



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:07 PM UTC

PDB ID : 1NDF / pdb_00001ndf
Title : Carnitine Acetyltransferase in Complex with Carnitine
Authors : Jogl, G.; Tong, L.
Deposited on : 2002-12-09
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

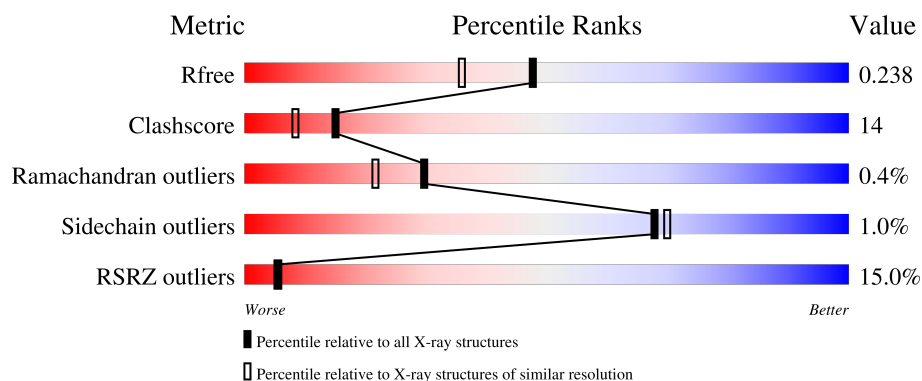
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	596	23% 71% 27% .
1	B	596	7% 75% 24% .

2 Entry composition [i](#)

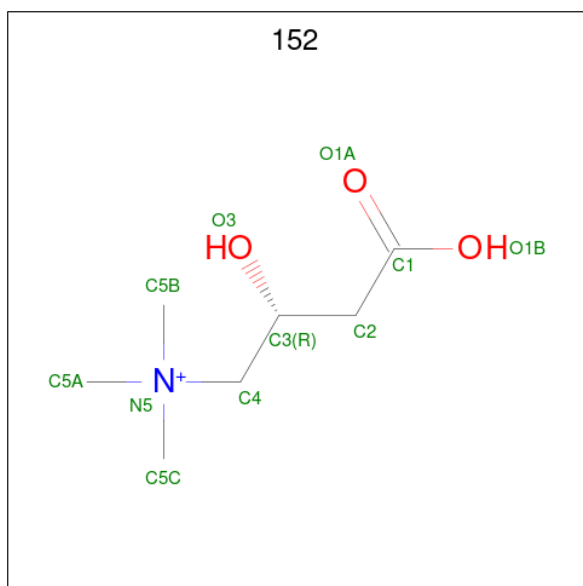
There are 3 unique types of molecules in this entry. The entry contains 10606 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Carnitine Acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	0	0
			4757	3034	820	875	28			
1	B	596	Total	C	N	O	S	0	0	0
			4757	3034	820	875	28			

- Molecule 2 is CARNITINE (CCD ID: 152) (formula: $C_7H_{16}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	7	1	3		
2	B	1	Total	C	N	O	0	0
			11	7	1	3		

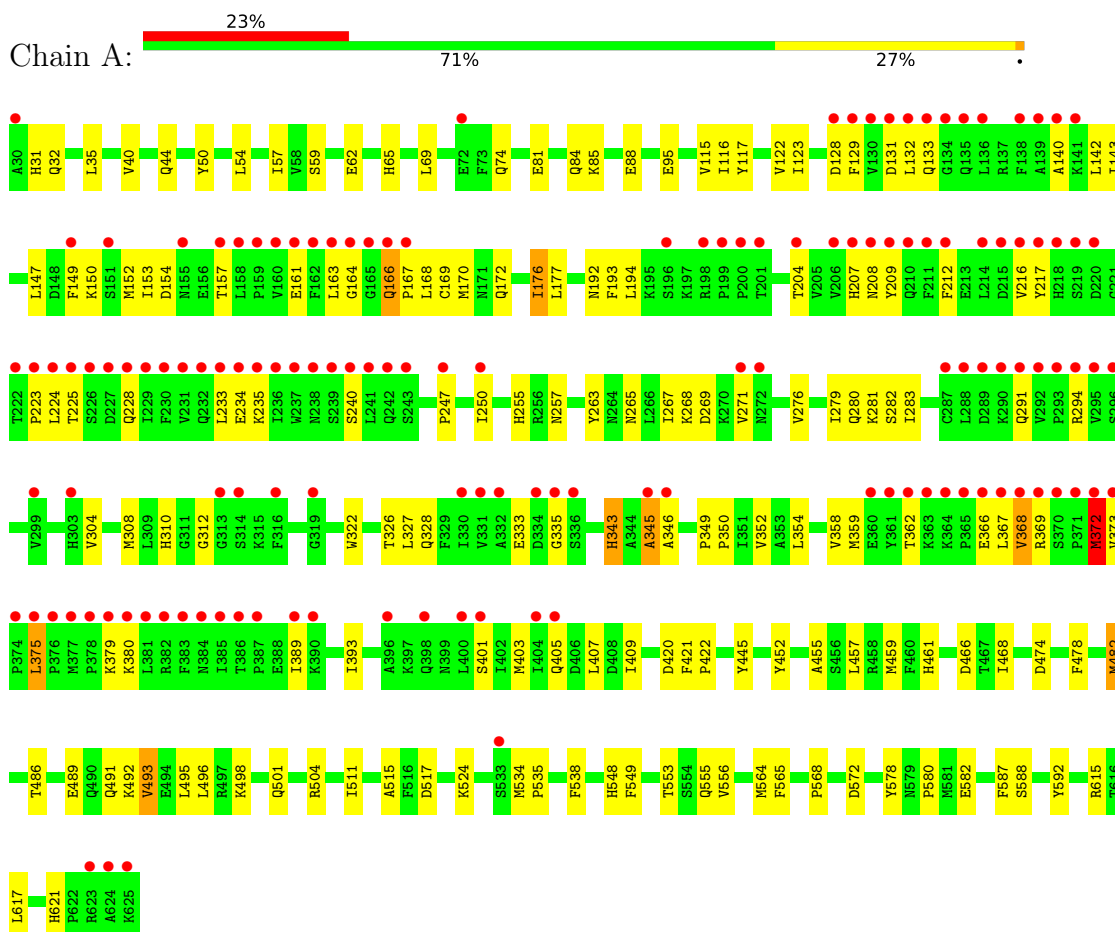
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	469	Total 469	O 469	0	0
3	B	601	Total 601	O 601	0	0

