ASP:HB2	1.99	0.62
1:B:133:LEU:CD2	1:B:135:ILE:HG13	2.29	0.62
1:B:323:ASN:ND2	1:B:324:LEU:N	2.48	0.62
1:A:297:GLY:HA2	1:A:308:ALA:HB2	1.83	0.61
1:B:23:THR:HG22	1:B:255:VAL:CG2	2.30	0.61
1:B:287:LEU:HG	1:B:289:ILE:HD11	1.81	0.61
1:B:368:HIS:C	1:B:370:ASN:H	2.07	0.61
1:B:379:GLN:O	1:B:386:GLN:HB2	2.01	0.61
1:B:116:ASP:HB2	1:B:120:VAL:N	2.16	0.61
1:A:38:MET:HG2	1:A:257:MET:HE2	1.82	0.61
1:A:18:ALA:HB3	1:A:50:VAL:HG12	1.83	0.60
1:B:41:ARG:NE	1:B:257:MET:HE3	2.16	0.60
1:B:364:MET:HE2	1:B:365:LEU:HA	1.82	0.60
1:B:396:LEU:N	1:B:396:LEU:HD23	2.15	0.60
1:B:107:HIS:HB3	1:B:148:LYS:HB2	1.83	0.60
1:B:138:LYS:O	1:B:139:VAL:HG23	2.02	0.60
1:B:340:VAL:CG1	1:B:345:ASP:HB2	2.32	0.60
1:A:151:THR:HG22	1:A:152:GLU:HG3	1.82	0.60
1:A:156:PRO:HD3	1:A:181:ASN:ND2	2.12	0.60
1:A:280:ARG:NH2	5:A:535:HOH:O	2.35	0.60
1:B:64:ASN:O	1:B:68:ASP:HB2	2.02	0.60
1:A:297:GLY:CA	1:A:308:ALA:HB2	2.32	0.59
1:B:50:VAL:HG22	1:B:90:ILE:CD1	2.33	0.59
1:B:110:ASN:HB3	1:B:127:LYS:HB2	1.86	0.58
1:B:135:ILE:CG2	1:B:138:LYS:HD2	2.31	0.58
1:B:301:PHE:O	1:B:302:ALA:HB3	2.04	0.57
1:B:320:VAL:HG13	1:B:334:VAL:HG22	1.86	0.57
1:B:67:ILE:HD11	1:B:106:ALA:CA	2.26	0.57
1:A:122:ARG:HG3	1:A:122:ARG:HH11	1.69	0.57
1:A:35:ALA:O	1:A:39:ILE:HG13	2.05	0.57
1:B:22:MET:O	1:B:224:GLN:HA	2.05	0.56
1:B:123:ALA:CB	1:B:157:VAL:HG21	2.35	0.56
1:B:36:LYS:HE2	1:B:40:GLU:OE1	2.05	0.56
1:B:434:VAL:HA	1:B:437:ARG:NH1	2.20	0.56
1:B:71:MET:SD	1:B:77:TYR:CD2	3.00	0.55
1:A:140:ARG:HG3	1:A:140:ARG:HH11	1.72	0.55
1:A:167:SER:O	1:A:192:PRO:HD2	2.07	0.55
1:A:362:GLN:HG3	1:A:374:THR:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:GLN:HE22	1:A:237:HIS:N	2.04	0.55
1:B:73:THR:HG23	1:B:113:LEU:HD21	1.89	0.55
1:B:431:GLU:O	1:B:434:VAL:HG22	2.06	0.55
1:A:56:PHE:CE2	1:A:94:LEU:HB3	2.42	0.54
1:B:63:LYS:C	1:B:65:GLU:H	2.13	0.54
1:B:396:LEU:HD23	1:B:396:LEU:H	1.71	0.54
1:A:107:HIS:HB3	1:A:148:LYS:HB2	1.89	0.54
1:A:201:LEU:HD23	1:A:201:LEU:C	2.33	0.54
1:B:210:ALA:O	1:B:214:GLU:HG3	2.08	0.53
1:B:324:LEU:HD13	1:B:325:LYS:HG3	1.90	0.53
1:A:96:GLY:HA2	1:A:111:THR:O	2.08	0.53
1:A:97:LEU:CD2	1:A:113:LEU:HD12	2.37	0.53
