



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:33 PM UTC

PDB ID : 4NWV / pdb_00004nwv
Title : Crystal structure of Orsay virus-like particle
Authors : Tao, Y.J.; Guo, Y.R.
Deposited on : 2013-12-06
Resolution : 3.25 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

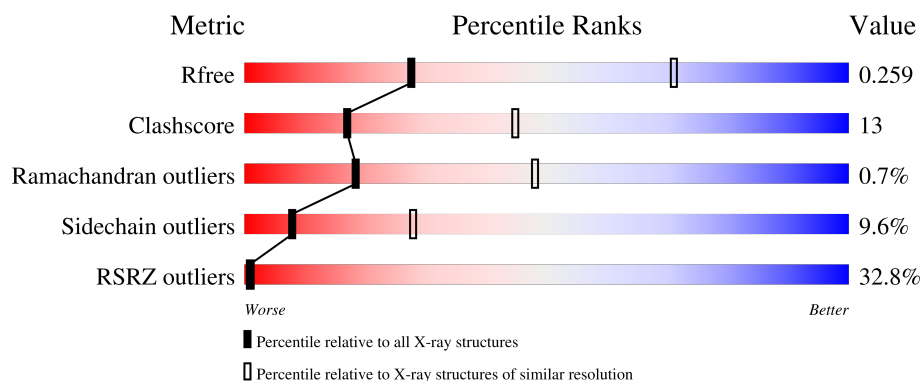
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	391	25% 63% 24% 9%
1	B	391	29% 63% 21% 12%
1	C	391	34% 60% 25% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8122 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2747	1763	462	516	6			
1	C	346	Total	C	N	O	S	0	0	0
			2689	1729	448	506	6			
1	B	345	Total	C	N	O	S	0	0	0
			2683	1726	447	504	6			

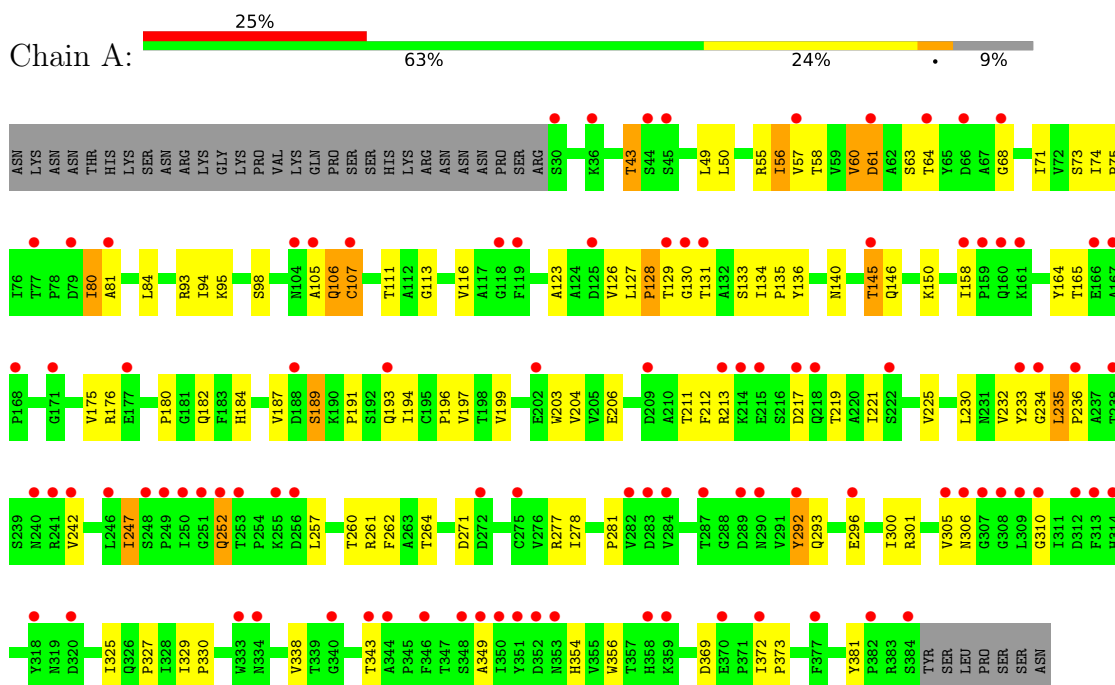
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

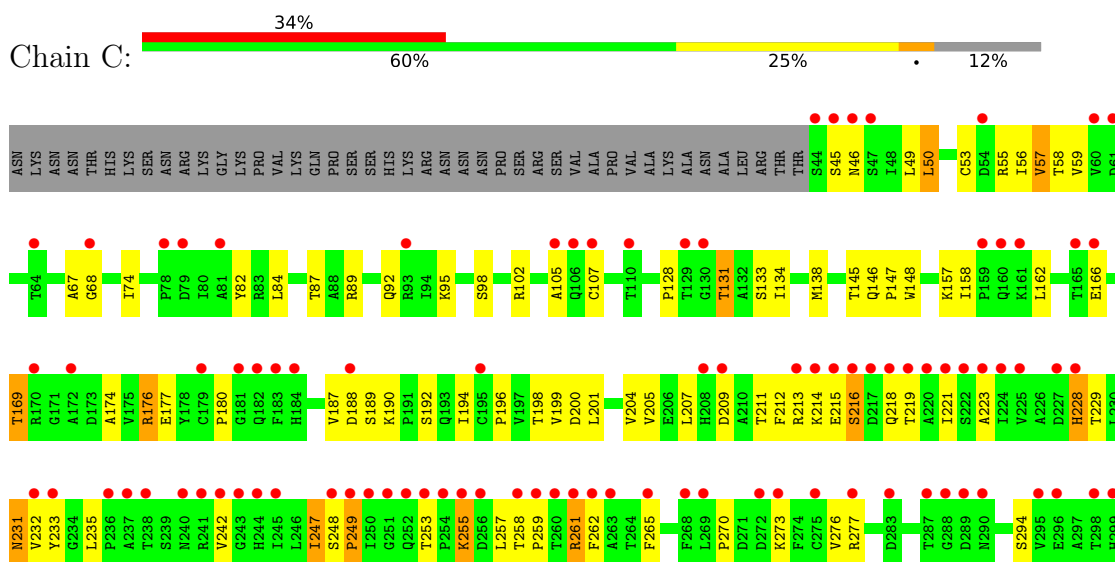
3 Residue-property plots [i](#)