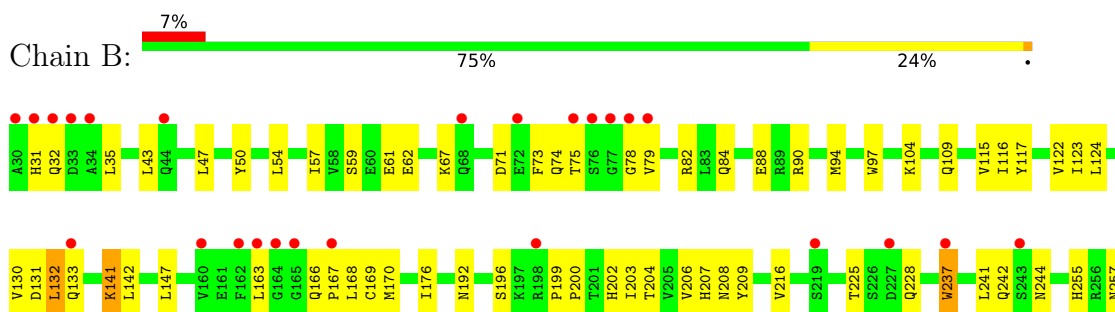
3 Residue-property plots [i](#)

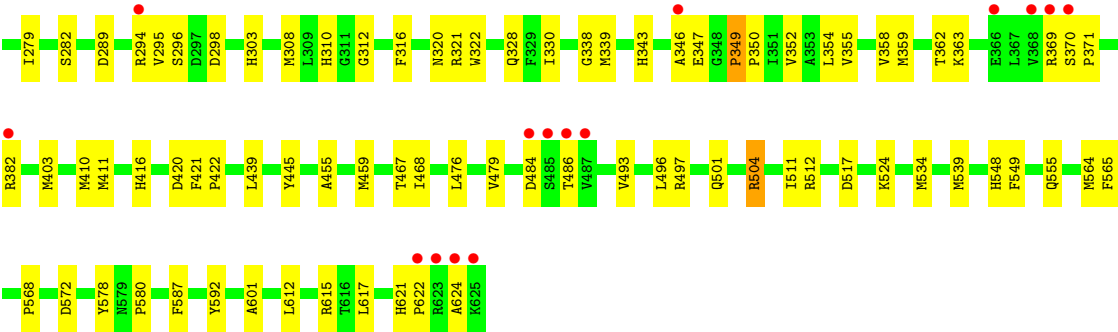
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Carnitine Acetyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	160.68Å 91.67Å 122.61Å 90.00° 128.84° 90.00°	Depositor
Resolution (Å)	19.95 – 1.90 19.95 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.7 (19.95-1.90) 96.6 (19.95-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.16 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.200 , 0.241 0.198 , 0.238	Depositor DCC
R_{free} test set	7946 reflections (7.33%)	wwPDB-VP
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10606	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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:
152

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	0.36	0/4872	0.86	11/6600 (0.2%)
1	B	0.39	0/4872	0.88	14/6600 (0.2%)
All	All	0.37	0/9744	0.87	25/13200 (0.2%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	HIS	N-CA-C	8.06	120.98	111.71
1	B	346	ALA	N-CA-C	7.48	119.06	108.74
1	B	517	ASP	N-CA-C	7.10	118.67	111.07
1	A	346	ALA	N-CA-C	6.99	117.47	108.24
1	A	40	VAL	N-CA-C	-6.71	100.42	107.60
1	B	57	ILE	N-CA-C	6.66	119.56	113.10
1	A	517	ASP	N-CA-C	6.11	117.61	111.07
1	B	343	HIS	N-CA-C	5.96	119.81	112.54
1	A	345	ALA	N-CA-C	5.70	117.57	111.36
1	B	349	PRO	N-CA-C	5.66	117.60	110.70
1	B	549	PHE	N-CA-C	5.65	118.62	108.17
1	A	549	PHE	N-CA-C	5.62	118.56	108.17
1	B	79	VAL	N-CA-C	5.59	116.23	110.36
1	A	445	TYR	N-CA-C	5.43	120.06	113.38
1	B	203	ILE	N-CA-C	-5.38	101.32	108.96
1	B	78	GLY	N-CA-C	5.29	120.10	111.27
1	B	316	PHE	N-CA-C	5.29	116.53	108.12
1	A	515	ALA	N-CA-C	-5.23	103.14	110.35
1	B	445	TYR	N-CA-C	5.15	119.84	113.50
1	A	57	ILE	N-CA-C	5.11	118.06	113.10
1	B	176	ILE	N-CA-C	5.09	119.53	112.35
1	A	553	THR	N-CA-C	5.08	116.71	109.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	289	ASP	N-CA-C	5.08	117.24	110.53
1	A	176	ILE	N-CA-C	5.05	118.20	111.44
1	B	467	THR	N-CA-C	5.05	117.19	109.07

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	4757	0	4733	145	0
1	B	4757	0	4733	114	0
2	A	11	0	15	2	0
2	B	11	0	15	1	0
3	A	469	0	0	8	0
3	B	601	0	0	9	0
All	All	10606	0	9496	261	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 14.