1:A:97:LEU:HD21	1:A:113:LEU:HD12	1.91	0.53
1:B:339:VAL:HA	1:B:390:HIS:CD2	2.43	0.53
1:B:156:PRO:HD3	1:B:181:ASN:ND2	2.24	0.53
1:B:197:LEU:O	1:B:201:LEU:HB3	2.09	0.53
1:B:364:MET:HE3	1:B:364:MET:O	2.09	0.53
1:A:22:MET:HG2	1:A:53:PRO:HG3	1.91	0.53
1:A:173:ARG:HD2	5:A:527:HOH:O	2.09	0.52
1:B:62:ASN:ND2	1:B:63:LYS:H	2.08	0.52
1:A:91:TRP:CH2	1:A:122:ARG:HG2	2.44	0.52
1:A:184:ARG:HH11	1:A:184:ARG:CB	2.22	0.52
1:B:156:PRO:HD3	1:B:181:ASN:HD22	1.73	0.52
1:B:51:PHE:C	1:B:52:LEU:HD12	2.35	0.52
1:A:196:THR:HG22	1:A:198:ASN:H	1.74	0.52
1:A:41:ARG:HB2	1:A:257:MET:CE	2.34	0.52
1:B:63:LYS:C	1:B:65:GLU:N	2.66	0.52
1:B:205:GLU:O	1:B:209:ARG:HG3	2.10	0.52
1:B:434:VAL:HA	1:B:437:ARG:HH12	1.75	0.52
1:A:302:ALA:HB2	1:A:388:VAL:HG23	1.92	0.52
1:A:142:MET:HB3	1:A:145:GLU:HG3	1.92	0.52
1:A:195:PHE:O	1:A:234:SER:HA	2.10	0.51
1:A:54:GLU:CB	1:A:193:SER:HA	2.27	0.51
1:B:72:ALA:C	1:B:74:ASP:H	2.19	0.51
1:B:235:TYR:O	1:B:237:HIS:HD2	1.94	0.51
1:A:20:CYS:O	1:A:222:ALA:HB1	2.11	0.50
1:A:142:MET:CB	1:A:145:GLU:HG3	2.40	0.50
1:A:173:ARG:O	1:A:175:PRO:HD3	2.11	0.50
1:A:78:MET:HE1	1:A:94:LEU:CD1	2.41	0.50
1:A:201:LEU:HA	1:A:235:TYR:CE1	2.47	0.50
1:B:369:HIS:O	1:B:371:VAL:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ASP:HB2	1:A:243:PRO:CD	2.42	0.50
1:B:207:LEU:O	1:B:211:ARG:HG2	2.12	0.50
1:B:169:CYS:HA	1:B:193:SER:OG	2.12	0.50
1:B:340:VAL:HG11	1:B:345:ASP:HB2	1.92	0.50
1:B:275:PRO:HG2	1:B:279:HIS:CE1	2.47	0.50
1:A:41:ARG:NE	1:A:257:MET:HE3	2.27	0.49
1:B:23:THR:HG22	1:B:255:VAL:HG22	1.93	0.49
1:A:263:ASP:OD2	1:B:254:ARG:NH2	2.35	0.49
1:B:52:LEU:HD12	1:B:52:LEU:N	2.28	0.49
1:A:323:ASN:HD22	1:A:324:LEU:N	2.11	0.49
1:B:368:HIS:C	1:B:370:ASN:N	2.71	0.49
1:A:173:ARG:HH22	1:A:203:HIS:CE1	2.28	0.49
1:B:57:ASP:CB	1:B:71:MET:HE1	2.42	0.49
1:B:50:VAL:HG22	1:B:90:ILE:HD11	1.93	0.49
1:B:38:MET:HA	1:B:257:MET:CE	2.42	0.49
1:B:424:ARG:NH2	1:B:429:MET:HG2	2.28	0.49
1:B:218:TYR:CD2	1:B:262:ILE:HG22	2.48	0.49
1:A:158:ASP:OD1	1:A:163:ARG:HD3	2.13	0.49
1:A:205:GLU:O	1:A:209:ARG:HG3	2.13	0.49
1:A:342:ARG:HG3	1:A:342:ARG:HH11	1.78	0.48
1:B:209:ARG:O	1:B:213:ILE:HG13	2.13	0.48
1:A:197:LEU:O	1:A:201:LEU:HB3	2.13	0.48