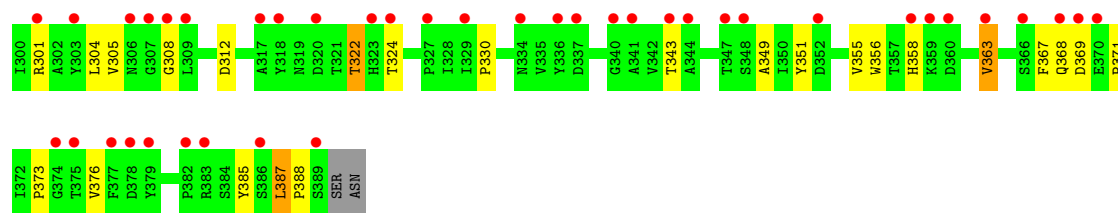
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

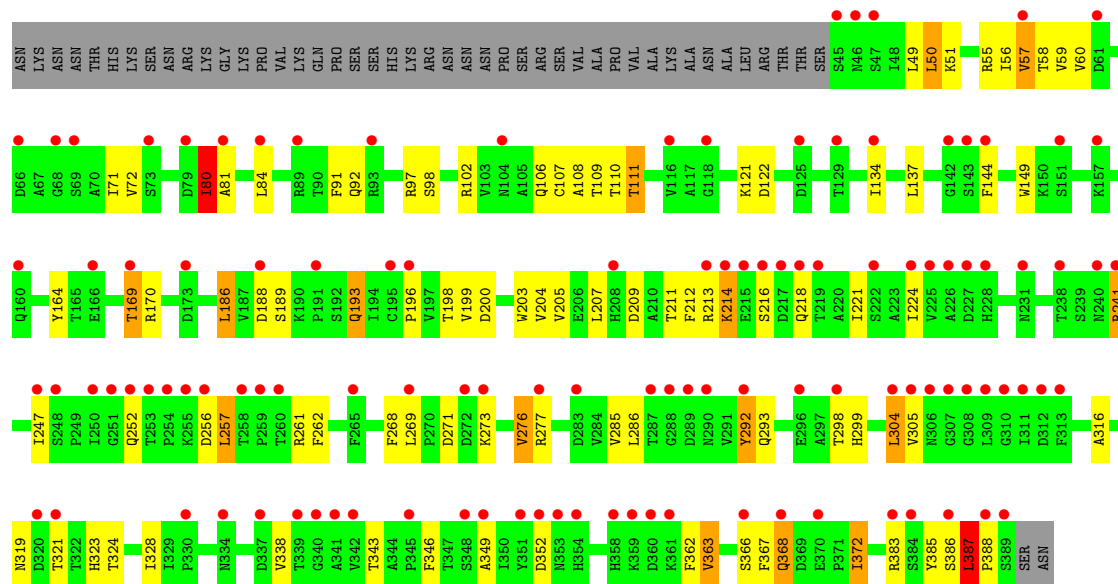


- Molecule 1: Capsid protein





● Molecule 1: Capsid protein



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	402.20Å 369.86Å 410.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.25 50.00 – 3.26	Depositor EDS
% Data completeness (in resolution range)	86.4 (50.00-3.25) 87.0 (50.00-3.26)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 3.25Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.278 , 0.279 0.258 , 0.259	Depositor DCC
R_{free} test set	20302 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.17	EDS
Total number of atoms	8122	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 1.68% 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: CA

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	0/2823	0.85	1/3873 (0.0%)
1	B	0.59	0/2760	0.88	6/3787 (0.2%)
1	C	0.57	0/2766	0.82	1/3795 (0.0%)
All	All	0.59	0/8349	0.85	8/11455 (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	B	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	387	LEU	CA-C-N	-7.56	111.84	119.93
1	B	387	LEU	C-N-CA	-7.56	111.84	119.93
1	B	372	ILE	CA-C-N	6.30	126.66	119.92
1	B	372	ILE	C-N-CA	6.30	126.66	119.92
1	C	228	HIS	N-CA-C	6.08	118.09	108.79
1	A	80	ILE	CB-CA-C	-5.95	104.10	112.14
1	B	386	SER	N-CA-C	-5.14	102.17	110.14
1	B	80	ILE	N-CA-C	5.06	115.29	110.53

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	144	PHE	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	2747	0	2709	74	0
1	B	2683	0	2634	58	0
1	C	2689	0	2641	82	0
2	A	2	0	0	0	0
2	C	1	0	0	0	0
All	All	8122	0	7984	203	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 13.