All (261) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ARG:HG2	1:B:94:MET:HE2	1.46	0.97
1:B:132:LEU:HD22	1:B:132:LEU:H	1.29	0.96
1:A:482:MET:HE2	1:A:482:MET:HA	1.50	0.93
1:B:308:MET:HE1	1:B:330:ILE:HB	1.50	0.93
1:B:534:MET:HB3	1:B:539:MET:HE3	1.49	0.91
1:A:534:MET:HE3	1:A:535:PRO:HD2	1.57	0.83
1:B:94:MET:CE	1:B:97:TRP:HA	2.09	0.83
1:A:310:HIS:HD2	1:A:312:GLY:H	1.25	0.82
1:B:94:MET:HE3	1:B:97:TRP:HA	1.63	0.80
1:B:310:HIS:HD2	1:B:312:GLY:H	1.29	0.79
1:A:489:GLU:O	1:A:493:VAL:HG23	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:ARG:HB3	1:A:504:ARG:HH11	1.49	0.78
1:B:308:MET:HE2	1:B:339:MET:N	1.98	0.78
1:B:539:MET:HE1	3:B:6523:HOH:O	1.85	0.76
1:A:482:MET:HE1	1:A:492:LYS:HB3	1.68	0.75
1:B:141:LYS:HD2	1:B:362:THR:HA	1.68	0.75
1:A:534:MET:CE	1:A:535:PRO:HD2	2.17	0.72
1:B:31:HIS:HE1	1:B:167:PRO:HB3	1.54	0.72
1:B:493:VAL:HG22	1:B:617:LEU:HG	1.73	0.70
1:A:122:VAL:HG22	1:A:564:MET:HG2	1.74	0.70
1:A:161:GLU:HB2	1:A:170:MET:HE1	1.73	0.70
1:B:32:GLN:HE22	1:B:170:MET:H	1.38	0.70
1:A:228:GLN:HB3	1:A:375:LEU:HD11	1.74	0.69
1:B:310:HIS:CD2	1:B:312:GLY:H	2.09	0.69
1:A:493:VAL:HG22	1:A:617:LEU:HG	1.75	0.68
1:B:349:PRO:O	1:B:352:VAL:HG22	1.94	0.68
1:A:457:LEU:HG	3:A:5100:HOH:O	1.94	0.68
1:B:555:GLN:HE21	1:B:580:PRO:HG2	1.59	0.68
1:A:265:ASN:HA	1:A:268:LYS:HE3	1.77	0.67
1:B:308:MET:HE2	1:B:338:GLY:C	2.20	0.67
1:A:161:GLU:H	1:A:170:MET:HE3	1.59	0.67
1:A:168:LEU:O	1:A:170:MET:HE2	1.95	0.67
1:A:310:HIS:CD2	1:A:312:GLY:H	2.11	0.67
1:B:131:ASP:OD1	1:B:133:GLN:HG3	1.94	0.66
1:A:504:ARG:HB3	1:A:504:ARG:NH1	2.10	0.66
1:B:524:LYS:HE3	1:B:534:MET:HE2	1.77	0.66
1:A:32:GLN:HE22	1:A:170:MET:H	1.44	0.66
1:A:161:GLU:H	1:A:170:MET:CE	2.09	0.66
1:B:308:MET:CE	1:B:330:ILE:HD12	2.26	0.66
1:A:204:THR:HG23	1:A:282:SER:HB3	1.78	0.65
1:A:255:HIS:HD2	1:A:257:ASN:H	1.44	0.65
1:B:308:MET:HE3	1:B:330:ILE:HD12	1.79	0.65
1:B:497:ARG:O	1:B:501:GLN:HG2	1.97	0.65
1:B:47:LEU:HD12	1:B:74:GLN:HB3	1.78	0.64
1:A:216:VAL:C	1:A:224:LEU:HD13	2.23	0.63
1:B:459:MET:HE3	1:B:511:ILE:HG22	1.80	0.63
1:A:534:MET:HE2	1:A:538:PHE:HD1	1.62	0.63
1:A:482:MET:CE	1:A:492:LYS:HB3	2.28	0.63
1:A:358:VAL:HG12	1:A:359:MET:HE2	1.79	0.63
1:B:410:MET:HE3	1:B:411:MET:O	1.99	0.62
1:A:349:PRO:HB2	1:A:350:PRO:HD3	1.80	0.62
1:A:491:GLN:HE21	1:A:495:LEU:HG	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:PRO:O	1:A:250:ILE:HG22	1.99	0.62
1:A:407:LEU:HD21	1:A:409:ILE:HD11	1.79	0.62
1:A:524:LYS:HG3	1:A:534:MET:HE1	1.82	0.61
1:A:31:HIS:HE1	1:A:167:PRO:HB3	1.64	0.61
1:A:421:PHE:HB3	1:A:422:PRO:HD3	1.82	0.61
1:A:534:MET:HE3	1:A:535:PRO:CD	2.31	0.61
1:B:132:LEU:H	1:B:132:LEU:CD2	2.06	0.60
1:A:225:THR:H	1:A:228:GLN:HE21	1.50	0.60
1:A:117:TYR:CE1	1:A:403:MET:HE3	2.37	0.59
1:B:370:SER:HB3	1:B:371:PRO:CD	2.31	0.59
1:B:47:LEU:CD1	1:B:74:GLN:HB3	2.31	0.59
1:A:225:THR:OG1	1:A:228:GLN:HG3	2.03	0.59
1:B:534:MET:HB3	1:B:539:MET:CE	2.29	0.59
1:A:276:VAL:O	1:A:280:GLN:HG3	2.03	0.59
