



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 01:56 AM UTC

PDB ID : 7QE1 / pdb_00007qe1
Title : Crystal structure of apo SN243
Authors : Neun, S.; Brear, P.; Campbell, E.; Omari, K.; Wagner, O.; Hyvonen, M.;
Hollfelder, F.
Deposited on : 2021-12-01
Resolution : 1.95 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

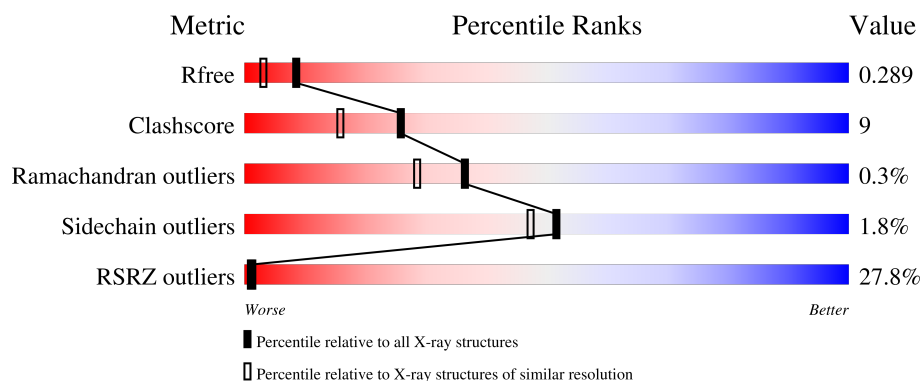
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	759	33% 74% 22% ..
1	B	759	21% 81% 14% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11334 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 SN243.

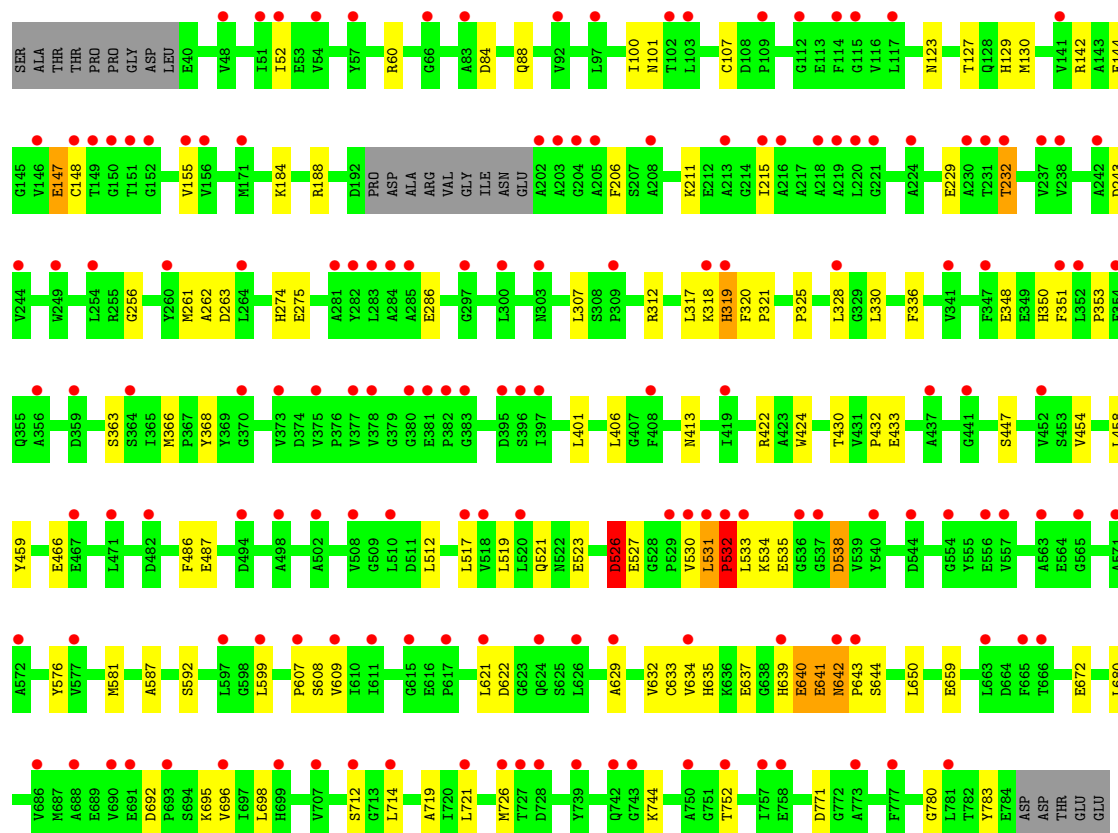
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	739	Total	C	N	O	S	0	0	0
			5618	3522	921	1155	20			
1	B	736	Total	C	N	O	S	0	0	0
			5598	3510	918	1150	20			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	14	Total	Zn	0	0
			14	14		
2	B	13	Total	Zn	0	0
			13	13		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total	O	0	0
			24	24		
3	B	67	Total	O	0	0
			67	67		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.28Å 90.76Å 103.29Å 67.22° 84.03° 76.91°	Depositor
Resolution (Å)	51.89 – 1.95 51.89 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.3 (51.89-1.95) 97.5 (51.89-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.240 , 0.290 0.247 , 0.289	Depositor DCC
R_{free} test set	6089 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11334	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% 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: ZN

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	0.57	0/5743	0.84	4/7831 (0.1%)
1	B	0.51	0/5722	0.82	10/7801 (0.1%)
All	All	0.54	0/11465	0.83	14/15632 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	535	GLU	CA-C-N	-13.29	112.63	122.33
1	B	535	GLU	C-N-CA	-13.29	112.63	122.33
1	A	532	PRO	N-CA-C	-7.28	97.48	112.47