1:B:366:GLU:O	1:B:370:ASN:HA	2.13	0.48
1:B:56:PHE:CZ	1:B:94:LEU:HB3	2.49	0.48
1:B:163:ARG:HB3	1:B:186:ALA:HA	1.95	0.48
1:B:36:LYS:HG3	1:B:84:LEU:HD11	1.96	0.48
1:B:126:ASN:O	1:B:127:LYS:C	2.56	0.48
1:B:303:ARG:HG2	1:B:303:ARG:HH11	1.78	0.48
1:A:138:LYS:O	1:A:139:VAL:HG13	2.14	0.47
1:A:163:ARG:HB3	1:A:186:ALA:HA	1.96	0.47
1:A:113:LEU:HD23	1:A:124:GLU:HG2	1.96	0.47
1:B:324:LEU:O	1:B:424:ARG:HG3	2.13	0.47
1:A:298:GLY:O	1:A:299:LEU:HB2	2.14	0.47
1:B:179:LEU:HD23	1:B:215:ASN:OD1	2.15	0.47
1:B:188:LEU:N	1:B:188:LEU:HD12	2.29	0.47
1:A:56:PHE:CZ	1:A:94:LEU:HB3	2.50	0.47
1:A:425:SER:OG	1:A:428:GLN:HG3	2.13	0.47
1:A:45:LYS:HE2	5:A:597:HOH:O	2.15	0.47
1:B:58:PHE:CZ	1:B:69:LEU:HB2	2.49	0.47
1:B:198:ASN:O	1:B:201:LEU:HD22	2.14	0.47
1:B:229:ASN:HB2	1:B:230:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:MET:HA	1:A:257:MET:CE	2.44	0.46
1:A:267:VAL:O	1:A:271:ARG:HG2	2.15	0.46
1:B:369:HIS:HD2	1:B:399:ARG:NH2	2.13	0.46
1:A:227:ALA:HA	1:A:233:GLN:NE2	2.31	0.46
1:B:328:THR:OG1	1:B:399:ARG:NH1	2.49	0.46
1:B:364:MET:HE1	1:B:436:TYR:CD1	2.50	0.46
1:A:86:ARG:HA	1:A:117:SER:O	2.16	0.46
1:B:335:SER:OG	1:B:392:HIS:HB3	2.16	0.46
1:A:301:PHE:O	1:A:304:PHE:HB2	2.16	0.46
1:A:196:THR:HG22	1:A:198:ASN:N	2.31	0.45
1:B:59:ILE:HG23	1:B:232:ARG:HH11	1.81	0.45
1:A:38:MET:HA	1:A:257:MET:HE1	1.97	0.45
1:B:401:GLY:O	1:B:402:ASP:C	2.59	0.45
1:B:51:PHE:HB3	5:B:471:HOH:O	2.16	0.45
1:B:111:THR:OG1	1:B:126:ASN:ND2	2.49	0.45
1:B:366:GLU:HG2	1:B:371:VAL:HG23	1.98	0.45
1:B:253:GLU:O	1:B:254:ARG:HB3	2.16	0.45
1:A:254:ARG:NH2	1:B:263:ASP:OD2	2.39	0.45
1:B:91:TRP:CD1	1:B:117:SER:HG	2.34	0.45
1:B:321:PHE:CE1	1:B:333:LEU:HD12	2.51	0.45
1:B:364:MET:HE3	1:B:364:MET:C	2.42	0.45
1:A:18:ALA:HB3	1:A:50:VAL:CG1	2.45	0.45
1:B:38:MET:HA	1:B:257:MET:HE1	1.97	0.45
1:B:181:ASN:HD22	1:B:181:ASN:HA	1.64	0.45
1:A:338:ARG:NH1	1:A:340:VAL:HG11	2.32	0.45
1:B:57:ASP:N	1:B:57:ASP:OD2	2.50	0.45
1:B:342:ARG:HA	1:B:380:ASP:OD2	2.16	0.45
1:A:134:GLU:OE2	1:A:140:ARG:NH1	2.50	0.45
1:B:114:ILE:C	1:B:115:ILE:HD12	2.42	0.45
1:A:292:LYS:HE2	1:A:313:TYR:HE1	1.83	0.44
1:A:376:ILE:CD1	1:A:395:ILE:HG12	2.47	0.44