1:A:493:VAL:HG22	1:A:617:LEU:CG	2.32	0.58
1:B:369:ARG:N	3:B:6100:HOH:O	2.36	0.58
1:A:84:GLN:O	1:A:88:GLU:HG3	2.04	0.57
1:A:478:PHE:CE1	1:A:482:MET:HE3	2.39	0.57
1:B:322:TRP:H	1:B:328:GLN:NE2	2.02	0.57
1:B:512:ARG:HG3	1:B:512:ARG:HH11	1.68	0.57
1:B:421:PHE:HB3	1:B:422:PRO:HD3	1.86	0.57
1:A:123:ILE:HG13	1:A:565:PHE:CE2	2.40	0.57
1:B:255:HIS:HD2	1:B:257:ASN:H	1.51	0.57
1:B:294:ARG:HG3	3:B:6232:HOH:O	2.04	0.57
2:A:5001:152:H5B3	2:A:5001:152:O3	2.05	0.56
1:B:59:SER:OG	1:B:62:GLU:HG3	2.05	0.56
1:A:163:LEU:HB3	1:A:166:GLN:OE1	2.05	0.56
1:A:534:MET:HE2	1:A:538:PHE:CD1	2.40	0.56
1:A:131:ASP:OD1	1:A:133:GLN:HG3	2.05	0.56
1:A:163:LEU:HD13	1:A:163:LEU:O	2.06	0.55
1:B:504:ARG:HH11	1:B:504:ARG:HB3	1.71	0.55
1:A:493:VAL:HG22	1:A:617:LEU:CD1	2.36	0.55
1:B:207:HIS:HE1	3:B:6426:HOH:O	1.90	0.55
1:A:482:MET:HA	1:A:482:MET:CE	2.31	0.55
1:B:568:PRO:HD2	1:B:592:TYR:CZ	2.42	0.55
1:B:294:ARG:HG3	1:B:294:ARG:HH11	1.72	0.55
1:B:382:ARG:HB2	1:B:382:ARG:NH1	2.21	0.55
1:B:370:SER:HB3	1:B:371:PRO:HD2	1.88	0.55
1:A:498:LYS:HD3	3:A:5054:HOH:O	2.07	0.54
1:A:555:GLN:HE21	1:A:580:PRO:HG2	1.72	0.54
1:A:132:LEU:H	1:A:132:LEU:HD22	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:VAL:HG11	1:A:556:VAL:HG12	1.90	0.54
1:B:358:VAL:O	1:B:362:THR:HG23	2.07	0.54
1:A:50:TYR:CZ	1:A:54:LEU:HD11	2.43	0.54
1:A:228:GLN:HG2	1:A:372:MET:HB3	1.90	0.54
1:A:501:GLN:NE2	3:A:5287:HOH:O	2.42	0.53
1:A:129:PHE:CZ	1:A:335:GLY:HA2	2.43	0.53
1:B:347:GLU:O	1:B:350:PRO:HD2	2.09	0.53
1:B:142:LEU:C	1:B:142:LEU:HD23	2.34	0.53
1:A:294:ARG:HG3	3:A:5409:HOH:O	2.08	0.53
1:A:255:HIS:CD2	1:A:257:ASN:H	2.25	0.53
1:B:548:HIS:HE1	1:B:572:ASP:OD1	1.91	0.52
1:A:349:PRO:HA	1:A:352:VAL:HG22	1.91	0.52
1:A:269:ASP:OD2	1:A:271:VAL:HB	2.10	0.52
1:A:486:THR:HG21	1:B:196:SER:HB3	1.91	0.52
1:A:161:GLU:CB	1:A:170:MET:HE1	2.39	0.52
1:A:372:MET:N	1:A:372:MET:HE3	2.25	0.52
1:A:496:LEU:HD23	1:A:496:LEU:C	2.34	0.52
1:A:568:PRO:HD2	1:A:592:TYR:CZ	2.45	0.52
1:B:192:ASN:HD22	1:B:192:ASN:C	2.17	0.52
1:A:193:PHE:CE2	1:A:281:LYS:HG2	2.45	0.52
1:A:115:VAL:HG12	1:A:116:ILE:HG13	1.90	0.52
1:A:132:LEU:HD22	1:A:132:LEU:N	2.25	0.52
1:A:291:GLN:HB2	1:A:333:GLU:HG3	1.92	0.52
1:B:496:LEU:C	1:B:496:LEU:HD23	2.35	0.51
1:B:35:LEU:HD11	1:B:169:CYS:HA	1.93	0.51
1:B:117:TYR:CE1	1:B:403:MET:HE3	2.46	0.51
1:B:132:LEU:HD22	1:B:132:LEU:N	2.11	0.51
1:A:44:GLN:HA	1:A:74:GLN:HE22	1.76	0.51
1:A:152:MET:HA	1:A:157:THR:OG1	2.11	0.51
1:A:455:ALA:HB2	1:A:468:ILE:HG13	1.93	0.51
1:A:225:THR:HG23	1:A:228:GLN:HE21	1.75	0.51
1:B:104:LYS:HD2	1:B:109:GLN:OE1	2.12	0.50
2:B:6001:152:H5B3	2:B:6001:152:O3	2.10	0.50
1:B:115:VAL:HG12	1:B:116:ILE:HG13	1.94	0.50
1:A:177:LEU:HD23	1:A:327:LEU:HD12	1.93	0.50
1:A:368:VAL:HG23	1:A:368:VAL:O	2.12	0.50
1:B:73:PHE:C	1:B:75:THR:H	2.18	0.50
1:A:132:LEU:H	1:A:132:LEU:CD2	2.25	0.49
1:A:457:LEU:HD21	1:A:466:ASP:HB2	1.94	0.49
1:B:202:HIS:HD2	3:B:6406:HOH:O	1.95	0.49
