



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2024 – 07:14 PM EST

PDB ID : 4NWV
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	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

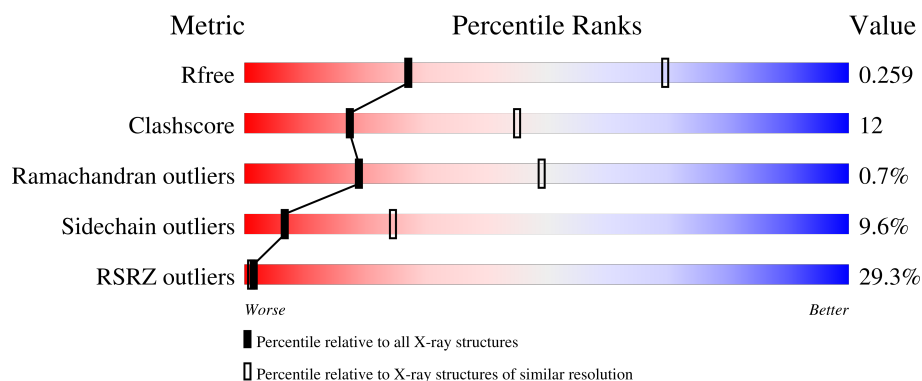
1 Overall quality at a glance

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}	164625	1482 (3.30-3.22)
Clashscore	180529	1546 (3.30-3.22)
Ramachandran outliers	177936	1536 (3.30-3.22)
Sidechain outliers	177891	1535 (3.30-3.22)
RSRZ outliers	164620	1483 (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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	391	<div> <div>21%</div> <div>62%</div> <div>26%</div> <div>9%</div> </div>
1	B	391	<div> <div>26%</div> <div>63%</div> <div>21%</div> <div>12%</div> </div>
1	C	391	<div> <div>30%</div> <div>60%</div> <div>25%</div> <div>12%</div> </div>

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			

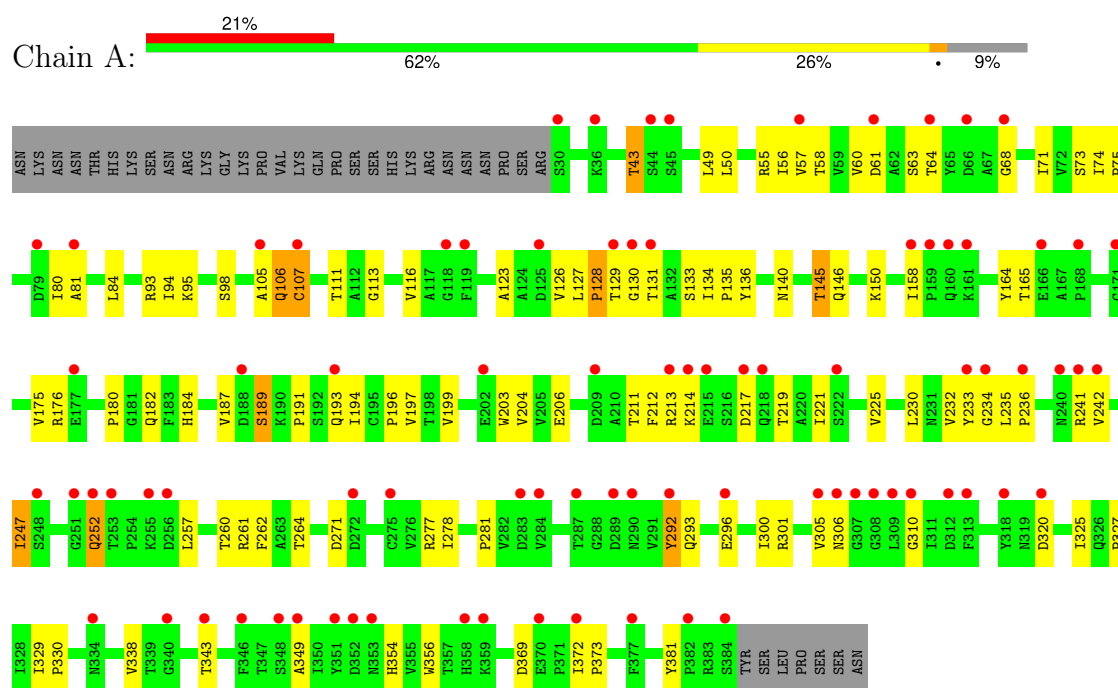
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