1:B:86:ARG:HA	1:B:117:SER:O	2.18	0.44
1:B:339:VAL:HA	1:B:390:HIS:NE2	2.33	0.44
1:A:140:ARG:HG3	1:A:140:ARG:NH1	2.31	0.44
1:A:204:TRP:CZ2	1:A:208:LEU:HD11	2.52	0.44
1:B:276:VAL:HG23	1:B:277:PHE:HD1	1.81	0.44
1:A:326:PRO:CD	1:A:424:ARG:HD2	2.47	0.44
1:B:324:LEU:HD22	1:B:324:LEU:O	2.16	0.44
1:A:398:ARG:HH11	1:A:398:ARG:HG3	1.82	0.44
1:A:58:PHE:CD1	1:A:58:PHE:C	2.96	0.44
1:A:113:LEU:CD2	1:A:124:GLU:HG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:THR:OG1	1:A:398:ARG:NH1	2.51	0.44
1:B:301:PHE:O	1:B:302:ALA:CB	2.64	0.44
1:B:424:ARG:HH21	1:B:429:MET:HG2	1.83	0.44
1:A:135:ILE:O	1:A:137:GLY:N	2.50	0.44
1:A:65:GLU:HG2	1:A:69:LEU:HD11	2.00	0.44
1:B:196:THR:HG22	1:B:199:THR:H	1.83	0.44
1:B:339:VAL:HG13	1:B:390:HIS:HD2	1.83	0.44
1:A:262:ILE:C	1:A:262:ILE:HD12	2.42	0.43
1:A:323:ASN:O	1:A:326:PRO:HD3	2.18	0.43
1:B:101:ASP:OD2	1:B:148:LYS:NZ	2.50	0.43
1:A:122:ARG:HH11	1:A:122:ARG:CG	2.31	0.43
1:B:56:PHE:CE1	1:B:94:LEU:HB3	2.53	0.43
1:A:297:GLY:HA3	1:A:308:ALA:HB2	2.00	0.43
1:B:59:ILE:HG23	1:B:232:ARG:NH1	2.33	0.43
1:B:238:SER:HB2	1:B:251:CYS:SG	2.58	0.43
1:A:113:LEU:C	1:A:114:ILE:HD12	2.44	0.43
1:A:127:LYS:HE2	1:A:129:HIS:O	2.19	0.43
1:B:61:LEU:HD12	1:B:61:LEU:N	2.34	0.43
1:B:375:THR:C	1:B:376:ILE:HD12	2.44	0.43
1:B:339:VAL:HG22	1:B:390:HIS:CD2	2.53	0.43
1:B:51:PHE:N	1:B:51:PHE:CD1	2.87	0.43
1:B:317:HIS:HB2	1:B:353:ASP:OD1	2.18	0.43
1:B:201:LEU:C	1:B:201:LEU:CD2	2.92	0.42
1:B:334:VAL:HB	1:B:393:ILE:HB	2.01	0.42
1:A:82:ARG:HD3	1:A:119:GLY:O	2.19	0.42
1:A:88:HIS:O	1:A:89:ASN:C	2.62	0.42
1:B:72:ALA:O	1:B:73:THR:CB	2.66	0.42
1:A:23:THR:HG23	1:A:225:THR:O	2.18	0.42
1:A:243:PRO:HB2	1:A:270:LEU:CD1	2.38	0.42
1:B:78:MET:HE2	1:B:78:MET:HA	2.01	0.42
1:B:130:LEU:HD13	1:B:149:ALA:HB2	2.02	0.42
1:A:107:HIS:O	1:A:148:LYS:HE2	2.19	0.42
1:A:243:PRO:CG	1:A:267:VAL:HG22	2.50	0.42
1:A:21:GLN:HG3	1:A:223:ALA:O	2.19	0.42
1:A:320:VAL:HA	1:A:333:LEU:O	2.19	0.42
1:B:281:ARG:NH1	1:B:283:ASP:OD1	2.53	0.42
1:B:53:PRO:O	1:B:56:PHE:HB3	2.20	0.42
1:B:326:PRO:HD2	1:B:424:ARG:HG3	2.01	0.42
1:B:392:HIS:CD2	1:B:392:HIS:N	2.88	0.42
1:A:57:ASP:O	1:A:58:PHE:HB3	2.20	0.41