1:B:204:THR:HG21	1:B:279:ILE:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:THR:HG23	1:A:345:ALA:HB3	1.93	0.49
1:B:82:ARG:HB3	3:B:6590:HOH:O	2.11	0.49
1:B:421:PHE:CZ	1:B:615:ARG:HG3	2.46	0.49
1:A:234:GLU:HB3	3:A:5184:HOH:O	2.13	0.49
1:A:59:SER:OG	1:A:62:GLU:HG3	2.12	0.49
1:B:354:LEU:C	1:B:354:LEU:HD23	2.38	0.49
1:A:81:GLU:O	1:A:85:LYS:HG2	2.11	0.49
1:A:123:ILE:HG13	1:A:565:PHE:HE2	1.78	0.49
1:A:163:LEU:HB2	1:A:168:LEU:HD21	1.94	0.49
1:A:322:TRP:H	1:A:328:GLN:HE22	1.59	0.49
1:B:339:MET:CE	1:B:355:VAL:HG22	2.43	0.49
1:A:366:GLU:HG2	1:A:369:ARG:NH2	2.29	0.48
1:B:493:VAL:HG12	1:B:497:ARG:NH1	2.28	0.48
1:A:366:GLU:HA	1:A:369:ARG:HH21	1.79	0.48
1:B:122:VAL:HG22	1:B:564:MET:HG2	1.94	0.48
1:B:320:ASN:C	1:B:321:ARG:HG2	2.38	0.48
1:A:35:LEU:HD11	1:A:169:CYS:HA	1.96	0.48
1:A:95:GLU:OE1	1:A:461:HIS:HE1	1.96	0.48
1:A:204:THR:HG21	1:A:279:ILE:HA	1.95	0.48
1:A:366:GLU:CB	1:A:369:ARG:HH21	2.26	0.48
1:A:493:VAL:HG22	1:A:617:LEU:HD11	1.96	0.48
1:A:578:TYR:HB3	1:A:587:PHE:CD1	2.48	0.48
1:B:84:GLN:O	1:B:88:GLU:HG3	2.14	0.48
1:A:217:TYR:CE1	1:A:223:PRO:HB3	2.49	0.47
1:A:459:MET:HE3	1:A:511:ILE:HG22	1.95	0.47
1:A:32:GLN:NE2	1:A:170:MET:H	2.12	0.47
1:A:482:MET:HE1	1:A:617:LEU:HD22	1.95	0.47
1:B:339:MET:HE1	1:B:355:VAL:HG22	1.95	0.47
1:B:382:ARG:HB2	1:B:382:ARG:CZ	2.44	0.47
1:B:455:ALA:HB2	1:B:468:ILE:HG13	1.96	0.47
1:B:61:GLU:CD	1:B:61:GLU:H	2.22	0.47
1:A:548:HIS:HE1	1:A:572:ASP:OD1	1.97	0.47
1:B:90:ARG:NE	1:B:94:MET:HE1	2.30	0.47
1:A:176:ILE:HB	1:A:327:LEU:HD11	1.97	0.46
1:B:416:HIS:CG	1:B:612:LEU:HD21	2.50	0.46
1:B:166:GLN:HA	1:B:167:PRO:HD3	1.84	0.46
1:A:225:THR:HG23	1:A:228:GLN:NE2	2.31	0.46
1:B:568:PRO:HB2	1:B:592:TYR:CE2	2.51	0.46
1:A:380:LYS:HD2	3:A:5425:HOH:O	2.14	0.46
1:A:143:ILE:O	1:A:147:LEU:HG	2.16	0.46
1:A:354:LEU:HD23	1:A:354:LEU:C	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ASN:C	1:A:192:ASN:HD22	2.22	0.46
1:A:128:ASP:O	1:A:129:PHE:C	2.59	0.46
1:B:578:TYR:HB3	1:B:587:PHE:CD1	2.51	0.46
1:A:207:HIS:NE2	1:A:208:ASN:ND2	2.64	0.46
1:A:367:LEU:O	1:A:369:ARG:HG2	2.16	0.45
1:B:43:LEU:O	1:B:47:LEU:HG	2.16	0.45
1:B:349:PRO:HB2	1:B:350:PRO:HD3	1.99	0.45
1:A:534:MET:HE3	1:A:534:MET:HA	1.97	0.45
1:B:130:VAL:HA	3:B:6223:HOH:O	2.16	0.45
1:A:263:TYR:O	1:A:267:ILE:HG12	2.17	0.45
1:A:326:THR:HG23	1:A:345:ALA:CB	2.47	0.45
1:B:308:MET:HE1	1:B:330:ILE:CB	2.35	0.45
1:A:140:ALA:HB2	1:A:233:LEU:HD12	1.99	0.45
1:A:322:TRP:H	1:A:328:GLN:NE2	2.15	0.45
1:A:401:SER:O	1:A:405:GLN:HG3	2.17	0.45
1:B:308:MET:CE	1:B:338:GLY:C	2.88	0.45
1:B:410:MET:HG2	1:B:601:ALA:HA	1.97	0.45
1:A:166:GLN:NE2	1:A:166:GLN:N	2.65	0.45
1:B:255:HIS:CD2	1:B:257:ASN:H	2.33	0.45
1:A:421:PHE:CZ	1:A:615:ARG:HG3	2.52	0.44
1:A:349:PRO:O	1:A:352:VAL:HG22	2.16	0.44
1:A:482:MET:HE2	1:A:492:LYS:HD3	1.99	0.44
1:A:172:GLN:OE1	1:A:350:PRO:HG2	2.18	0.44
1:A:225:THR:N	1:A:228:GLN:HE21	2.14	0.44
1:A:65:HIS:CE1	1:A:69:LEU:HD11	2.53	0.44
1:A:150:LYS:HE3	1:A:283:ILE:HD13	2.00	0.44