1	B	532	PRO	N-CA-C	-6.30	99.48	112.47
1	A	758	GLU	N-CA-CB	-6.21	102.31	110.88
1	B	526	ASP	N-CA-C	-6.21	104.60	111.36
1	B	538	ASP	N-CA-C	-5.73	99.95	109.46
1	B	639	HIS	N-CA-C	-5.53	106.74	112.93
1	B	319	HIS	CB-CA-C	5.46	121.29	110.42
1	A	425	GLY	N-CA-C	-5.35	107.94	115.32
1	B	52	ILE	CA-C-N	5.25	129.75	122.77
1	B	52	ILE	C-N-CA	5.25	129.75	122.77
1	A	758	GLU	CB-CA-C	5.12	117.98	109.38
1	B	318	LYS	N-CA-C	5.10	117.72	109.40

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	5618	0	5286	131	0
1	B	5598	0	5273	77	0
2	A	14	0	0	0	0
2	B	13	0	0	0	0
3	A	24	0	0	0	0
3	B	67	0	0	3	0
All	All	11334	0	10559	207	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 9.

All (207) 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:635:HIS:HD2	1:B:637:GLU:H	1.12	0.91
1:A:592:SER:O	1:A:599:LEU:HD13	1.77	0.85
1:A:611:ILE:O	1:A:611:ILE:HD12	1.81	0.81
1:A:744:LYS:HD3	1:A:780:GLY:HA3	1.66	0.78
1:A:754:GLU:O	1:A:758:GLU:HB2	1.85	0.77
1:B:531:LEU:O	1:B:533:LEU:N	2.17	0.76
1:A:592:SER:O	1:A:599:LEU:CD1	2.33	0.76
1:A:371:VAL:HG21	1:A:610:ILE:HD13	1.68	0.76
1:B:592:SER:O	1:B:599:LEU:HD13	1.87	0.74
1:A:587:ALA:HB1	1:A:650:LEU:HD12	1.68	0.73
1:A:531:LEU:O	1:A:533:LEU:N	2.22	0.72
1:B:129:HIS:ND1	3:B:903:HOH:O	2.24	0.71
1:A:142:ARG:HD2	1:A:146:VAL:HG11	1.73	0.70
1:B:635:HIS:CD2	1:B:637:GLU:H	2.04	0.68
1:A:501:GLY:O	1:A:506:ARG:NH1	2.25	0.67
1:B:744:LYS:HD3	1:B:780:GLY:HA3	1.77	0.66
1:A:635:HIS:HD2	1:A:637:GLU:H	1.43	0.64
1:A:418:ILE:HA	1:A:422:ARG:HB2	1.80	0.64
1:A:531:LEU:HD22	1:A:719:ALA:HB1	1.79	0.63
1:A:144:GLU:HB3	1:B:144:GLU:CD	2.24	0.63
1:B:527:GLU:H	1:B:527:GLU:CD	2.07	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ILE:HD13	1:B:512:LEU:HD23	1.81	0.62
1:B:517:LEU:HD13	1:B:726:MET:SD	2.40	0.61
1:B:752:THR:HG21	1:B:771:ASP:HB2	1.82	0.61
1:A:191:ILE:O	1:A:211:LYS:HE2	2.01	0.61
1:A:387:PRO:HB2	1:A:389:THR:HG22	1.82	0.61
1:A:525:THR:OG1	1:A:528:GLY:N	2.34	0.61