1:B:133:LEU:HD21	1:B:135:ILE:HG13	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASP:OD2	1:A:148:LYS:NZ	2.53	0.41
1:A:78:MET:HE1	1:A:94:LEU:HD12	2.02	0.41
1:B:192:PRO:HA	1:B:222:ALA:O	2.21	0.41
1:B:204:TRP:CE2	1:B:208:LEU:HD11	2.55	0.41
1:A:343:LEU:HD11	1:A:378:VAL:HG11	2.02	0.41
1:B:115:ILE:CG2	1:B:116:ASP:N	2.83	0.41
1:A:57:ASP:OD2	1:A:58:PHE:N	2.54	0.41
1:A:299:LEU:HD12	1:A:311:ILE:HD13	2.02	0.41
1:B:242:ASP:C	1:B:242:ASP:OD1	2.63	0.41
1:B:21:GLN:HB2	1:B:238:SER:OG	2.20	0.41
1:A:253:GLU:O	1:A:254:ARG:HB3	2.21	0.41
1:B:135:ILE:O	1:B:136:PRO:C	2.64	0.41
1:B:307:PRO:HD2	1:B:310:HIS:ND1	2.35	0.41
1:B:396:LEU:HA	1:B:397:PRO:HD2	1.89	0.40
1:A:227:ALA:HB2	1:A:233:GLN:HE22	1.86	0.40
1:B:35:ALA:O	1:B:39:ILE:HG13	2.21	0.40
1:A:179:LEU:HD23	1:A:215:ASN:OD1	2.21	0.40
1:A:218:TYR:CD2	1:A:242:ASP:HA	2.56	0.40
1:A:424:ARG:NH2	1:A:432:GLU:OE1	2.48	0.40
1:A:21:GLN:NE2	1:A:237:HIS:N	2.69	0.40
1:A:323:ASN:HD22	1:A:324:LEU:H	1.67	0.40
1:B:95:GLY:HA2	1:B:192:PRO:HG3	2.04	0.40
1:B:198:ASN:HA	1:B:201:LEU:HD13	2.04	0.40
1:B:229:ASN:HB2	1:B:230:PRO:CD	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	408/440 (93%)	376 (92%)	23 (6%)	9 (2%)	5 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	406/440 (92%)	359 (88%)	36 (9%)	11 (3%)	4	15
All	All	814/880 (92%)	735 (90%)	59 (7%)	20 (2%)	4	16

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	CYS
1	A	402	ASP
1	B	136	PRO
1	A	54	GLU
1	A	95	GLY
1	A	424	ARG
1	B	170	TYR
1	B	302	ALA
1	A	96	GLY
1	B	67	ILE
1	B	95	GLY
1	B	370	ASN
1	B	401	GLY
1	A	136	PRO
1	A	170	TYR
1	A	299	LEU
1	B	204	TRP
1	B	96	GLY
1	B	369	HIS
1	B	341	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	357/383 (93%)	341 (96%)	16 (4%)	24	58
1	B	353/383 (92%)	332 (94%)	21 (6%)	18	48
All	All	710/766 (93%)	673 (95%)	37 (5%)	21	53

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	VAL
1	A	122	ARG
1	A	139	VAL
1	A	141	LEU
1	A	151	THR
1	A	157	VAL
1	A	172	VAL
1	A	177	LEU
1	A	184	ARG
1	A	193	SER
1	A	201	LEU
1	A	230	PRO
1	A	287	LEU
1	A	296	THR
1	A	388	VAL
1	A	402	ASP
1	B	23	THR
1	B	50	VAL
1	B	76	GLU
1	B	83	GLU
1	B	133	LEU
1	B	139	VAL
1	B	154	ILE
