



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:44 PM UTC

PDB ID : 2HXG / pdb_00002hxg
Title : Crystal Structure of Mn²⁺ bound ECAI
Authors : Manjasetty, B.A.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2006-08-03
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
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

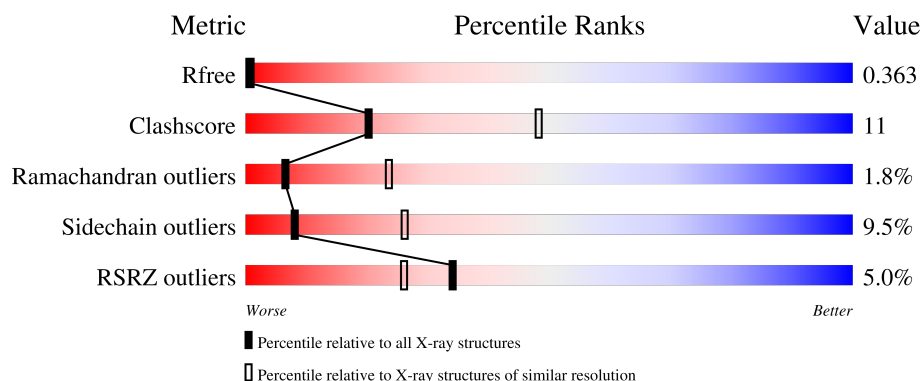
1 Overall quality at a glance

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	500	4% 76% 20% .
1	B	500	4% 74% 22% .
1	C	500	7% 72% 23% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11565 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 L-arabinose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	0	0
			3829	2431	669	705	24			
1	B	498	Total	C	N	O	S	0	0	0
			3895	2474	680	717	24			
1	C	498	Total	C	N	O	S	0	0	0
			3735	2353	650	708	24			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	PRO	ARG	SEE REMARK 999	UNP Q8FL89
B	72	PRO	ARG	SEE REMARK 999	UNP Q8FL89
C	72	PRO	ARG	SEE REMARK 999	UNP Q8FL89

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	41	Total	O	0	0
			41	41		
3	B	37	Total	O	0	0
			37	37		

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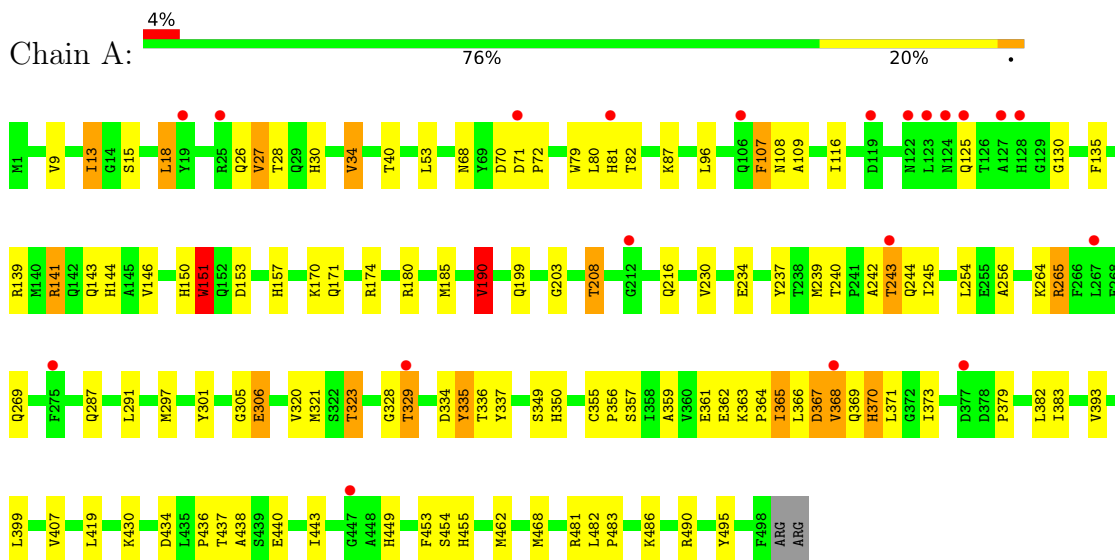
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	25	Total	O	0	0
			25	25		