1:A:389:THR:HG23	1:A:394:SER:OG	2.01	0.60
1:A:263:ASP:OD1	1:A:319:HIS:HB2	2.01	0.60
1:B:232:THR:HB	1:B:286:GLU:HG3	1.84	0.59
1:A:125:ILE:HG21	1:A:171:MET:HG2	1.84	0.59
1:A:144:GLU:H	1:A:144:GLU:CD	2.11	0.59
1:B:531:LEU:O	1:B:532:PRO:C	2.44	0.59
1:A:752:THR:HG21	1:A:771:ASP:HB3	1.84	0.58
1:A:49:LYS:HG3	1:A:62:LEU:HA	1.85	0.57
1:A:626:LEU:H	1:A:626:LEU:HD12	1.68	0.57
1:B:430:THR:HG23	1:B:433:GLU:H	1.70	0.57
1:A:149:THR:C	1:A:151:THR:H	2.13	0.56
1:B:632:VAL:HA	1:B:635:HIS:NE2	2.20	0.56
1:A:531:LEU:O	1:A:532:PRO:C	2.47	0.56
1:B:526:ASP:N	1:B:526:ASP:OD1	2.39	0.56
1:A:377:VAL:HA	1:A:386:TYR:CE2	2.40	0.55
1:B:262:ALA:HB1	1:B:353:PRO:HB2	1.89	0.55
1:A:191:ILE:O	1:A:211:LYS:CD	2.56	0.54
1:A:193:PRO:HD3	1:A:211:LYS:CE	2.37	0.54
1:A:325:PRO:HD3	1:A:350:HIS:ND1	2.23	0.54
1:B:629:ALA:HA	1:B:634:VAL:HG21	1.90	0.54
1:A:148:CYS:SG	1:A:148:CYS:O	2.64	0.54
1:A:521:GLN:O	1:A:719:ALA:HA	2.07	0.54
1:A:247:GLU:HG2	1:A:312:ARG:NH1	2.23	0.54
1:A:531:LEU:HD21	1:A:721:LEU:HD11	1.89	0.54
1:B:632:VAL:HA	1:B:635:HIS:CE1	2.43	0.54
1:B:633:CYS:HA	1:B:643:PRO:HG2	1.88	0.54
1:B:609:VAL:HG12	1:B:622:ASP:C	2.33	0.54
1:A:147:GLU:H	1:A:147:GLU:CD	2.15	0.54
1:A:78:THR:HG21	1:A:482:ASP:OD1	2.09	0.53
1:A:84:ASP:O	1:A:88:GLN:HG3	2.08	0.53
1:A:59:PHE:HZ	1:A:75:ARG:HE	1.56	0.53
1:B:319:HIS:HA	1:B:368:TYR:HB2	1.90	0.53
1:B:328:LEU:HD11	1:B:607:PRO:HG2	1.91	0.53
1:B:531:LEU:HD11	1:B:721:LEU:HD21	1.90	0.53
1:A:632:VAL:HA	1:A:635:HIS:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:ILE:HD12	1:A:611:ILE:C	2.34	0.52
1:A:519:LEU:HD13	1:A:531:LEU:HD23	1.92	0.52
1:B:60:ARG:HD2	1:B:487:GLU:O	2.10	0.52
1:A:687:MET:HG2	1:A:696:VAL:HG21	1.92	0.52
1:B:641:GLU:O	1:B:642:ASN:C	2.51	0.52
1:B:107:CYS:SG	1:B:148:CYS:HB3	2.50	0.52
1:A:635:HIS:HD2	1:A:637:GLU:N	2.08	0.52
1:A:49:LYS:HE2	1:A:173:GLU:O	2.10	0.51
1:A:338:LYS:O	1:A:371:VAL:HG22	2.11	0.51