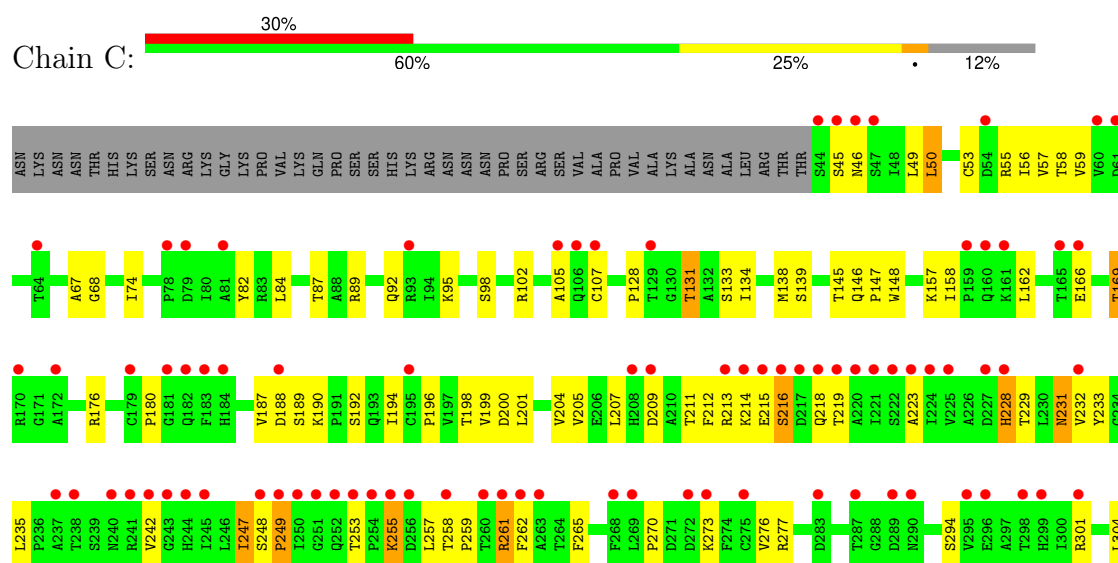
3 Residue-property plots

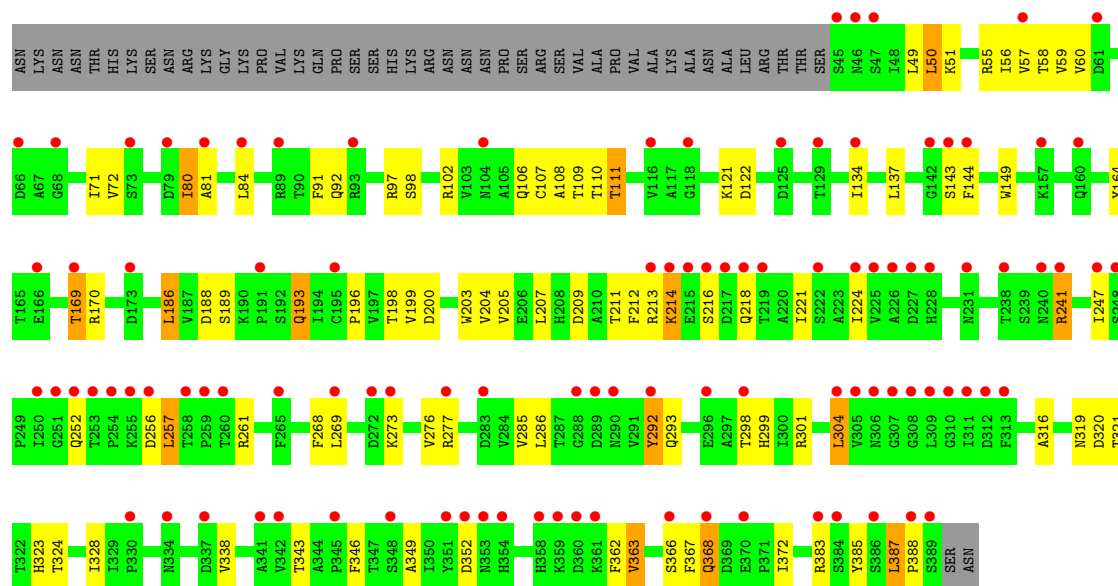
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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