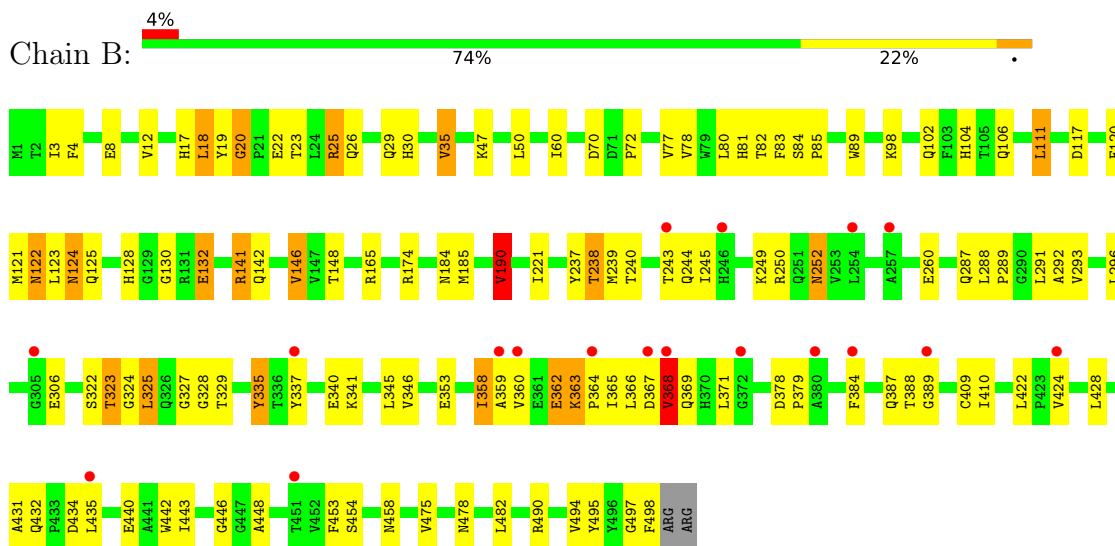
3 Residue-property plots

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.

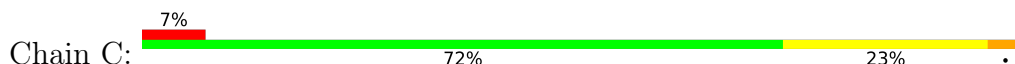
- Molecule 1: L-arabinose isomerase

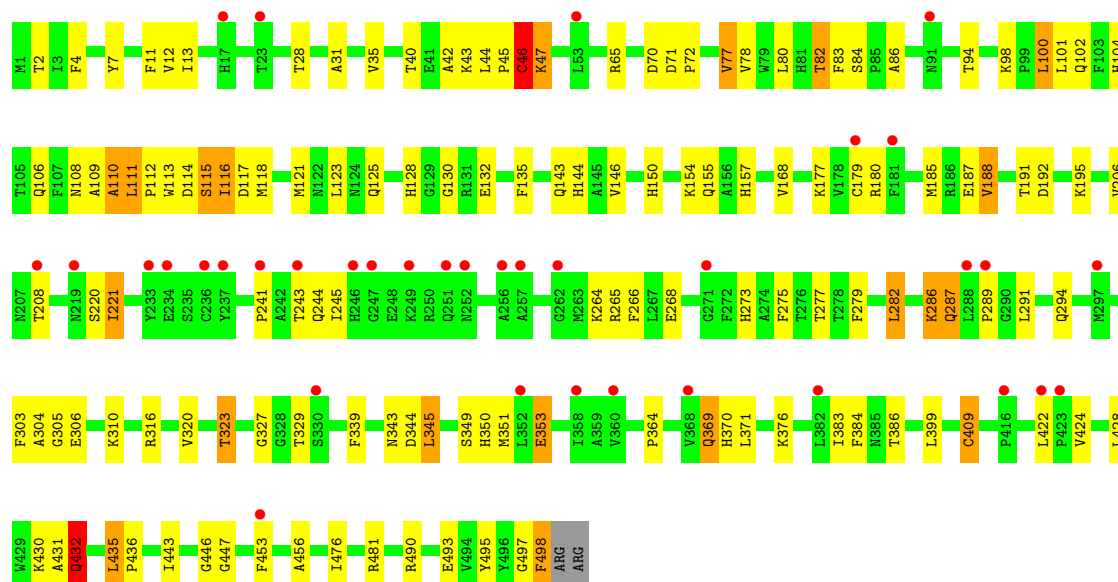


- Molecule 1: L-arabinose isomerase



- Molecule 1: L-arabinose isomerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	116.87Å 116.87Å 215.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.3 (20.00-2.80) 92.0 (20.00-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.13 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.229 , 0.288 0.317 , 0.363	Depositor DCC
R_{free} test set	1988 reflections (4.04%)	wwPDB-VP
Wilson B-factor (Å ²)	53.8	Xtriage
Anisotropy	0.683	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11565	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: MN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.61	0/3922	0.84	1/5325 (0.0%)
1	B	0.62	0/3991	0.87	2/5424 (0.0%)
1	C	0.57	0/3826	0.85	5/5203 (0.1%)
All	All	0.60	0/11739	0.85	8/15952 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
1	C	0	3
All	All	0	7

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	190	VAL	CB-CA-C	-7.47	102.25	112.04
1	A	190	VAL	CB-CA-C	-6.68	102.30	112.05
1	C	84	SER	CA-C-N	6.28	126.65	119.93
1	C	84	SER	C-N-CA	6.28	126.65	119.93
1	C	369	GLN	CA-C-N	5.74	132.03	121.70
1	C	369	GLN	C-N-CA	5.74	132.03	121.70
1	C	208	THR	N-CA-C	5.66	117.96	108.73
1	B	454	SER	N-CA-C	5.00	116.53	108.32

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	PHE	Peptide
1	B	327	GLY	Peptide
1	B	362	GLU	Peptide
1	B	368	VAL	Peptide
1	C	369	GLN	Peptide
1	C	431	ALA	Peptide
1	C	46	CYS	Peptide

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	3829	0	3686	97	0
1	B	3895	0	3783	94	0
1	C	3735	0	3440	90	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	41	0	0	3	0
3	B	37	0	0	2	0
3	C	25	0	0	0	0
All	All	11565	0	10909	253	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 11.