1:A:150:LYS:HG2	1:A:154:ASP:OD2	2.18	0.44
1:B:124:LEU:HD11	1:B:339:MET:CE	2.47	0.44
1:A:294:ARG:HG3	1:A:294:ARG:HH11	1.83	0.43
1:B:295:VAL:HG11	1:B:303:HIS:CD2	2.54	0.43
1:A:176:ILE:HA	1:A:326:THR:HG21	2.00	0.43
1:B:308:MET:HE1	1:B:330:ILE:HD12	2.00	0.43
1:B:512:ARG:HG3	1:B:512:ARG:NH1	2.31	0.43
1:B:296:SER:OG	1:B:298:ASP:OD1	2.29	0.43
1:B:439:LEU:HA	1:B:479:VAL:HG12	2.01	0.43
1:B:242:GLN:HB3	1:B:244:ASN:OD1	2.19	0.43
1:B:204:THR:HG23	1:B:282:SER:HB3	2.00	0.43
1:A:489:GLU:HB3	1:A:621:HIS:NE2	2.33	0.42
1:B:163:LEU:HD13	1:B:163:LEU:C	2.43	0.42
1:A:142:LEU:HD23	1:A:142:LEU:C	2.44	0.42
1:A:474:ASP:OD1	1:A:498:LYS:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:TYR:CZ	1:B:54:LEU:HD11	2.55	0.42
1:B:123:ILE:HG13	1:B:565:PHE:CE2	2.55	0.42
1:A:565:PHE:HB3	1:A:588:SER:HB2	2.01	0.42
1:B:82:ARG:HD2	3:B:6590:HOH:O	2.18	0.42
1:B:147:LEU:HD11	1:B:216:VAL:HB	2.02	0.42
1:B:163:LEU:HB2	1:B:168:LEU:HD11	2.02	0.42
1:B:322:TRP:H	1:B:328:GLN:HE22	1.66	0.42
1:A:304:VAL:O	1:A:308:MET:HG2	2.20	0.42
1:A:358:VAL:O	1:A:362:THR:HG23	2.20	0.42
1:B:310:HIS:HE1	3:B:6396:HOH:O	2.03	0.42
1:B:104:LYS:HG2	1:B:109:GLN:CD	2.45	0.42
1:B:124:LEU:HD11	1:B:339:MET:HE3	2.01	0.42
1:B:208:ASN:O	1:B:209:TYR:HB2	2.19	0.42
1:B:32:GLN:NE2	1:B:170:MET:H	2.11	0.42
1:A:129:PHE:C	1:A:129:PHE:CD1	2.98	0.42
1:B:484:ASP:C	1:B:486:THR:H	2.28	0.42
1:A:235:LYS:NZ	1:A:375:LEU:O	2.53	0.41
1:A:212:PHE:CZ	1:A:240:SER:HB3	2.54	0.41
1:B:225:THR:H	1:B:228:GLN:NE2	2.17	0.41
2:A:5001:152:H5A2	2:A:5001:152:H3	1.82	0.41
1:B:308:MET:CE	1:B:339:MET:N	2.77	0.41
1:A:166:GLN:HA	1:A:167:PRO:HD3	1.89	0.41
1:A:209:TYR:N	1:A:209:TYR:CD2	2.89	0.41
1:A:420:ASP:HB3	1:A:582:GLU:OE2	2.21	0.41
1:A:310:HIS:HE1	3:A:5315:HOH:O	2.02	0.41
1:B:61:GLU:CD	1:B:61:GLU:N	2.79	0.41
1:B:67:LYS:HE2	1:B:71:ASP:OD2	2.20	0.41
1:B:82:ARG:HG3	1:B:82:ARG:HH11	1.86	0.41
1:B:420:ASP:OD1	1:B:421:PHE:N	2.54	0.41
1:B:621:HIS:N	1:B:622:PRO:HD3	2.35	0.41
1:A:192:ASN:ND2	1:A:194:LEU:H	2.18	0.40
1:A:482:MET:HE1	1:A:617:LEU:CD2	2.51	0.40
1:A:255:HIS:CD2	1:A:257:ASN:HB2	2.56	0.40
1:A:372:MET:HB2	1:A:373:VAL:H	1.64	0.40
1:A:389:ILE:O	1:A:393:ILE:HG13	2.22	0.40
1:B:294:ARG:HG3	1:B:294:ARG:NH1	2.35	0.40
1:A:373:VAL:O	1:A:375:LEU:N	2.44	0.40
1:A:149:PHE:HE1	1:A:153:ILE:HD11	1.87	0.40
1:A:379:LYS:HG3	3:A:5451:HOH:O	2.22	0.40
1:A:421:PHE:CE1	1:A:615:ARG:HG3	2.57	0.40
1:B:199:PRO:HA	1:B:200:PRO:HD3	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:TYR:C	1:A:452:TYR:CD2	3.00	0.40
1:B:237:TRP:CE2	1:B:241:LEU:HD21	2.57	0.40
1:B:359:MET:O	1:B:363:LYS:HG2	2.21	0.40
1:B:476:LEU:HA	1:B:479:VAL:HG22	2.03	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	594/596 (100%)	569 (96%)	21 (4%)	4 (1%)	18	10
1	B	594/596 (100%)	575 (97%)	18 (3%)	1 (0%)	43	36
All	All	1188/1192 (100%)	1144 (96%)	39 (3%)	5 (0%)	30	22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	372	MET
1	B	624	ALA
1	A	164	GLY
1	A	375	LEU
1	A	368	VAL