All (203) 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:228:HIS:HB3	1:C:249:PRO:HA	1.42	1.00
1:C:228:HIS:CB	1:C:249:PRO:HA	1.99	0.91
1:C:107:CYS:SG	1:C:148:TRP:HB3	2.12	0.89
1:A:176:ARG:HG2	1:B:164:TYR:CE2	2.22	0.73
1:A:247:ILE:HD11	1:A:257:LEU:HA	1.71	0.72
1:C:247:ILE:HD11	1:C:257:LEU:HG	1.72	0.71
1:C:82:TYR:HH	1:C:385:TYR:HH	1.36	0.70
1:A:130:GLY:HA2	1:A:133:SER:OG	1.91	0.70
1:A:164:TYR:CE2	1:C:176:ARG:HG2	2.28	0.69
1:C:211:THR:HG22	1:C:212:PHE:N	2.08	0.69
1:A:43:THR:HG21	1:C:138:MET:O	1.94	0.68
1:A:158:ILE:HD13	1:A:180:PRO:HB2	1.76	0.67
1:C:247:ILE:HD13	1:C:261:ARG:HG2	1.76	0.66
1:B:49:LEU:HD12	1:B:205:VAL:O	1.95	0.66
1:C:218:GLN:HG2	1:C:371:PRO:HB3	1.77	0.66
1:B:387:LEU:O	1:B:388:PRO:C	2.36	0.65
1:B:57:VAL:HA	1:B:388:PRO:HD3	1.77	0.65
1:B:81:ALA:HB3	1:B:84:LEU:HB3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:PRO:HB2	1:C:270:PRO:HG2	1.79	0.64
1:C:218:GLN:HG2	1:C:371:PRO:CB	2.29	0.63
1:B:109:THR:HG22	1:B:149:TRP:CD2	2.34	0.62
1:B:211:THR:HG22	1:B:212:PHE:N	2.14	0.62
1:C:67:ALA:HA	1:C:187:VAL:HG23	1.81	0.61
1:A:176:ARG:HG2	1:B:164:TYR:CZ	2.35	0.61
1:A:123:ALA:HB1	1:A:175:VAL:HG22	1.81	0.61
1:C:262:PHE:CD2	1:C:270:PRO:HG3	2.36	0.61
1:C:57:VAL:CG1	1:C:199:VAL:HB	2.32	0.60
1:C:211:THR:HG22	1:C:212:PHE:H	1.67	0.60
1:C:223:ALA:HB2	1:C:265:PHE:CZ	2.37	0.60
1:A:234:GLY:HA2	1:A:242:VAL:HG22	1.83	0.60
1:B:277:ARG:HB3	1:B:363:VAL:HG13	1.83	0.59
1:C:134:ILE:HD13	1:C:188:ASP:HA	1.83	0.59
1:C:262:PHE:CG	1:C:270:PRO:HG3	2.38	0.59
1:A:211:THR:HG22	1:A:212:PHE:N	2.18	0.59
1:C:55:ARG:HD2	1:C:200:ASP:OD2	2.03	0.57
1:C:57:VAL:HG12	1:C:199:VAL:HB	1.86	0.57
1:C:105:ALA:HB1	1:C:148:TRP:O	2.04	0.57
1:B:211:THR:HG22	1:B:212:PHE:H	1.70	0.57
1:C:257:LEU:N	1:C:257:LEU:HD12	2.19	0.56
1:C:128:PRO:HG2	1:C:133:SER:HA	1.86	0.55
1:C:95:LYS:HB2	1:C:162:LEU:HD23	1.89	0.54
1:C:228:HIS:HB2	1:C:249:PRO:HA	1.88	0.54
1:B:107:CYS:HB2	1:B:111:THR:HG21	1.89	0.54
1:A:57:VAL:HG12	1:A:199:VAL:HB	1.90	0.54
1:A:75:PRO:O	1:A:80:ILE:HD11	2.07	0.54
1:C:55:ARG:CD	1:C:200:ASP:OD2	2.55	0.54
1:C:387:LEU:HD23	1:C:388:PRO:HA	1.90	0.54
1:A:64:THR:HG21	1:A:225:VAL:HG23	1.90	0.53
1:B:58:THR:HG23	1:B:387:LEU:HB2	1.89	0.53
1:B:286:LEU:HB3	1:B:346:PHE:CD1	2.44	0.53
1:A:277:ARG:NH1	1:A:369:ASP:OD1	2.42	0.53
1:C:305:VAL:HG21	1:C:312:ASP:HB2	1.90	0.53
1:B:213:ARG:HE	1:B:214:LYS:H	1.55	0.53
1:C:49:LEU:HD12	1:C:205:VAL:O	2.09	0.52
1:C:277:ARG:HB3	1:C:363:VAL:HG13	1.92	0.52
1:C:231:ASN:HD21	1:C:248:SER:HB2	1.73	0.52
1:A:194:ILE:HG22	1:A:196:PRO:HD3	1.92	0.52
1:A:330:PRO:HG3	1:A:349:ALA:HB2	1.92	0.52
1:A:165:THR:OG1	1:A:213:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ALA:O	1:B:170:ARG:NH1	2.44	0.51
1:A:305:VAL:HG12	1:A:310:GLY:HA3	1.92	0.51
1:C:56:ILE:CG1	1:C:201:LEU:HB2	2.40	0.51
1:A:49:LEU:C	1:A:49:LEU:HD23	2.34	0.51
1:B:80:ILE:HD12	1:B:80:ILE:O	2.11	0.51
1:C:187:VAL:HG23	1:C:187:VAL:O	2.10	0.51
1:B:292:TYR:C	1:B:292:TYR:CD2	2.88	0.51
1:C:50:LEU:HD11	1:C:87:THR:HG21	1.91	0.51
1:C:211:THR:CG2	1:C:212:PHE:N	2.73	0.51