All (253) 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:C:180:ARG:HD2	1:C:195:LYS:HZ2	1.26	0.99
1:B:360:VAL:HG22	1:B:387:GLN:HG2	1.52	0.90
1:C:109:ALA:HB2	1:C:150:HIS:CG	2.12	0.85
1:A:364:PRO:HD2	1:A:383:ILE:O	1.80	0.79
1:C:180:ARG:HD2	1:C:195:LYS:NZ	1.97	0.79
1:B:102:GLN:NE2	1:B:104:HIS:HD2	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ARG:NH2	1:B:323:THR:O	2.21	0.74
1:B:337:TYR:OH	1:C:104:HIS:HE1	1.72	0.73
1:A:366:LEU:HD11	1:A:368:VAL:HG23	1.71	0.73
1:C:112:PRO:O	1:C:116:ILE:HG13	1.88	0.73
1:A:170:LYS:HD2	1:A:468:MET:HG3	1.73	0.71
1:A:367:ASP:O	1:A:368:VAL:C	2.34	0.71
1:A:367:ASP:O	1:A:369:GLN:N	2.25	0.70
1:A:107:PHE:HB3	1:A:108:ASN:HD22	1.55	0.69
1:A:321:MET:SD	1:A:462:MET:HE1	2.32	0.69
1:B:497:GLY:O	1:B:498:PHE:CD2	2.46	0.68
1:A:234:GLU:OE2	1:A:239:MET:HE2	1.94	0.68
1:B:102:GLN:HE22	1:B:104:HIS:CD2	2.11	0.67
1:B:102:GLN:NE2	1:B:104:HIS:CD2	2.62	0.66
1:B:102:GLN:HE22	1:B:104:HIS:HD2	1.41	0.66
1:A:449:HIS:HB2	1:B:128:HIS:HB2	1.76	0.66
1:A:13:ILE:HD12	1:A:13:ILE:H	1.59	0.66
1:A:107:PHE:CB	1:A:108:ASN:HD22	2.08	0.65
1:C:195:LYS:NZ	1:C:206:VAL:CB	2.60	0.65
1:B:125:GLN:HB2	1:B:128:HIS:CE1	2.31	0.65
1:C:80:LEU:HD13	1:C:130:GLY:HA2	1.78	0.63
1:C:100:LEU:HD12	1:C:101:LEU:N	2.13	0.63
1:C:109:ALA:HB2	1:C:150:HIS:CD2	2.32	0.63
1:C:82:THR:HG22	1:C:83:PHE:O	1.99	0.63
1:A:369:GLN:O	1:A:370:HIS:C	2.40	0.63
1:C:121:MET:O	1:C:125:GLN:HG2	1.98	0.63
1:C:102:GLN:HE22	1:C:104:HIS:HD2	1.46	0.63
1:C:498:PHE:C	1:C:498:PHE:CD2	2.77	0.62
1:B:121:MET:HE3	1:B:121:MET:HA	1.81	0.62
1:A:13:ILE:CD1	1:A:53:LEU:HA	2.30	0.62
1:A:355:CYS:SG	1:A:357:SER:HB2	2.40	0.62
1:C:185:MET:HB3	1:C:188:VAL:HG21	1.80	0.62
1:C:364:PRO:HD2	1:C:383:ILE:O	1.99	0.61
1:C:195:LYS:HZ3	1:C:206:VAL:CB	2.13	0.61
1:B:252:ASN:N	1:B:252:ASN:HD22	1.98	0.61
1:A:151:TRP:O	1:A:157:HIS:NE2	2.33	0.61
1:A:436:PRO:O	1:A:440:GLU:HG3	2.00	0.61
1:B:239:MET:SD	1:B:365:ILE:HG21	2.40	0.61
1:C:46:CYS:CB	1:C:47:LYS:HB2	2.30	0.61
1:A:356:PRO:HG3	1:A:382:LEU:HD12	1.82	0.61
1:B:30:HIS:ND1	1:B:81:HIS:NE2	2.42	0.60
1:C:185:MET:HB3	1:C:188:VAL:CG2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:GLN:HA	1:B:29:GLN:HE21	1.66	0.60
1:A:240:THR:HG21	1:A:366:LEU:HD13	1.83	0.59
1:A:237:TYR:CB	1:A:365:ILE:HG22	2.33	0.59
1:A:13:ILE:HD13	1:A:53:LEU:HA	1.83	0.59
1:C:316:ARG:O	1:C:320:VAL:HG23	2.03	0.59
1:A:337:TYR:H	1:B:106:GLN:HE22	1.51	0.58
1:B:360:VAL:HG22	1:B:387:GLN:HE21	1.69	0.58
1:B:360:VAL:HG22	1:B:387:GLN:CG	2.29	0.58
1:B:367:ASP:O	1:B:368:VAL:C	2.46	0.58
1:B:125:GLN:OE1	1:B:128:HIS:NE2	2.36	0.58
1:A:230:VAL:HG21	1:A:254:LEU:HD23	1.86	0.58
1:C:46:CYS:HB2	1:C:47:LYS:HB2	1.86	0.58
1:B:328:GLY:HA3	1:B:358:ILE:HG22	1.85	0.57
1:A:151:TRP:HE3	1:A:151:TRP:N	2.03	0.57
1:B:329:THR:HA	1:B:453:PHE:O	2.04	0.57
1:B:360:VAL:HG12	1:B:360:VAL:O	2.04	0.57