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	524/524 (100%)	519 (99%)	5 (1%)	68	70
1	B	524/524 (100%)	519 (99%)	5 (1%)	68	70
All	All	1048/1048 (100%)	1038 (99%)	10 (1%)	68	70

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	A	343	HIS
1	A	372	MET
1	A	482	MET
1	A	493	VAL
1	B	132	LEU
1	B	141	LYS
1	B	206	VAL
1	B	237	TRP
1	B	504	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	32	GLN
1	A	65	HIS
1	A	74	GLN
1	A	84	GLN
1	A	133	GLN
1	A	135	GLN
1	A	187	GLN
1	A	192	ASN
1	A	208	ASN
1	A	210	GLN
1	A	228	GLN
1	A	255	HIS
1	A	277	ASN
1	A	303	HIS
1	A	307	GLN
1	A	310	HIS
1	A	328	GLN
1	A	357	HIS
1	A	447	GLN

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Mol	Chain	Res	Type
1	A	461	HIS
1	A	491	GLN
1	A	501	GLN
1	A	503	HIS
1	A	526	GLN
1	A	548	HIS
1	A	550	ASN
1	A	555	GLN
1	A	586	ASN
1	A	619	GLN
1	A	620	ASN
1	B	32	GLN
1	B	44	GLN
1	B	55	GLN
1	B	68	GLN
1	B	84	GLN
1	B	112	GLN
1	B	135	GLN
1	B	155	ASN
1	B	166	GLN
1	B	192	ASN
1	B	202	HIS
1	B	207	HIS
1	B	228	GLN
1	B	255	HIS
1	B	307	GLN
1	B	310	HIS
1	B	328	GLN
1	B	357	HIS
1	B	405	GLN
1	B	461	HIS
1	B	503	HIS
1	B	526	GLN
1	B	548	HIS
1	B	555	GLN
1	B	586	ASN
1	B	619	GLN
1	B	620	ASN