1:C:294:SER:HB3	1:B:352:ASP:OD2	2.11	0.51
1:B:276:VAL:HG11	1:B:362:PHE:HB3	1.92	0.51
1:B:304:LEU:H	1:B:304:LEU:HD23	1.75	0.50
1:B:109:THR:HG22	1:B:149:TRP:CE3	2.46	0.50
1:B:319:ASN:ND2	1:B:321:THR:HB	2.27	0.50
1:A:74:ILE:HD12	1:A:80:ILE:HD13	1.94	0.50
1:C:92:GLN:HE21	1:C:211:THR:HB	1.77	0.50
1:B:111:THR:HB	1:B:193:GLN:HG2	1.91	0.50
1:B:55:ARG:HD3	1:B:200:ASP:OD1	2.11	0.50
1:B:276:VAL:CG1	1:B:362:PHE:HB3	2.42	0.49
1:A:232:VAL:HG23	1:A:356:TRP:HZ3	1.76	0.49
1:B:56:ILE:HG23	1:B:80:ILE:HG12	1.94	0.49
1:C:134:ILE:CD1	1:C:188:ASP:HA	2.42	0.49
1:A:211:THR:HG22	1:A:212:PHE:H	1.78	0.49
1:A:217:ASP:HA	1:A:373:PRO:HA	1.95	0.49
1:C:247:ILE:HD12	1:C:255:LYS:O	2.13	0.49
1:A:252:GLN:HE21	1:A:252:GLN:N	2.10	0.49
1:C:146:GLN:HG3	1:C:147:PRO:HD2	1.95	0.49
1:B:366:SER:C	1:B:367:PHE:O	2.48	0.48
1:C:242:VAL:HG12	1:C:351:TYR:CD2	2.47	0.48
1:C:89:ARG:NE	1:C:215:GLU:HG3	2.28	0.48
1:A:140:ASN:HD21	1:B:211:THR:HG23	1.79	0.48
1:C:258:THR:N	1:C:259:PRO:HA	2.29	0.48
1:B:134:ILE:HG12	1:B:186:LEU:HD23	1.95	0.48
1:A:292:TYR:C	1:A:292:TYR:CD2	2.91	0.48
1:A:128:PRO:HG2	1:A:136:TYR:CD2	2.49	0.47
1:C:166:GLU:OE1	1:C:213:ARG:HG2	2.13	0.47
1:C:223:ALA:HB3	1:C:358:HIS:HA	1.96	0.47
1:A:235:LEU:HB3	1:A:236:PRO:HD3	1.96	0.47
1:A:260:THR:O	1:A:264:THR:HG23	2.14	0.47
1:A:130:GLY:O	1:A:131:THR:C	2.58	0.47
1:C:258:THR:OG1	1:C:261:ARG:NH1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:GLN:NE2	1:B:211:THR:OG1	2.47	0.47
1:A:63:SER:HA	1:A:191:PRO:HG2	1.96	0.47
1:A:73:SER:HB3	1:A:184:HIS:CD2	2.50	0.47
1:C:128:PRO:O	1:C:133:SER:HB3	2.14	0.47
1:A:127:LEU:C	1:A:128:PRO:O	2.57	0.47
1:C:214:LYS:HB3	1:C:216:SER:N	2.30	0.47
1:C:262:PHE:CD2	1:C:262:PHE:C	2.92	0.47
1:B:134:ILE:CD1	1:B:188:ASP:HA	2.45	0.47
1:A:106:GLN:CG	1:A:196:PRO:HG2	2.45	0.47
1:C:194:ILE:HG22	1:C:196:PRO:HD3	1.97	0.47
1:A:105:ALA:HB1	1:A:107:CYS:SG	2.55	0.46
1:A:116:VAL:HG21	1:A:134:ILE:HG23	1.96	0.46
1:A:232:VAL:HG23	1:A:356:TRP:CZ3	2.50	0.46
1:C:53:CYS:HA	1:C:201:LEU:O	2.14	0.46
1:B:108:ALA:O	1:B:111:THR:CG2	2.64	0.46
1:C:232:VAL:HG23	1:C:356:TRP:CZ3	2.51	0.46
1:A:233:TYR:HB2	1:B:338:VAL:HG12	1.96	0.46
1:C:211:THR:CG2	1:C:212:PHE:H	2.29	0.46
1:C:74:ILE:HG23	1:C:74:ILE:O	2.16	0.46
1:B:247:ILE:HD12	1:B:261:ARG:HB3	1.96	0.46
1:A:111:THR:HG22	1:A:193:GLN:HB2	1.97	0.46
1:A:126:VAL:HG12	1:B:169:THR:HB	1.97	0.46
1:C:330:PRO:HG3	1:C:349:ALA:HB2	1.98	0.45
1:B:91:PHE:CG	1:B:207:LEU:HB3	2.51	0.45
1:A:128:PRO:HG2	1:A:136:TYR:CG	2.51	0.45
1:C:59:VAL:HA	1:C:198:THR:HG22	1.98	0.45
1:B:108:ALA:O	1:B:111:THR:HG23	2.16	0.45
1:A:271:ASP:OD1	1:A:381:TYR:CE1	2.69	0.45
1:B:268:PHE:HB3	1:B:383:ARG:HG3	1.99	0.45
1:C:242:VAL:HG12	1:C:351:TYR:HD2	1.82	0.45
1:A:68:GLY:HA3	1:A:130:GLY:C	2.41	0.45
1:A:194:ILE:HD12	1:A:194:ILE:H	1.81	0.45
1:B:50:LEU:HB3	1:B:203:TRP:HZ3	1.82	0.44
1:A:60:VAL:O	1:A:61:ASP:C	2.59	0.44
1:B:51:LYS:HG2	1:B:204:VAL:HG22	1.99	0.44
1:A:50:LEU:HB3	1:A:203:TRP:HZ3	1.82	0.44
1:B:323:HIS:O	1:B:368:GLN:NE2	2.50	0.44
1:A:94:ILE:HB	1:A:165:THR:HG22	1.99	0.44
1:B:137:LEU:CD2	1:B:186:LEU:HD22	2.48	0.44