1:B:369:GLN:CB	1:B:378:ASP:HB3	2.34	0.57
1:C:195:LYS:HZ3	1:C:206:VAL:C	2.13	0.57
1:A:87:LYS:HB2	1:C:187:GLU:O	2.05	0.57
1:C:12:VAL:O	1:C:78:VAL:HA	2.05	0.57
1:C:180:ARG:CD	1:C:195:LYS:HZ2	2.11	0.56
1:B:494:VAL:HG21	1:C:495:TYR:HA	1.88	0.56
1:C:102:GLN:HE22	1:C:104:HIS:CD2	2.22	0.56
1:A:13:ILE:HD12	1:A:13:ILE:N	2.20	0.56
1:A:369:GLN:CB	1:A:379:PRO:HD2	2.35	0.56
1:B:120:PHE:O	1:B:123:LEU:O	2.24	0.56
1:C:350:HIS:ND1	1:C:353:GLU:OE1	2.38	0.56
1:A:70:ASP:CG	1:A:72:PRO:HD2	2.30	0.55
1:B:409:CYS:O	1:B:432:GLN:HB2	2.06	0.55
1:B:322:SER:O	1:B:323:THR:C	2.50	0.55
1:C:264:LYS:O	1:C:268:GLU:HG3	2.07	0.55
1:C:71:ASP:OD1	1:C:72:PRO:HD3	2.07	0.55
1:A:237:TYR:HB3	1:A:365:ILE:HG22	1.88	0.55
1:B:249:LYS:NZ	1:B:378:ASP:OD1	2.40	0.55
1:B:324:GLY:C	1:B:325:LEU:HD23	2.32	0.55
1:C:498:PHE:C	1:C:498:PHE:HD2	2.13	0.55
1:A:71:ASP:N	1:A:72:PRO:CD	2.70	0.55
1:C:409:CYS:HB2	1:C:432:GLN:HG3	1.90	0.54
1:C:2:THR:HG23	1:C:323:THR:HG21	1.88	0.54
1:A:335:TYR:CD2	1:B:121:MET:HG3	2.43	0.54
1:A:18:LEU:N	1:A:18:LEU:HD23	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:HIS:CD2	1:A:107:PHE:CZ	2.96	0.54
1:B:360:VAL:CG2	1:B:387:GLN:HG2	2.30	0.54
1:A:367:ASP:O	1:A:369:GLN:CA	2.56	0.53
1:B:368:VAL:O	1:B:368:VAL:HG12	2.09	0.53
1:B:337:TYR:H	1:C:106:GLN:HE22	1.57	0.53
1:B:70:ASP:OD1	1:B:72:PRO:HD2	2.09	0.53
1:A:151:TRP:N	1:A:151:TRP:CE3	2.77	0.53
1:B:422:LEU:HD13	1:C:116:ILE:HG22	1.90	0.53
1:B:240:THR:HG21	1:B:366:LEU:HB2	1.91	0.52
1:B:35:VAL:HG21	1:B:50:LEU:HB2	1.91	0.52
1:A:79:TRP:CZ2	1:A:81:HIS:HD2	2.27	0.52
1:A:30:HIS:CG	1:A:107:PHE:CZ	2.98	0.52
1:A:180:ARG:HB2	1:A:208:THR:HG22	1.92	0.51
1:B:190:VAL:HG23	1:C:132:GLU:OE2	2.10	0.51
1:A:27:VAL:HG23	1:A:81:HIS:ND1	2.26	0.51
1:B:122:ASN:OD1	1:B:122:ASN:C	2.54	0.51
1:A:334:ASP:O	1:B:128:HIS:HB3	2.11	0.51
1:B:190:VAL:HG13	1:C:135:PHE:CG	2.46	0.50
1:C:70:ASP:CG	1:C:72:PRO:HD2	2.37	0.50
1:A:495:TYR:CZ	1:C:490:ARG:HG2	2.47	0.50
1:B:20:GLY:N	3:B:525:HOH:O	2.43	0.50
1:B:322:SER:O	1:B:325:LEU:HB2	2.12	0.50
1:C:241:PRO:HA	1:C:244:GLN:HE21	1.77	0.50
1:A:367:ASP:O	1:A:369:GLN:CB	2.59	0.50
1:C:108:ASN:ND2	1:C:110:ALA:O	2.39	0.50
1:A:363:LYS:HD2	1:A:363:LYS:N	2.26	0.49
1:A:490:ARG:HD2	1:B:495:TYR:CE2	2.46	0.49
1:A:329:THR:HA	1:A:453:PHE:O	2.12	0.49
1:C:101:LEU:HD23	1:C:101:LEU:C	2.38	0.49
1:C:112:PRO:HB2	1:C:115:SER:OG	2.12	0.49
1:B:365:ILE:HG12	1:B:365:ILE:O	2.13	0.49
1:B:432:GLN:HG2	1:B:478:ASN:ND2	2.27	0.48
1:C:279:PHE:HA	1:C:282:LEU:HD12	1.95	0.48
1:B:190:VAL:CG2	1:C:132:GLU:OE2	2.61	0.48
1:C:102:GLN:NE2	1:C:104:HIS:HD2	2.10	0.48
1:C:42:ALA:O	1:C:44:LEU:HG	2.13	0.48
1:C:82:THR:CG2	1:C:83:PHE:N	2.76	0.48
1:C:179:CYS:O	1:C:275:PHE:HA	2.12	0.48
1:B:490:ARG:HG2	1:C:495:TYR:CE2	2.49	0.48
1:C:279:PHE:CE2	1:C:306:GLU:HG2	2.48	0.48