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 [i](#)

5.1 Standard geometry [i](#)

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	0.43	0/2823	0.65	0/3873
1	B	0.42	0/2760	0.66	0/3787
1	C	0.41	0/2766	0.64	0/3795
All	All	0.42	0/8349	0.65	0/11455

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.

There are no bond angle outliers.

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 [i](#)

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	72	0
1	B	2683	0	2634	56	0
1	C	2689	0	2641	80	0
2	A	2	0	0	0	0
2	C	1	0	0	0	0
All	All	8122	0	7984	197	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 12.

All (197) 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: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
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:B:387:LEU:O	1:B:388:PRO:C	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:HD23	1:B:304:LEU:H	1.75	0.50
1:B:109:THR:HG22	1:B:149:TRP:CE3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:258:THR:OG1	1:C:261:ARG:NH1	2.46	0.47
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:C:214:LYS:HB3	1:C:216:SER:N	2.30	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:A:49:LEU:C	1:A:49:LEU:HD23	2.34	0.46
1:B:108:ALA:O	1:B:111:THR:CG2	2.64	0.46
1:B:292:TYR:CD2	1:B:292:TYR:C	2.88	0.46
1:C:232:VAL:HG23	1:C:356:TRP:CZ3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:366:SER:C	1:B:367:PHE:O	2.48	0.46
1:C:74:ILE:O	1:C:74:ILE:HG23	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: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: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
1:C:169:THR:HG21	1:C:213:ARG:CZ	2.47	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:292:TYR:C	1:A:292:TYR:CD2	2.91	0.43
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:B:97:ARG:HH11	1:B:97:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:130:GLY:O	1:A:131:THR:C	2.58	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:127:LEU:C	1:A:128:PRO:O	2.57	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:C:262:PHE:CD2	1:C:262:PHE:C	2.92	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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	353/391 (90%)	334 (95%)	17 (5%)	2 (1%)	22	52
1	B	343/391 (88%)	324 (94%)	17 (5%)	2 (1%)	22	52
1	C	344/391 (88%)	322 (94%)	19 (6%)	3 (1%)	14	43
All	All	1040/1173 (89%)	980 (94%)	53 (5%)	7 (1%)	19	49

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%)	278 (92%)	25 (8%)	9	30
1	B	297/338 (88%)	264 (89%)	33 (11%)	5	19
1	C	298/338 (88%)	270 (91%)	28 (9%)	7	25
All	All	898/1014 (89%)	812 (90%)	86 (10%)	7	24

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	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
1	A	214	LYS
1	A	219	THR
1	A	221	ILE
1	A	230	LEU
1	A	241	ARG
1	A	247	ILE
1	A	252	GLN
1	A	292	TYR
1	A	293	GLN
1	A	320	ASP
1	A	343	THR
1	A	372	ILE
1	C	50	LEU
1	C	84	LEU
1	C	98	SER
1	C	131	THR
1	C	139	SER