1:A:71:ILE:CD1	1:A:197:VAL:HG21	2.48	0.44
1:A:93:ARG:HH11	1:A:93:ARG:HG2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:THR:HG21	1:C:213:ARG:CZ	2.47	0.44
1:C:257:LEU:C	1:C:259:PRO:HA	2.43	0.44
1:C:301:ARG:CZ	1:C:367:PHE:HE2	2.30	0.44
1:C:45:SER:OG	1:C:46:ASN:N	2.51	0.44
1:A:301:ARG:NH1	1:A:325:ILE:O	2.50	0.43
1:A:330:PRO:HG3	1:A:349:ALA:CB	2.48	0.43
1:A:56:ILE:HD12	1:A:56:ILE:HA	1.90	0.43
1:C:174:ALA:HB3	1:C:177:GLU:CD	2.43	0.43
1:B:97:ARG:HG2	1:B:97:ARG:HH11	1.82	0.43
1:A:146:GLN:HG3	1:A:150:LYS:HB2	2.00	0.43
1:A:257:LEU:HD22	1:A:262:PHE:HB2	1.99	0.43
1:B:247:ILE:CG1	1:B:257:LEU:HG	2.48	0.43
1:C:322:THR:HB	1:C:324:THR:HG22	1.99	0.43
1:C:213:ARG:HG3	1:C:215:GLU:HA	2.01	0.43
1:C:58:THR:HG23	1:C:387:LEU:HB3	2.01	0.43
1:C:373:PRO:HB2	1:C:376:VAL:HG23	2.01	0.43
1:B:57:VAL:HG22	1:B:199:VAL:HG23	2.01	0.43
1:A:305:VAL:HG13	1:A:306:ASN:N	2.34	0.43
1:A:354:HIS:HD2	1:A:356:TRP:CE2	2.37	0.43
1:C:92:GLN:OE1	1:B:122:ASP:HB2	2.19	0.43
1:C:102:ARG:HB2	1:C:102:ARG:NH1	2.34	0.43
1:A:281:PRO:HB3	1:A:296:GLU:HG3	2.00	0.43
1:C:158:ILE:HD12	1:C:180:PRO:HB2	2.00	0.43
1:C:229:THR:HB	1:C:356:TRP:O	2.19	0.43
1:B:316:ALA:HA	1:B:328:ILE:HG13	2.00	0.43
1:A:95:LYS:HB3	1:A:206:GLU:HB2	2.01	0.42
1:A:338:VAL:HG23	1:C:235:LEU:O	2.18	0.42
1:C:68:GLY:HA3	1:C:131:THR:HA	2.00	0.42
1:C:304:LEU:HB3	1:C:308:GLY:HA2	2.01	0.42
1:B:59:VAL:HG22	1:B:198:THR:HG22	2.01	0.42
1:A:278:ILE:HD12	1:A:278:ILE:HA	1.91	0.42
1:B:299:HIS:O	1:B:316:ALA:N	2.50	0.42
1:B:385:TYR:OH	1:B:387:LEU:HD13	2.20	0.42
1:A:56:ILE:HG13	1:A:80:ILE:HG21	2.01	0.42
1:A:123:ALA:CB	1:A:175:VAL:HG22	2.46	0.42
1:A:116:VAL:HG22	1:A:145:THR:HB	2.02	0.42
1:A:278:ILE:HD13	1:A:300:ILE:HG13	2.02	0.42
1:C:56:ILE:CG2	1:C:74:ILE:HD13	2.50	0.42
1:B:57:VAL:HG11	1:B:72:VAL:HG22	2.02	0.42
1:C:261:ARG:HB2	1:C:261:ARG:HH11	1.85	0.41
1:C:231:ASN:ND2	1:C:233:TYR:OH	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ARG:NH1	1:B:256:ASP:HB3	2.34	0.41
1:A:134:ILE:N	1:A:135:PRO:HD2	2.35	0.41
1:C:187:VAL:O	1:C:187:VAL:CG2	2.68	0.41
1:A:327:PRO:HB2	1:A:329:ILE:HD13	2.01	0.41
1:C:231:ASN:HB3	1:C:355:VAL:HA	2.02	0.41
1:B:261:ARG:O	1:B:262:PHE:C	2.63	0.41
1:C:367:PHE:H	1:C:367:PHE:HD1	1.68	0.41
1:B:71:ILE:HG13	1:B:72:VAL:HG23	2.02	0.41
1:A:56:ILE:HG23	1:A:74:ILE:HD11	2.03	0.41
1:A:68:GLY:O	1:A:130:GLY:HA3	2.20	0.41
1:A:113:GLY:HA2	1:A:189:SER:HB3	2.03	0.41
1:A:278:ILE:HD11	1:A:356:TRP:CE2	2.56	0.41
1:B:285:VAL:O	1:B:349:ALA:HA	2.21	0.41
1:A:305:VAL:HG12	1:A:310:GLY:CA	2.51	0.41
1:C:218:GLN:HG2	1:C:371:PRO:HB2	2.03	0.40
1:C:102:ARG:HB2	1:C:102:ARG:HH11	1.86	0.40
1:B:60:VAL:O	1:B:196:PRO:HA	2.22	0.40
1:B:269:LEU:HD12	1:B:269:LEU:HA	1.92	0.40
1:A:81:ALA:HB3	1:A:84:LEU:HB3	2.03	0.40
1:A:247:ILE:HD13	1:A:261:ARG:HD2	2.02	0.40
1:B:271:ASP:OD1	1:B:271:ASP:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	353/391 (90%)	334 (95%)	17 (5%)	2 (1%)	21	51
1	B	343/391 (88%)	324 (94%)	17 (5%)	2 (1%)	21	51
1	C	344/391 (88%)	322 (94%)	19 (6%)	3 (1%)	14	42
All	All	1040/1173 (89%)	980 (94%)	53 (5%)	7 (1%)	18	48