1:A:427:GLU:HA	1:A:434:ARG:HH21	1.75	0.51
1:A:635:HIS:CD2	1:A:637:GLU:H	2.26	0.51
1:B:101:ASN:HB2	1:B:130:MET:HE1	1.93	0.51
1:B:659:GLU:OE2	1:B:672:GLU:HG2	2.11	0.51
1:A:331:ASP:OD2	1:A:333:HIS:HD2	1.93	0.50
1:A:517:LEU:HD21	1:A:721:LEU:HD22	1.93	0.50
1:A:454:VAL:O	1:A:458:LEU:HG	2.11	0.50
1:A:348:GLU:HA	1:A:351:PHE:CE2	2.46	0.50
1:A:149:THR:O	1:A:151:THR:N	2.43	0.50
1:A:231:THR:HG23	1:A:232:THR:H	1.77	0.50
1:B:184:LYS:HA	1:B:256:GLY:O	2.12	0.49
1:A:159:ALA:O	1:A:163:THR:HG23	2.12	0.49
1:B:432:PRO:HB3	1:B:458:LEU:HD21	1.93	0.49
1:B:534:LYS:HG2	1:B:576:TYR:OH	2.12	0.49
1:B:100:ILE:HG23	1:B:447:SER:HA	1.95	0.49
1:A:369:TYR:HD1	1:A:418:ILE:HD13	1.77	0.49
1:A:193:PRO:HD3	1:A:211:LYS:HE2	1.94	0.49
1:B:147:GLU:H	1:B:147:GLU:CD	2.20	0.49
1:B:348:GLU:HA	1:B:351:PHE:CE2	2.47	0.49
1:B:609:VAL:HA	1:B:621:LEU:O	2.13	0.49
1:A:261:MET:HE2	1:A:319:HIS:HE1	1.77	0.49
1:A:518:VAL:HG22	1:A:743:GLY:C	2.38	0.49
1:B:692:ASP:HB3	1:B:695:LYS:HG3	1.93	0.49
1:A:247:GLU:HG2	1:A:312:ARG:HH11	1.78	0.48
1:A:422:ARG:NH1	1:A:646:THR:OG1	2.46	0.48
1:A:646:THR:HG23	1:A:647:ASP:OD1	2.13	0.48
1:B:608:SER:HB3	1:B:621:LEU:HD12	1.94	0.48
1:B:263:ASP:OD1	1:B:319:HIS:HB2	2.13	0.48
1:B:401:LEU:O	1:B:406:LEU:HG	2.13	0.48
1:B:243:ASP:OD1	1:B:312:ARG:NH2	2.43	0.48
1:A:120:GLN:HG2	1:A:124:TYR:CZ	2.49	0.48
1:A:641:GLU:H	1:A:641:GLU:CD	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ILE:HG23	1:A:447:SER:HA	1.96	0.48
1:A:425:GLY:C	1:A:426:LEU:HD12	2.39	0.48
1:A:261:MET:HE1	1:A:275:GLU:OE2	2.14	0.47
1:B:696:VAL:HG12	1:B:698:LEU:CD1	2.44	0.47
1:A:105:ALA:HB3	1:A:137:ASN:ND2	2.29	0.47
1:A:108:ASP:HB3	1:A:111:THR:HB	1.95	0.47
1:A:120:GLN:HG2	1:A:124:TYR:CE1	2.48	0.47
1:B:261:MET:HE1	1:B:275:GLU:CD	2.39	0.47
1:A:332:PRO:HG3	1:A:368:TYR:CE2	2.50	0.47
1:B:88:GLN:OE1	3:B:901:HOH:O	2.20	0.47
1:A:100:ILE:HD12	1:A:132:ARG:HB3	1.96	0.47
1:A:85:LEU:O	1:A:89:MET:HG3	2.15	0.47