1:C:329:THR:HA	1:C:453:PHE:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:VAL:HA	1:C:101:LEU:O	2.14	0.47
1:A:135:PHE:HA	1:C:446:GLY:HA2	1.96	0.47
1:A:239:MET:HE3	1:A:243:THR:CG2	2.44	0.47
1:C:100:LEU:HD12	1:C:100:LEU:C	2.39	0.47
1:A:141:ARG:HH22	1:C:399:LEU:HB3	1.79	0.47
1:B:22:GLU:HA	1:B:25:ARG:HG3	1.96	0.47
1:B:165:ARG:HH21	1:B:325:LEU:HG	1.79	0.47
1:B:371:LEU:HD21	1:C:118:MET:HE3	1.96	0.47
1:B:366:LEU:HD11	1:B:368:VAL:HG23	1.97	0.47
1:B:442:TRP:O	1:B:446:GLY:O	2.32	0.47
1:B:17:HIS:O	1:B:18:LEU:C	2.57	0.47
1:B:346:VAL:HG22	1:B:435:LEU:HD21	1.96	0.47
1:A:320:VAL:O	1:A:323:THR:OG1	2.32	0.46
1:B:293:VAL:HG11	1:B:353:GLU:HG2	1.96	0.46
1:A:68:ASN:HD21	1:A:96:LEU:HA	1.80	0.46
1:A:27:VAL:CG2	1:A:81:HIS:ND1	2.79	0.46
1:A:190:VAL:HG22	1:B:132:GLU:OE2	2.16	0.46
1:A:462:MET:HE2	1:A:462:MET:N	2.30	0.46
1:C:177:LYS:H	1:C:273:HIS:HD2	1.64	0.46
1:B:237:TYR:HB3	1:B:363:LYS:O	2.16	0.46
1:A:305:GLY:O	1:A:306:GLU:C	2.59	0.45
1:C:291:LEU:O	1:C:291:LEU:HG	2.16	0.45
1:A:170:LYS:HD2	1:A:468:MET:CG	2.44	0.45
1:A:109:ALA:O	1:C:339:PHE:HB2	2.16	0.45
1:A:239:MET:O	1:A:244:GLN:NE2	2.50	0.45
1:A:443:ILE:HG21	1:B:146:VAL:HG11	1.98	0.45
1:C:112:PRO:HG2	1:C:116:ILE:HG12	1.98	0.45
1:A:13:ILE:HD13	1:A:53:LEU:HD22	1.98	0.45
1:A:141:ARG:HD3	1:C:493:GLU:OE2	2.17	0.45
1:A:265:ARG:HG2	1:A:269:GLN:HE22	1.82	0.45
1:B:443:ILE:HA	3:B:524:HOH:O	2.16	0.45
1:A:70:ASP:C	1:A:72:PRO:HD2	2.41	0.45
1:A:80:LEU:HD13	1:A:130:GLY:HA2	1.99	0.45
1:B:117:ASP:OD1	1:B:117:ASP:C	2.59	0.45
1:B:345:LEU:HD13	1:B:428:LEU:HD21	1.99	0.45
1:C:185:MET:O	1:C:188:VAL:HG23	2.17	0.45
1:A:366:LEU:HD12	1:A:367:ASP:H	1.81	0.45
1:C:13:ILE:CD1	1:C:31:ALA:HB2	2.46	0.45
1:C:192:ASP:O	1:C:310:LYS:NZ	2.46	0.45
1:A:26:GLN:O	1:A:30:HIS:NE2	2.50	0.45
1:B:84:SER:O	1:B:85:PRO:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:THR:O	1:B:364:PRO:HA	2.17	0.45
1:C:349:SER:OG	1:C:350:HIS:N	2.48	0.45
1:A:185:MET:HE3	1:A:306:GLU:HG3	1.98	0.44
1:B:260:GLU:HA	1:B:292:ALA:HB1	1.99	0.44
1:A:239:MET:HB3	1:A:243:THR:HG22	1.98	0.44
1:A:364:PRO:HB2	3:A:520:HOH:O	2.17	0.44
1:B:80:LEU:CD1	1:B:130:GLY:HA2	2.47	0.44
1:A:150:HIS:O	1:A:153:ASP:N	2.36	0.44
1:A:337:TYR:OH	1:B:104:HIS:HE1	2.01	0.44
1:B:4:PHE:HD1	1:B:323:THR:HG21	1.83	0.44
1:C:46:CYS:CA	1:C:47:LYS:HB2	2.48	0.44
1:B:335:TYR:CD2	1:C:121:MET:SD	3.11	0.44
1:B:388:THR:HG22	1:B:389:GLY:N	2.33	0.44
1:B:111:LEU:C	1:B:111:LEU:HD12	2.43	0.43
1:C:11:PHE:CD2	1:C:35:VAL:HG23	2.52	0.43
1:C:112:PRO:HG2	1:C:116:ILE:CG1	2.48	0.43
1:A:368:VAL:O	1:A:368:VAL:HG12	2.18	0.43
1:C:435:LEU:N	1:C:436:PRO:HD2	2.33	0.43
1:A:264:LYS:O	1:A:265:ARG:C	2.61	0.43
1:A:436:PRO:HA	1:B:148:THR:HB	2.00	0.43
1:B:81:HIS:HE1	1:B:124:ASN:HD22	1.67	0.43
1:A:71:ASP:N	1:A:72:PRO:HD3	2.34	0.43
1:B:287:GLN:NE2	1:B:379:PRO:HA	2.33	0.43
1:A:30:HIS:CD2	1:A:107:PHE:HZ	2.35	0.43