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	PRO
1	C	369	ASP
1	C	209	ASP
1	A	61	ASP
1	B	209	ASP
1	C	249	PRO
1	B	387	LEU

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	303/338 (90%)	279 (92%)	24 (8%)	11	35
1	B	297/338 (88%)	264 (89%)	33 (11%)	6	23
1	C	298/338 (88%)	269 (90%)	29 (10%)	8	27
All	All	898/1014 (89%)	812 (90%)	86 (10%)	8	28

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	THR
1	A	55	ARG
1	A	56	ILE
1	A	58	THR
1	A	60	VAL
1	A	98	SER
1	A	106	GLN
1	A	107	CYS
1	A	129	THR
1	A	145	THR
1	A	182	GLN
1	A	187	VAL
1	A	189	SER
1	A	204	VAL

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Mol	Chain	Res	Type
1	A	219	THR
1	A	221	ILE
1	A	230	LEU
1	A	235	LEU
1	A	247	ILE
1	A	252	GLN
1	A	292	TYR
1	A	293	GLN
1	A	343	THR
1	A	372	ILE
1	C	50	LEU
1	C	57	VAL
1	C	84	LEU
1	C	98	SER
1	C	131	THR
1	C	145	THR
1	C	157	LYS
1	C	169	THR
1	C	176	ARG
1	C	189	SER
1	C	190	LYS
1	C	192	SER
1	C	204	VAL
1	C	207	LEU
1	C	216	SER
1	C	219	THR
1	C	221	ILE
1	C	231	ASN
1	C	247	ILE
1	C	253	THR
1	C	255	LYS
1	C	261	ARG
1	C	273	LYS
1	C	276	VAL
1	C	322	THR
1	C	343	THR
1	C	363	VAL
1	C	368	GLN
1	C	387	LEU
1	B	50	LEU
1	B	57	VAL
1	B	80	ILE

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Mol	Chain	Res	Type
1	B	98	SER
1	B	102	ARG
1	B	106	GLN
1	B	110	THR
1	B	111	THR
1	B	121	LYS
1	B	169	THR
1	B	186	LEU
1	B	189	SER
1	B	193	GLN
1	B	214	LYS
1	B	216	SER
1	B	218	GLN
1	B	221	ILE
1	B	224	ILE
1	B	241	ARG
1	B	252	GLN
1	B	257	LEU
1	B	273	LYS
1	B	276	VAL
1	B	292	TYR
1	B	293	GLN
1	B	298	THR
1	B	304	LEU
1	B	305	VAL
1	B	324	THR
1	B	343	THR
1	B	363	VAL
1	B	368	GLN
1	B	372	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	140	ASN
1	A	184	HIS
1	A	252	GLN
1	A	354	HIS
1	C	154	HIS
1	C	182	GLN
1	C	231	ASN

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Mol	Chain	Res	Type
1	C	326	GLN
1	C	368	GLN
1	B	140	ASN
1	B	182	GLN
1	B	228	HIS
1	B	244	HIS
1	B	293	GLN
1	B	368	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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 [i](#)

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	355/391 (90%)	1.63	97 (27%)  	15, 39, 82, 185	0
1	B	345/391 (88%)	1.82	114 (33%)  	14, 43, 84, 127	0
1	C	346/391 (88%)	1.93	132 (38%)  	15, 47, 95, 162	0
All	All	1046/1173 (89%)	1.79	343 (32%)  	14, 43, 91, 185	0