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Mol	Chain	Res	Type
1	C	145	THR
1	C	157	LYS
1	C	169	THR
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	228	HIS
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	80	ILE
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	143	SER
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

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Mol	Chain	Res	Type
1	B	252	GLN
1	B	257	LEU
1	B	273	LYS
1	B	292	TYR
1	B	293	GLN
1	B	298	THR
1	B	301	ARG
1	B	304	LEU
1	B	320	ASP
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 (14) 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	319	ASN
1	A	354	HIS
1	C	182	GLN
1	C	231	ASN
1	C	326	GLN
1	B	140	ASN
1	B	228	HIS
1	B	244	HIS
1	B	319	ASN
1	B	368	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 [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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Warning: The R factor obtained from EDS is 0.5734, which does not match the depositor's R factor of 0.2778. Please interpret the results in this section carefully.

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%)	1.48	84 (23%) 2 2	15, 39, 82, 185	0
1	B	345/391 (88%)	1.67	103 (29%) 1 1	14, 43, 84, 127	0
1	C	346/391 (88%)	1.78	119 (34%) 1 1	15, 47, 95, 162	0
All	All	1046/1173 (89%)	1.64	306 (29%) 1 1	14, 43, 91, 185	0

All (306) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	GLY	9.0
1	B	310	GLY	8.3
1	B	289	ASP	8.1
1	A	160	GLN	8.1
1	C	308	GLY	8.0
1	B	306	ASN	7.1
1	C	289	ASP	7.0
1	C	306	ASN	6.9
1	B	252	GLN	6.9
1	C	258	THR	6.7
1	B	251	GLY	6.3
1	A	289	ASP	6.2
1	C	252	GLN	6.2
1	C	389	SER	6.1
1	A	384	SER	6.0
1	B	309	LEU	5.9
1	A	129	THR	5.7
1	C	307	GLY	5.6
1	A	283	ASP	5.6
1	B	290	ASN	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	252	GLN	5.4
1	B	240	ASN	5.4
1	C	220	ALA	5.3
1	B	215	GLU	5.3
1	B	370	GLU	5.3
1	B	253	THR	5.2
1	A	305	VAL	5.1
1	C	216	SER	5.0
1	A	290	ASN	5.0
1	B	218	GLN	5.0
1	C	290	ASN	4.9
1	C	352	ASP	4.9
1	C	44	SER	4.9
1	C	374	GLY	4.9
1	A	159	PRO	4.8
1	C	296	GLU	4.7
1	B	389	SER	4.7
1	C	366	SER	4.6
1	C	161	LYS	4.5
1	C	359	LYS	4.5
1	C	283	ASP	4.5
1	C	253	THR	4.4
1	C	320	ASP	4.4
1	B	368	GLN	4.4
1	C	378	ASP	4.3
1	A	306	ASN	4.3
1	C	54	ASP	4.3
1	C	250	ILE	4.3
1	C	219	THR	4.2
1	B	219	THR	4.2
1	C	240	ASN	4.2
1	A	308	GLY	4.2