1:A:101:ASN:HD22	1:A:450:SER:HB3	1.80	0.47
1:B:188:ARG:HD3	1:B:206:PHE:CE2	2.49	0.47
1:A:261:MET:HE2	1:A:319:HIS:CE1	2.50	0.46
1:A:358:ILE:HA	1:A:362:VAL:HG12	1.97	0.46
1:A:170:GLU:HA	1:A:490:TYR:OH	2.15	0.46
1:A:85:LEU:HD21	1:A:179:ILE:HD11	1.97	0.46
1:A:470:ASP:O	1:A:474:GLU:HG3	2.16	0.46
1:A:63:ASN:HD21	1:A:65:ASN:ND2	2.14	0.45
1:A:460:GLU:C	1:A:462:ASP:H	2.24	0.45
1:B:521:GLN:O	1:B:719:ALA:HA	2.14	0.45
1:A:331:ASP:OD2	1:A:333:HIS:CD2	2.69	0.45
1:B:454:VAL:O	1:B:458:LEU:HG	2.16	0.45
1:B:640:GLU:HG3	1:B:641:GLU:O	2.17	0.45
1:B:744:LYS:NZ	1:B:780:GLY:O	2.46	0.45
1:B:325:PRO:HD3	1:B:350:HIS:CD2	2.52	0.45
1:A:191:ILE:O	1:A:193:PRO:HD3	2.17	0.45
1:A:632:VAL:HA	1:A:635:HIS:NE2	2.31	0.45
1:B:672:GLU:OE1	3:B:902:HOH:O	2.21	0.45
1:B:692:ASP:O	1:B:695:LYS:HG3	2.16	0.45
1:A:63:ASN:HD21	1:A:65:ASN:CG	2.25	0.45
1:A:366:MET:HA	1:A:413:ASN:O	2.17	0.45
1:B:531:LEU:HB3	1:B:783:TYR:CE1	2.52	0.45
1:B:307:LEU:HD21	1:B:363:SER:HB2	1.99	0.44
1:B:641:GLU:O	1:B:643:PRO:N	2.51	0.44
1:A:534:LYS:HG2	1:A:576:TYR:HE2	1.82	0.44
1:A:613:ASP:N	1:A:613:ASP:OD1	2.50	0.44
1:A:777:PHE:C	1:A:777:PHE:CD1	2.96	0.44
1:A:60:ARG:NH1	1:A:486:PHE:O	2.47	0.44
1:A:411:TYR:HB3	1:A:475:ARG:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:680:LEU:HD11	1:B:714:LEU:HD21	2.00	0.44
1:A:124:TYR:CE1	1:A:450:SER:HB2	2.53	0.44
1:A:369:TYR:CE1	1:A:418:ILE:HG21	2.53	0.44
1:A:270:TRP:CZ3	1:A:324:GLY:HA2	2.53	0.44
1:B:60:ARG:NH1	1:B:486:PHE:O	2.45	0.44
1:B:123:ASN:OD1	1:B:127:THR:OG1	2.36	0.44
1:A:139:VAL:HA	1:A:156:VAL:O	2.18	0.43
1:B:84:ASP:O	1:B:88:GLN:HG3	2.18	0.43
1:B:459:TYR:HE1	1:B:466:GLU:HB3	1.83	0.43
1:B:581:MET:HE3	1:B:581:MET:HB3	1.81	0.43
1:A:65:ASN:ND2	1:A:67:GLU:HB2	2.33	0.43
1:A:369:TYR:CD1	1:A:418:ILE:HG21	2.53	0.43
1:B:752:THR:HG21	1:B:771:ASP:CB	2.48	0.43
1:A:371:VAL:O	1:A:371:VAL:HG23	2.19	0.43
1:A:191:ILE:O	1:A:211:LYS:CE	2.65	0.43
1:B:330:LEU:HD22	1:B:336:PHE:CE1	2.54	0.43