All (343) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	GLY	9.2
1	B	310	GLY	8.5
1	B	289	ASP	8.3
1	C	308	GLY	8.3
1	A	160	GLN	8.2
1	B	306	ASN	7.3
1	C	289	ASP	7.1
1	C	306	ASN	7.0
1	B	252	GLN	7.0
1	C	258	THR	6.9
1	B	251	GLY	6.5
1	A	289	ASP	6.4
1	C	252	GLN	6.3
1	C	389	SER	6.3
1	A	384	SER	6.2
1	B	309	LEU	6.1
1	A	129	THR	5.9
1	C	307	GLY	5.8
1	A	283	ASP	5.8
1	B	290	ASN	5.5
1	B	240	ASN	5.5
1	A	252	GLN	5.5
1	C	220	ALA	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	253	THR	5.4
1	B	215	GLU	5.4
1	B	370	GLU	5.3
1	A	305	VAL	5.2
1	C	216	SER	5.2
1	A	290	ASN	5.1
1	B	218	GLN	5.1
1	C	352	ASP	5.1
1	C	44	SER	5.1
1	C	290	ASN	5.1
1	C	374	GLY	5.1
1	A	159	PRO	5.0
1	B	389	SER	4.9
1	C	366	SER	4.8
1	C	296	GLU	4.8
1	C	283	ASP	4.7
1	C	161	LYS	4.6
1	C	359	LYS	4.6
1	C	253	THR	4.6
1	C	320	ASP	4.6
1	C	378	ASP	4.5
1	B	368	GLN	4.5
1	C	54	ASP	4.5
1	A	306	ASN	4.5
1	C	250	ILE	4.4
1	C	219	THR	4.4
1	B	219	THR	4.4
1	A	308	GLY	4.4
1	B	195	CYS	4.4
1	C	240	ASN	4.4
1	B	125	ASP	4.3
1	C	209	ASP	4.3
1	B	227	ASP	4.3
1	B	79	ASP	4.2
1	A	66	ASP	4.2
1	C	263	ALA	4.2
1	A	251	GLY	4.2
1	C	341	ALA	4.1
1	B	352	ASP	4.1
1	B	341	ALA	4.1
1	A	348	SER	4.0
1	B	217	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	348	SER	4.0
1	C	334	ASN	4.0
1	A	292	TYR	4.0
1	C	343	THR	4.0
1	C	383	ARG	4.0
1	C	382	PRO	3.9
1	C	47	SER	3.9
1	A	79	ASP	3.9
1	B	366	SER	3.9
1	C	129	THR	3.8
1	C	238	THR	3.8
1	C	375	THR	3.8
1	B	231	ASN	3.8
1	A	193	GLN	3.8
1	B	334	ASN	3.8
1	B	308	GLY	3.8
1	C	337	ASP	3.8
1	A	158	ILE	3.8
1	A	130	GLY	3.7
1	A	215	GLU	3.7
1	C	222	SER	3.7
1	C	227	ASP	3.7
1	C	215	GLU	3.7
1	A	240	ASN	3.7
1	C	255	LYS	3.7
1	B	248	SER	3.6
1	B	46	ASN	3.6
1	B	360	ASP	3.6
1	C	360	ASP	3.6
1	A	45	SER	3.6
1	C	228	HIS	3.6
1	C	369	ASP	3.6
1	A	168	PRO	3.5
1	B	104	ASN	3.5
1	A	320	ASP	3.5
1	A	287	THR	3.5
1	B	272	ASP	3.5
1	B	351	TYR	3.5
1	A	334	ASN	3.5
1	A	64	THR	3.5
1	C	298	THR	3.5
1	A	309	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	318	TYR	3.4
1	C	165	THR	3.4
1	B	312	ASP	3.4
1	A	296	GLU	3.4
1	B	358	HIS	3.4
1	B	166	GLU	3.4
1	C	214	LYS	3.4
1	C	249	PRO	3.4
1	A	107	CYS	3.3
1	C	251	GLY	3.3
1	B	214	LYS	3.3
1	A	68	GLY	3.3
1	C	241	ARG	3.3
1	A	242	VAL	3.3
1	A	61	ASP	3.3
1	B	304	LEU	3.3
1	A	312	ASP	3.2
1	A	352	ASP	3.2
1	C	256	ASP	3.2
1	B	68	GLY	3.2
1	C	344	ALA	3.2
1	A	370	GLU	3.2
1	A	233	TYR	3.2
1	C	93	ARG	3.2
1	B	157	LYS	3.1
1	A	377	PHE	3.1
1	C	348	SER	3.1
1	C	272	ASP	3.1
1	B	288	GLY	3.1
1	C	166	GLU	3.1
1	B	296	GLU	3.1
1	B	305	VAL	3.1
1	A	275	CYS	3.1
1	C	243	GLY	3.1
1	B	116	VAL	3.1
1	B	313	PHE	3.1
1	A	359	LYS	3.0
1	A	166	GLU	3.0
1	B	256	ASP	3.0
1	C	368	GLN	3.0
1	C	386	SER	3.0
1	B	224	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	311	ILE	3.0
1	C	183	PHE	3.0
1	B	129	THR	3.0
1	B	222	SER	3.0
1	B	118	GLY	3.0
1	C	260	THR	3.0
1	A	105	ALA	2.9
1	C	105	ALA	2.9
1	A	310	GLY	2.9
1	B	225	VAL	2.9
1	A	177	GLU	2.9
1	C	370	GLU	2.9
1	B	384	SER	2.9
1	C	358	HIS	2.9
1	A	213	ARG	2.9
1	C	213	ARG	2.9
1	B	361	LYS	2.9
1	B	241	ARG	2.9
1	C	254	PRO	2.9
1	B	259	PRO	2.9
1	A	256	ASP	2.8
1	B	238	THR	2.8
1	C	225	VAL	2.8
1	A	346	PHE	2.8
1	B	388	PRO	2.8
1	B	359	LYS	2.8
1	C	159	PRO	2.8