1:A:329:THR:HA	1:A:454:SER:HA	2.01	0.43
1:B:83:PHE:CZ	1:B:132:GLU:HG3	2.54	0.43
1:B:324:GLY:O	1:B:325:LEU:HD23	2.19	0.43
1:C:345:LEU:HD11	1:C:430:LYS:HE2	2.00	0.43
1:B:184:ASN:O	1:B:185:MET:C	2.62	0.42
1:C:4:PHE:CD2	1:C:45:PRO:HB2	2.54	0.42
1:C:286:LYS:O	1:C:287:GLN:CB	2.67	0.42
1:A:482:LEU:N	1:A:483:PRO:HD2	2.34	0.42
1:B:190:VAL:HG13	1:C:135:PHE:CD1	2.54	0.42
1:A:242:ALA:HA	3:A:531:HOH:O	2.19	0.42
1:A:70:ASP:C	1:A:72:PRO:CD	2.92	0.42
1:A:199:GLN:O	1:A:203:GLY:HA2	2.20	0.42
1:A:34:VAL:CG1	1:A:151:TRP:CD1	3.03	0.42
1:A:297:MET:HA	1:A:301:TYR:O	2.19	0.42
1:B:82:THR:HB	1:B:125:GLN:HE21	1.84	0.42
1:B:288:LEU:HD12	1:B:289:PRO:HD2	2.01	0.42
1:C:154:LYS:HA	1:C:157:HIS:ND1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:LEU:HA	1:C:294:GLN:HB2	2.02	0.42
1:A:146:VAL:HG21	1:C:443:ILE:CG2	2.50	0.42
1:A:349:SER:OG	1:A:350:HIS:N	2.52	0.42
1:A:109:ALA:N	1:A:151:TRP:HH2	2.18	0.42
1:A:171:GLN:O	1:A:174:ARG:HB2	2.20	0.42
1:A:180:ARG:HD3	1:A:208:THR:HG22	2.00	0.42
1:C:11:PHE:CD2	1:C:35:VAL:CG2	3.02	0.42
1:C:7:TYR:CD2	1:C:168:VAL:HG13	2.55	0.42
1:C:497:GLY:O	1:C:498:PHE:HB3	2.19	0.42
1:B:239:MET:HA	1:B:365:ILE:HG22	2.03	0.41
1:B:243:THR:HG21	1:B:365:ILE:HG23	2.02	0.41
1:B:340:GLU:O	1:B:341:LYS:C	2.63	0.41
1:B:185:MET:HB2	1:B:306:GLU:HB2	2.02	0.41
1:C:71:ASP:N	1:C:72:PRO:CD	2.83	0.41
1:C:327:GLY:HA3	1:C:456:ALA:HB2	2.01	0.41
1:C:344:ASP:HB3	1:C:435:LEU:HD12	2.02	0.41
1:B:19:TYR:O	1:B:20:GLY:O	2.38	0.41
1:A:256:ALA:HB2	1:A:287:GLN:NE2	2.36	0.41
1:A:437:THR:O	1:A:438:ALA:C	2.64	0.41
1:B:125:GLN:OE1	1:B:128:HIS:CE1	2.73	0.41
1:B:190:VAL:HG11	1:B:448:ALA:HB2	2.01	0.41
1:C:82:THR:HA	1:C:125:GLN:HB2	2.03	0.41
1:A:237:TYR:HB2	1:A:365:ILE:HG22	2.02	0.41
1:C:86:ALA:HB2	1:C:132:GLU:HG3	2.03	0.41
1:C:303:PHE:CE1	1:C:304:ALA:O	2.74	0.41
1:A:359:ALA:HB3	1:A:363:LYS:HE3	2.03	0.41
1:A:486:LYS:NZ	3:A:529:HOH:O	2.30	0.41
1:B:60:ILE:HG21	1:B:89:TRP:HA	2.03	0.41
1:C:111:LEU:O	1:C:113:TRP:N	2.54	0.41
1:A:371:LEU:HD22	1:A:373:ILE:HB	2.03	0.41
1:B:434:ASP:O	1:B:435:LEU:C	2.63	0.41
1:C:266:PHE:CD2	1:C:266:PHE:C	2.98	0.40
1:A:305:GLY:C	1:A:306:GLU:HG2	2.46	0.40
1:A:399:LEU:O	1:B:141:ARG:NH2	2.54	0.40
1:B:359:ALA:HB2	1:B:384:PHE:CD2	2.56	0.40
1:A:30:HIS:CE1	1:A:107:PHE:CE1	3.09	0.40
1:B:292:ALA:O	1:B:296:LEU:HG	2.20	0.40
1:C:83:PHE:H	1:C:125:GLN:HE21	1.69	0.40
1:A:239:MET:HE3	1:A:243:THR:HG22	2.02	0.40
1:B:410:ILE:HG22	1:B:431:ALA:HA	2.03	0.40
1:A:328:GLY:O	1:A:329:THR:CB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:SER:C	1:C:221:ILE:HG22	2.46	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	496/500 (99%)	453 (91%)	36 (7%)	7 (1%)	9	30
1	B	496/500 (99%)	451 (91%)	41 (8%)	4 (1%)	16	44
1	C	496/500 (99%)	418 (84%)	62 (12%)	16 (3%)	3	11
All	All	1488/1500 (99%)	1322 (89%)	139 (9%)	27 (2%)	6	23