1	B	163	ARG
1	B	177	LEU
1	B	181	ASN
1	B	195	PHE
1	B	196	THR
1	B	201	LEU
1	B	281	ARG
1	B	338	ARG
1	B	364	MET
1	B	370	ASN
1	B	388	VAL
1	B	392	HIS
1	B	396	LEU
1	B	425	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	99	HIS
1	A	126	ASN
1	A	181	ASN
1	A	233	GLN
1	A	323	ASN
1	A	370	ASN
1	A	438	ASN
1	B	37	ASN
1	B	62	ASN
1	B	64	ASN
1	B	66	GLN
1	B	126	ASN
1	B	181	ASN
1	B	237	HIS
1	B	323	ASN
1	B	331	HIS
1	B	370	ASN
1	B	390	HIS
1	B	392	HIS
1	B	438	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](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	EMC	A	451	1	1,2,2	0.72	0	-		
2	EMC	B	452	1	1,2,2	0.61	0	-		
2	EMC	A	454	1	1,2,2	0.75	0	-		
4	MPD	A	502	-	7,7,7	0.45	0	9,10,10	0.52	0
2	EMC	A	453	1	1,2,2	0.55	0	-		
2	EMC	B	455	1	1,2,2	0.51	0	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPD	A	502	-	-	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	412/440 (93%)	-0.36	6 (1%) 72 63	7, 18, 41, 63	0
1	B	410/440 (93%)	0.27	22 (5%) 31 24	9, 33, 69, 88	0
All	All	822/880 (93%)	-0.05	28 (3%) 48 39	7, 23, 64, 88	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	73	THR	3.7
1	A	423	PRO	3.5
1	B	66	GLN	3.5
1	B	402	ASP	3.4
1	A	233	GLN	3.2
1	A	296	THR	3.2
1	B	63	LYS	3.1
1	B	62	ASN	3.1
1	B	72	ALA	2.9
1	B	146	PHE	2.8
1	B	430	ALA	2.7
1	B	368	HIS	2.6
1	B	375	THR	2.6
1	A	136	PRO	2.5
1	B	10	MET	2.5
1	B	308	ALA	2.5
1	B	294	SER	2.3
1	B	398	ARG	2.3
1	B	295	GLU	2.3
1	B	400	ALA	2.2
1	B	431	GLU	2.2
1	B	330	GLY	2.2
1	A	10	MET	2.2
1	B	296	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	323	ASN	2.1
1	B	329	ASP	2.1
1	A	298	GLY	2.0
1	B	74	ASP	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
4	MPD	A	502	8/8	0.74	0.18	40,43,45,45	0
3	NA	A	456	1/1	0.92	0.06	16,16,16,16	0
3	NA	B	458	1/1	0.96	0.23	20,20,20,20	0
2	EMC	B	452	3/3	0.99	0.18	23,23,23,23	3
2	EMC	B	455	3/3	0.99	0.19	24,24,24,24	3
2	EMC	A	451	3/3	0.99	0.20	24,24,24,24	3
3	NA	A	457	1/1	0.99	0.04	19,19,19,19	0
3	NA	A	459	1/1	0.99	0.21	11,11,11,11	0
2	EMC	A	453	3/3	0.99	0.20	25,25,25,25	3
2	EMC	A	454	3/3	0.99	0.20	25,25,25,25	3

6.5 Other polymers [i](#)

There are no such residues in this entry.