1	A	36	LYS	2.8
1	A	188	ASP	2.8
1	B	255	LYS	2.8
1	B	228	HIS	2.8
1	A	349	ALA	2.8
1	A	44	SER	2.8
1	A	313	PHE	2.7
1	A	118	GLY	2.7
1	B	66	ASP	2.7
1	B	307	GLY	2.7
1	B	250	ILE	2.7
1	B	142	GLY	2.7
1	A	214	LYS	2.7
1	C	273	LYS	2.7
1	C	81	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	298	THR	2.7
1	C	223	ALA	2.7
1	B	354	HIS	2.7
1	C	299	HIS	2.7
1	B	213	ARG	2.7
1	C	195	CYS	2.7
1	B	226	ALA	2.7
1	C	379	TYR	2.7
1	C	217	ASP	2.7
1	A	236	PRO	2.6
1	C	269	LEU	2.6
1	A	125	ASP	2.6
1	C	237	ALA	2.6
1	A	222	SER	2.6
1	C	45	SER	2.6
1	B	342	VAL	2.6
1	B	330	PRO	2.6
1	C	188	ASP	2.6
1	C	295	VAL	2.6
1	B	173	ASP	2.6
1	C	184	HIS	2.5
1	C	106	GLN	2.5
1	B	383	ARG	2.5
1	B	144	PHE	2.5
1	C	244	HIS	2.5
1	C	336	TYR	2.5
1	C	248	SER	2.5
1	C	218	GLN	2.5
1	A	81	ALA	2.5
1	A	217	ASP	2.5
1	C	172	ALA	2.5
1	B	247	ILE	2.5
1	A	382	PRO	2.5
1	B	269	LEU	2.5
1	B	292	TYR	2.5
1	A	218	GLN	2.5
1	C	317	ALA	2.5
1	A	353	ASN	2.5
1	C	262	PHE	2.5
1	B	353	ASN	2.5
1	A	253	THR	2.5
1	C	347	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	161	LYS	2.5
1	A	284	VAL	2.5
1	B	216	SER	2.4
1	C	79	ASP	2.4
1	B	283	ASP	2.4
1	C	232	VAL	2.4
1	C	160	GLN	2.4
1	C	245	ILE	2.4
1	A	119	PHE	2.4
1	A	131	THR	2.4
1	A	343	THR	2.4
1	B	57	VAL	2.4
1	A	241	ARG	2.4
1	C	377	PHE	2.4
1	C	287	THR	2.4
1	C	46	ASN	2.4
1	A	358	HIS	2.4
1	B	386	SER	2.4
1	C	261	ARG	2.3
1	B	81	ALA	2.3
1	B	265	PHE	2.3
1	B	45	SER	2.3
1	B	273	LYS	2.3
1	C	275	CYS	2.3
1	B	93	ARG	2.3
1	C	208	HIS	2.3
1	C	61	ASP	2.3
1	B	160	GLN	2.3
1	B	191	PRO	2.3
1	B	254	PRO	2.3
1	B	134	ILE	2.3
1	C	323	HIS	2.3
1	A	272	ASP	2.3
1	B	61	ASP	2.3
1	C	170	ARG	2.3
1	B	143	SER	2.3
1	C	179	CYS	2.3
1	C	182	GLN	2.3
1	A	171	GLY	2.3
1	A	340	GLY	2.3
1	C	268	PHE	2.3
1	C	107	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	89	ARG	2.3
1	B	337	ASP	2.3
1	B	260	THR	2.2
1	A	30	SER	2.2
1	A	351	TYR	2.2
1	A	372	ILE	2.2
1	C	78	PRO	2.2
1	C	181	GLY	2.2
1	A	318	TYR	2.2
1	A	248	SER	2.2
1	C	60	VAL	2.2
1	C	221	ILE	2.2
1	C	327	PRO	2.2
1	B	84	LEU	2.2
1	B	345	PRO	2.2
1	C	64	THR	2.2
1	C	324	THR	2.2
1	C	242	VAL	2.2
1	B	47	SER	2.2
1	B	73	SER	2.2
1	A	234	GLY	2.2
1	A	209	ASP	2.2
1	B	169	THR	2.2
1	B	258	THR	2.2
1	A	57	VAL	2.2
1	C	303	TYR	2.2
1	C	309	LEU	2.2
1	A	202	GLU	2.2
1	A	255	LYS	2.2
1	C	301	ARG	2.2
1	A	333	TRP	2.2
1	A	238	THR	2.1
1	C	110	THR	2.1
1	C	224	ILE	2.1
1	A	246	LEU	2.1
1	C	130	GLY	2.1
1	A	104	ASN	2.1
1	B	188	ASP	2.1
1	A	250	ILE	2.1
1	A	344	ALA	2.1
1	B	277	ARG	2.1
1	A	249	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	320	ASP	2.1
1	A	314	HIS	2.1
1	A	77	THR	2.1
1	B	321	THR	2.1
1	A	167	ALA	2.1
1	B	349	ALA	2.1
1	C	68	GLY	2.1
1	C	265	PHE	2.1
1	A	350	ILE	2.1
1	C	329	ILE	2.1
1	C	233	TYR	2.1
1	B	287	THR	2.1
1	C	340	GLY	2.1
1	C	259	PRO	2.1
1	C	288	GLY	2.1
1	B	340	GLY	2.1
1	C	236	PRO	2.1
1	B	151	SER	2.0
1	C	277	ARG	2.0
1	A	145	THR	2.0
1	A	282	VAL	2.0
1	B	69	SER	2.0
1	B	208	HIS	2.0
1	B	339	THR	2.0
1	B	196	PRO	2.0
1	C	363	VAL	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	CA	A	901	1/1	0.91	0.21	94,94,94,94	0
2	CA	A	902	1/1	0.92	0.19	80,80,80,80	0
2	CA	C	901	1/1	0.96	0.16	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.