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	TRP
1	A	368	VAL
1	A	370	HIS
1	B	245	ILE
1	C	287	GLN
1	C	370	HIS
1	C	371	LEU
1	B	20	GLY
1	C	43	LYS
1	C	376	LYS
1	C	447	GLY
1	C	40	THR
1	C	144	HIS
1	C	386	THR
1	A	143	GLN
1	C	110	ALA

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Mol	Chain	Res	Type
1	C	143	GLN
1	C	351	MET
1	A	144	HIS
1	A	329	THR
1	B	18	LEU
1	C	47	LYS
1	C	305	GLY
1	C	432	GLN
1	A	82	THR
1	B	368	VAL
1	C	289	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	394/419 (94%)	359 (91%)	35 (9%)	9	29
1	B	410/419 (98%)	374 (91%)	36 (9%)	9	29
1	C	369/419 (88%)	329 (89%)	40 (11%)	6	21
All	All	1173/1257 (93%)	1062 (90%)	111 (10%)	8	26

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	13	ILE
1	A	15	SER
1	A	18	LEU
1	A	27	VAL
1	A	28	THR
1	A	34	VAL
1	A	40	THR
1	A	116	ILE
1	A	125	GLN
1	A	139	ARG

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Mol	Chain	Res	Type
1	A	141	ARG
1	A	151	TRP
1	A	190	VAL
1	A	208	THR
1	A	216	GLN
1	A	243	THR
1	A	245	ILE
1	A	265	ARG
1	A	291	LEU
1	A	306	GLU
1	A	323	THR
1	A	335	TYR
1	A	336	THR
1	A	361	GLU
1	A	362	GLU
1	A	365	ILE
1	A	367	ASP
1	A	393	VAL
1	A	407	VAL
1	A	419	LEU
1	A	430	LYS
1	A	434	ASP
1	A	455	HIS
1	A	481	ARG
1	B	3	ILE
1	B	8	GLU
1	B	12	VAL
1	B	23	THR
1	B	25	ARG
1	B	35	VAL
1	B	47	LYS
1	B	77	VAL
1	B	78	VAL
1	B	98	LYS
1	B	111	LEU
1	B	122	ASN
1	B	124	ASN
1	B	132	GLU
1	B	141	ARG
1	B	142	GLN
1	B	146	VAL
1	B	174	ARG

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Mol	Chain	Res	Type
1	B	190	VAL
1	B	221	ILE
1	B	238	THR
1	B	244	GLN
1	B	250	ARG
1	B	252	ASN
1	B	291	LEU
1	B	323	THR
1	B	325	LEU
1	B	335	TYR
1	B	358	ILE
1	B	362	GLU
1	B	363	LYS
1	B	424	VAL
1	B	440	GLU
1	B	458	ASN
1	B	475	VAL
1	B	482	LEU
1	C	28	THR
1	C	46	CYS
1	C	65	ARG
1	C	77	VAL
1	C	82	THR
1	C	94	THR
1	C	98	LYS
1	C	100	LEU
1	C	111	LEU
1	C	114	ASP
1	C	115	SER
1	C	116	ILE
1	C	117	ASP
1	C	123	LEU
1	C	128	HIS
1	C	146	VAL
1	C	155	GLN
1	C	188	VAL
1	C	191	THR
1	C	221	ILE
1	C	243	THR
1	C	245	ILE
1	C	265	ARG
1	C	277	THR