5.3.3 RNA ⓘ

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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	152	A	5001	-	10,10,10	1.21	1 (10%)	13,14,14	1.09	1 (7%)
2	152	B	6001	-	10,10,10	1.19	1 (10%)	13,14,14	1.00	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	152	A	5001	-	-	0/9/9/9	-
2	152	B	6001	-	-	0/9/9/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6001	152	C4-N5	-2.18	1.47	1.52
2	A	5001	152	C4-N5	-2.13	1.47	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5001	152	C3-C4-N5	-3.23	110.75	116.70
2	B	6001	152	C3-C4-N5	-2.83	111.49	116.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5001	152	2	0
2	B	6001	152	1	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	596/596 (100%)	0.90	139 (23%) 2 2	9, 23, 57, 90	0
1	B	596/596 (100%)	0.13	40 (6%) 24 25	7, 17, 39, 73	0
All	All	1192/1192 (100%)	0.51	179 (15%) 5 5	7, 19, 53, 90	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	77	GLY	10.9
1	B	624	ALA	9.9
1	B	78	GLY	9.2
1	A	373	VAL	8.4
1	B	76	SER	8.0
1	A	375	LEU	6.9
1	A	231	VAL	6.5
1	A	370	SER	6.4
1	A	624	ALA	6.3
1	B	75	THR	6.2
1	A	368	VAL	5.9
1	A	625	LYS	5.9
1	A	130	VAL	5.5
1	A	237	TRP	5.4
1	A	163	LEU	5.4
1	A	227	ASP	5.2
1	B	30	ALA	5.2
1	A	376	PRO	5.2
1	A	372	MET	5.0
1	A	378	PRO	5.0
1	A	374	PRO	4.9
1	A	162	PHE	4.8
1	A	371	PRO	4.8
1	A	166	GLN	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	377	MET	4.6
1	B	625	LYS	4.6
1	B	369	ARG	4.5
1	B	368	VAL	4.2
1	A	236	ILE	4.2
1	A	233	LEU	4.2
1	A	165	GLY	4.1
1	B	31	HIS	4.1
1	A	241	LEU	4.1
1	A	129	PHE	4.1
1	A	224	LEU	4.1
1	A	293	PRO	4.1
1	A	217	TYR	4.0
1	A	365	PRO	4.0
1	A	296	SER	4.0
1	A	134	GLY	4.0
1	A	379	LYS	3.9
1	A	164	GLY	3.9
1	A	369	ARG	3.8
1	A	208	ASN	3.8
1	A	229	ILE	3.8
1	B	370	SER	3.8
1	A	131	ASP	3.8
1	A	361	TYR	3.8
1	A	623	ARG	3.8
1	A	216	VAL	3.7
1	A	292	VAL	3.7
1	A	230	PHE	3.7
1	A	367	LEU	3.7
1	A	225	THR	3.7
1	A	206	VAL	3.7
1	A	198	ARG	3.6
1	A	405	GLN	3.5
1	B	164	GLY	3.5
1	A	362	THR	3.5
1	A	160	VAL	3.4
1	A	243	SER	3.4
1	B	68	GLN	3.4
1	A	239	SER	3.4
1	A	232	GLN	3.3
1	B	32	GLN	3.3
1	A	132	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	214	LEU	3.3
1	A	139	ALA	3.2
1	B	79	VAL	3.2
1	A	346	ALA	3.2
1	A	226	SER	3.2
1	B	243	SER	3.2
1	A	128	ASP	3.2
1	A	219	SER	3.2
1	A	316	PHE	3.2
1	A	207	HIS	3.2
1	A	295	VAL	3.1
1	A	390	LYS	3.1
1	A	167	PRO	3.1
1	A	223	PRO	3.1
1	A	136	LEU	3.1
1	A	332	ALA	3.1
1	A	228	GLN	3.1
1	A	290	LYS	3.0
1	A	381	LEU	3.0
1	A	299	VAL	3.0
1	B	160	VAL	3.0
1	A	533	SER	3.0
1	A	387	PRO	3.0
1	A	242	GLN	3.0
1	A	288	LEU	3.0
1	A	398	GLN	2.9
1	B	163	LEU	2.9
1	B	237	TRP	2.9
1	A	389	ILE	2.9
1	B	294	ARG	2.8
1	B	623	ARG	2.8
1	A	366	GLU	2.8
1	A	345	ALA	2.8
1	A	238	ASN	2.8
1	B	487	VAL	2.8
1	A	383	PHE	2.8
1	A	218	HIS	2.8
1	B	622	PRO	2.8
1	A	271	VAL	2.8
1	B	133	GLN	2.7
1	B	162	PHE	2.7
1	A	334	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	401	SER	2.7
1	A	291	GLN	2.7
1	B	486	THR	2.7
1	B	167	PRO	2.7
1	A	289	ASP	2.7
1	A	234	GLU	2.7
1	B	72	GLU	2.6
1	A	220	ASP	2.6
1	B	33	ASP	2.6
1	B	346	ALA	2.6
1	A	360	GLU	2.6
1	A	364	LYS	2.6
1	A	380	LYS	2.6
1	A	204	THR	2.6
1	B	227	ASP	2.6
1	A	363	LYS	2.6
1	A	331	VAL	2.6
1	A	303	HIS	2.5
1	B	366	GLU	2.5
1	A	384	ASN	2.5
1	A	240	SER	2.5
1	A	159	PRO	2.5
1	A	209	TYR	2.5
1	A	210	GLN	2.4
1	A	386	THR	2.4
1	A	215	ASP	2.4
1	B	219	SER	2.4
1	B	34	ALA	2.4
1	A	294	ARG	2.4
1	A	319	GLY	2.4
1	B	485	SER	2.4
1	A	138	PHE	2.4
1	A	149	PHE	2.4
1	A	250	ILE	2.4
1	A	382	ARG	2.4
1	A	196	SER	2.4
1	A	140	ALA	2.3
1	A	385	ILE	2.3
1	A	161	GLU	2.3
1	A	157	THR	2.3
1	A	212	PHE	2.3
1	A	155	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	235	LYS	2.3
1	A	133	GLN	2.3
1	A	135	GLN	2.3
1	A	151	SER	2.2
1	A	404	ILE	2.2
1	A	272	ASN	2.2
1	A	222	THR	2.2
1	A	287	CYS	2.2
1	A	158	LEU	2.2
1	A	335	GLY	2.2
1	A	396	ALA	2.2
1	A	211	PHE	2.2
1	A	330	ILE	2.2
1	B	165	GLY	2.2
1	A	247	PRO	2.2
1	A	30	ALA	2.2
1	A	141	LYS	2.1
1	B	382	ARG	2.1
1	A	201	THR	2.1
1	B	198	ARG	2.1
1	A	400	LEU	2.1
1	B	44	GLN	2.1
1	B	484	ASP	2.1
1	A	313	GLY	2.1
1	A	200	PRO	2.1
1	A	72	GLU	2.0
1	A	336	SER	2.0
1	A	199	PRO	2.0
1	A	314	SER	2.0

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

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

6.3 Carbohydrates ⓘ

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	152	A	5001	11/11	0.95	0.07	9,14,18,18	0
2	152	B	6001	11/11	0.95	0.06	12,14,17,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.