1	B	195	CYS	4.2
1	B	125	ASP	4.1
1	C	209	ASP	4.1
1	B	227	ASP	4.1
1	B	79	ASP	4.1
1	C	263	ALA	4.0
1	C	341	ALA	4.0
1	A	66	ASP	4.0
1	A	251	GLY	4.0
1	B	352	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	341	ALA	3.9
1	C	383	ARG	3.9
1	B	217	ASP	3.9
1	A	348	SER	3.9
1	B	348	SER	3.9
1	C	334	ASN	3.9
1	C	343	THR	3.8
1	A	292	TYR	3.8
1	C	382	PRO	3.8
1	C	47	SER	3.7
1	A	79	ASP	3.7
1	A	193	GLN	3.7
1	B	366	SER	3.7
1	B	231	ASN	3.7
1	C	129	THR	3.7
1	C	238	THR	3.7
1	C	375	THR	3.7
1	B	334	ASN	3.7
1	B	308	GLY	3.6
1	A	215	GLU	3.6
1	A	158	ILE	3.6
1	C	337	ASP	3.6
1	C	215	GLU	3.6
1	A	130	GLY	3.6
1	C	255	LYS	3.6
1	C	222	SER	3.5
1	A	240	ASN	3.5
1	C	227	ASP	3.5
1	B	46	ASN	3.5
1	B	248	SER	3.5
1	B	360	ASP	3.5
1	C	360	ASP	3.4
1	C	228	HIS	3.4
1	A	45	SER	3.4
1	B	104	ASN	3.4
1	C	369	ASP	3.4
1	A	168	PRO	3.4
1	A	320	ASP	3.4
1	A	287	THR	3.4
1	B	272	ASP	3.3
1	A	334	ASN	3.3
1	B	351	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	64	THR	3.3
1	C	298	THR	3.3
1	A	296	GLU	3.3
1	A	309	LEU	3.3
1	C	214	LYS	3.2
1	B	166	GLU	3.2
1	C	165	THR	3.2
1	B	214	LYS	3.2
1	C	318	TYR	3.2
1	B	312	ASP	3.2
1	B	358	HIS	3.2
1	C	241	ARG	3.2
1	C	249	PRO	3.2
1	C	251	GLY	3.2
1	A	107	CYS	3.2
1	A	68	GLY	3.1
1	A	242	VAL	3.1
1	B	304	LEU	3.1
1	A	61	ASP	3.1
1	A	312	ASP	3.1
1	A	352	ASP	3.1
1	C	256	ASP	3.1
1	C	344	ALA	3.1
1	B	68	GLY	3.1
1	C	93	ARG	3.1
1	A	370	GLU	3.0
1	B	157	LYS	3.0
1	C	166	GLU	3.0
1	A	233	TYR	3.0
1	B	288	GLY	3.0
1	B	296	GLU	3.0
1	C	272	ASP	3.0
1	A	377	PHE	3.0
1	C	348	SER	3.0
1	B	305	VAL	2.9
1	A	359	LYS	2.9
1	B	116	VAL	2.9
1	A	166	GLU	2.9
1	C	243	GLY	2.9
1	A	275	CYS	2.9
1	C	368	GLN	2.9
1	B	224	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	311	ILE	2.9
1	B	313	PHE	2.9
1	B	256	ASP	2.9
1	C	386	SER	2.8
1	B	129	THR	2.8
1	A	105	ALA	2.8
1	A	213	ARG	2.8
1	C	105	ALA	2.8
1	C	213	ARG	2.8
1	A	177	GLU	2.8
1	C	370	GLU	2.8
1	B	361	LYS	2.8
1	C	260	THR	2.8
1	B	225	VAL	2.8
1	B	118	GLY	2.8
1	C	183	PHE	2.8
1	B	222	SER	2.8
1	B	241	ARG	2.8
1	A	310	GLY	2.8
1	C	358	HIS	2.7
1	B	384	SER	2.7
1	C	254	PRO	2.7
1	B	359	LYS	2.7
1	C	225	VAL	2.7
1	A	36	LYS	2.7
1	B	238	THR	2.7
1	B	255	LYS	2.7
1	B	259	PRO	2.7
1	A	256	ASP	2.7
1	A	346	PHE	2.6
1	B	388	PRO	2.6
1	A	188	ASP	2.6
1	A	349	ALA	2.6
1	C	159	PRO	2.6
1	A	214	LYS	2.6
1	C	273	LYS	2.6
1	B	228	HIS	2.6
1	B	250	ILE	2.6
1	A	118	GLY	2.6
1	B	307	GLY	2.6