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Mol	Chain	Res	Type
1	C	282	LEU
1	C	286	LYS
1	C	323	THR
1	C	343	ASN
1	C	345	LEU
1	C	353	GLU
1	C	384	PHE
1	C	409	CYS
1	C	422	LEU
1	C	424	VAL
1	C	428	LEU
1	C	432	GLN
1	C	435	LEU
1	C	476	ILE
1	C	481	ARG
1	C	498	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	26	GLN
1	A	108	ASN
1	A	125	GLN
1	A	143	GLN
1	A	152	GLN
1	A	244	GLN
1	A	251	GLN
1	A	269	GLN
1	A	298	GLN
1	A	343	ASN
1	A	370	HIS
1	A	464	GLN
1	A	478	ASN
1	B	6	ASN
1	B	16	GLN
1	B	29	GLN
1	B	97	ASN
1	B	102	GLN
1	B	104	HIS
1	B	106	GLN
1	B	124	ASN

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Mol	Chain	Res	Type
1	B	142	GLN
1	B	171	GLN
1	B	251	GLN
1	B	252	ASN
1	B	269	GLN
1	B	287	GLN
1	B	298	GLN
1	B	343	ASN
1	B	387	GLN
1	B	464	GLN
1	B	478	ASN
1	C	16	GLN
1	C	29	GLN
1	C	102	GLN
1	C	104	HIS
1	C	106	GLN
1	C	125	GLN
1	C	128	HIS
1	C	142	GLN
1	C	143	GLN
1	C	207	ASN
1	C	244	GLN
1	C	246	HIS
1	C	273	HIS
1	C	343	ASN
1	C	369	GLN
1	C	408	ASN
1	C	460	ASN
1	C	464	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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

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	498/500 (99%)	0.68	20 (4%) 42 33	42, 49, 55, 65	0
1	B	498/500 (99%)	0.63	18 (3%) 46 37	39, 47, 55, 71	0
1	C	498/500 (99%)	0.85	36 (7%) 21 16	36, 46, 53, 64	0
All	All	1494/1500 (99%)	0.72	74 (4%) 34 26	36, 47, 54, 71	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	246	HIS	3.9
1	A	123	LEU	3.8
1	B	424	VAL	3.6
1	C	237	TYR	3.6
1	B	384	PHE	3.5
1	B	360	VAL	3.5
1	A	19	TYR	3.3
1	A	106	GLN	3.3
1	C	416	PRO	3.2
1	B	367	ASP	3.1
1	A	122	ASN	3.0
1	A	124	ASN	3.0
1	C	251	GLN	3.0
1	C	352	LEU	2.8
1	C	241	PRO	2.8
1	A	128	HIS	2.8
1	B	435	LEU	2.7
1	C	257	ALA	2.7
1	C	247	GLY	2.7
1	A	119	ASP	2.7
1	C	243	THR	2.6
1	C	256	ALA	2.6
1	B	337	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	382	LEU	2.5
1	C	288	LEU	2.5
1	A	243	THR	2.5
1	A	329	THR	2.5
1	C	234	GLU	2.5
1	B	359	ALA	2.5
1	B	246	HIS	2.5
1	C	297	MET	2.4
1	A	368	VAL	2.4
1	B	368	VAL	2.4
1	C	368	VAL	2.4
1	C	453	PHE	2.4
1	B	254	LEU	2.4
1	C	236	CYS	2.4
1	A	125	GLN	2.4
1	C	208	THR	2.4
1	A	25	ARG	2.4
1	C	233	TYR	2.4
1	C	23	THR	2.4
1	C	330	SER	2.3
1	C	252	ASN	2.3
1	C	53	LEU	2.3
1	B	372	GLY	2.3
1	A	377	ASP	2.3
1	B	305	GLY	2.3
1	C	249	LYS	2.2
1	B	451	THR	2.2
1	A	275	PHE	2.2
1	B	257	ALA	2.2
1	C	179	CYS	2.2
1	C	422	LEU	2.2
1	C	219	ASN	2.2
1	C	17	HIS	2.2
1	C	289	PRO	2.2
1	C	262	GLY	2.2
1	C	360	VAL	2.1
1	C	423	PRO	2.1
1	A	81	HIS	2.1
1	A	447	GLY	2.1
1	B	380	ALA	2.1
1	C	91	ASN	2.1
1	A	267	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	181	PHE	2.1
1	C	271	GLY	2.1
1	A	212	GLY	2.0
1	B	389	GLY	2.0
1	B	243	THR	2.0
1	C	358	ILE	2.0
1	A	127	ALA	2.0
1	B	364	PRO	2.0
1	A	71	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
2	MN	C	501	1/1	0.93	0.11	71,71,71,71	0
2	MN	B	501	1/1	0.96	0.04	50,50,50,50	0
2	MN	A	501	1/1	0.98	0.03	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.