1	C	81	ALA	2.6
1	A	44	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	66	ASP	2.6
1	A	313	PHE	2.6
1	B	142	GLY	2.6
1	C	223	ALA	2.6
1	B	213	ARG	2.6
1	B	298	THR	2.6
1	B	354	HIS	2.5
1	B	226	ALA	2.5
1	C	299	HIS	2.5
1	C	269	LEU	2.5
1	C	195	CYS	2.5
1	C	217	ASP	2.5
1	C	379	TYR	2.5
1	C	237	ALA	2.5
1	A	236	PRO	2.5
1	A	125	ASP	2.5
1	B	342	VAL	2.5
1	A	222	SER	2.4
1	C	45	SER	2.4
1	C	295	VAL	2.4
1	B	383	ARG	2.4
1	C	188	ASP	2.4
1	B	330	PRO	2.4
1	C	106	GLN	2.4
1	B	173	ASP	2.4
1	C	184	HIS	2.4
1	A	81	ALA	2.4
1	C	172	ALA	2.4
1	C	218	GLN	2.4
1	B	247	ILE	2.4
1	C	244	HIS	2.4
1	C	336	TYR	2.3
1	B	269	LEU	2.3
1	A	161	LYS	2.3
1	C	248	SER	2.3
1	B	144	PHE	2.3
1	A	217	ASP	2.3
1	C	317	ALA	2.3
1	A	218	GLN	2.3
1	A	382	PRO	2.3
1	A	353	ASN	2.3
1	B	353	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	284	VAL	2.3
1	A	253	THR	2.3
1	C	347	THR	2.3
1	B	292	TYR	2.3
1	C	232	VAL	2.3
1	C	245	ILE	2.3
1	C	160	GLN	2.3
1	C	262	PHE	2.3
1	A	241	ARG	2.3
1	B	57	VAL	2.3
1	B	216	SER	2.3
1	C	79	ASP	2.3
1	B	283	ASP	2.3
1	A	131	THR	2.3
1	A	343	THR	2.3
1	A	119	PHE	2.2
1	C	261	ARG	2.2
1	C	46	ASN	2.2
1	C	287	THR	2.2
1	B	93	ARG	2.2
1	B	273	LYS	2.2
1	B	81	ALA	2.2
1	A	358	HIS	2.2
1	C	377	PHE	2.2
1	C	170	ARG	2.2
1	B	386	SER	2.2
1	B	160	GLN	2.2
1	B	134	ILE	2.2
1	C	208	HIS	2.2
1	B	265	PHE	2.2
1	B	45	SER	2.2
1	C	61	ASP	2.2
1	C	275	CYS	2.1
1	B	89	ARG	2.1
1	C	323	HIS	2.1
1	B	191	PRO	2.1
1	B	254	PRO	2.1
1	A	272	ASP	2.1
1	B	61	ASP	2.1
1	C	182	GLN	2.1
1	B	143	SER	2.1
1	A	171	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	340	GLY	2.1
1	C	179	CYS	2.1
1	A	372	ILE	2.1
1	B	260	THR	2.1
1	B	337	ASP	2.1
1	C	268	PHE	2.1
1	C	107	CYS	2.1
1	C	60	VAL	2.1
1	C	221	ILE	2.1
1	C	181	GLY	2.1
1	A	30	SER	2.1
1	A	351	TYR	2.1
1	B	84	LEU	2.1
1	C	78	PRO	2.1
1	C	242	VAL	2.1
1	A	255	LYS	2.0
1	C	301	ARG	2.0
1	A	318	TYR	2.0
1	C	64	THR	2.0
1	C	324	THR	2.0
1	A	248	SER	2.0
1	A	57	VAL	2.0
1	C	327	PRO	2.0
1	B	345	PRO	2.0
1	A	202	GLU	2.0
1	A	234	GLY	2.0
1	B	169	THR	2.0
1	B	258	THR	2.0
1	C	309	LEU	2.0
1	B	47	SER	2.0
1	B	73	SER	2.0
1	A	209	ASP	2.0
1	B	277	ARG	2.0
1	C	224	ILE	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 [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
2	CA	A	901	1/1	0.90	0.23	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	0.17	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.