1:B:519:LEU:HD13	1:B:531:LEU:HD12	1.99	0.43
1:A:262:ALA:HA	1:A:288:MET:HE3	2.01	0.43
1:B:430:THR:HG22	1:B:433:GLU:HB2	2.00	0.43
1:A:222:GLU:OE1	1:A:742:GLN:NE2	2.49	0.42
1:A:641:GLU:CD	1:A:642:ASN:H	2.27	0.42
1:B:430:THR:HG23	1:B:432:PRO:HD2	2.01	0.42
1:A:270:TRP:O	1:A:273:THR:HG23	2.20	0.42
1:A:620:GLY:C	1:A:621:LEU:HD23	2.44	0.42
1:B:523:GLU:O	1:B:530:VAL:HG23	2.19	0.42
1:A:261:MET:HE3	1:A:261:MET:HB2	1.81	0.42
1:A:616:GLU:HG3	1:A:617:PRO:HD2	2.01	0.42
1:B:142:ARG:HG2	1:B:155:VAL:HB	2.00	0.42
1:B:422:ARG:HG2	1:B:424:TRP:CZ2	2.54	0.42
1:B:587:ALA:HB1	1:B:650:LEU:HD12	2.02	0.42
1:A:515:LYS:HD3	1:A:742:GLN:NE2	2.34	0.42
1:A:326:GLN:HB3	1:A:330:LEU:O	2.20	0.42
1:A:191:ILE:O	1:A:211:LYS:HD2	2.20	0.42
1:A:325:PRO:HD3	1:A:350:HIS:CE1	2.55	0.42
1:A:649:ARG:O	1:A:650:LEU:C	2.62	0.42
1:B:531:LEU:HD23	1:B:531:LEU:HA	1.62	0.42
1:A:369:TYR:CD1	1:A:418:ILE:HD13	2.54	0.42
1:A:63:ASN:ND2	1:A:69:ASP:CG	2.78	0.41
1:A:46:ALA:HB2	1:A:60:ARG:HE	1.85	0.41
1:A:503:ASP:OD1	1:A:506:ARG:NH2	2.47	0.41
1:A:531:LEU:HD11	1:A:735:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:775:TYR:CD1	1:A:779:TYR:CE2	3.08	0.41
1:B:211:LYS:HD3	1:B:274:HIS:O	2.20	0.41
1:A:209:PHE:CE2	1:A:512:LEU:HD22	2.56	0.41
1:A:401:LEU:O	1:A:406:LEU:HG	2.20	0.41
1:B:430:THR:CG2	1:B:433:GLU:H	2.33	0.41
1:A:53:GLU:HG2	1:A:57:TYR:O	2.21	0.41
1:A:577:VAL:N	1:A:695:LYS:O	2.44	0.41
1:A:413:ASN:C	1:A:413:ASN:HD22	2.29	0.41
1:B:413:ASN:C	1:B:413:ASN:HD22	2.29	0.41
1:A:320:PHE:CE1	1:A:402:LEU:HB2	2.56	0.41
1:A:752:THR:HG21	1:A:771:ASP:CB	2.49	0.41
1:B:712:SER:OG	1:B:714:LEU:HG	2.21	0.41
1:A:562:VAL:HG11	1:A:568:ARG:HA	2.03	0.41
1:A:611:ILE:O	1:A:611:ILE:CD1	2.60	0.41
1:B:366:MET:HA	1:B:413:ASN:O	2.21	0.41
1:A:85:LEU:HD21	1:A:179:ILE:CD1	2.51	0.40
1:A:175:THR:O	1:A:176:ARG:C	2.63	0.40
1:A:609:VAL:HG12	1:A:622:ASP:C	2.47	0.40
1:A:298:GLU:O	1:A:300:LEU:HD12	2.21	0.40
1:A:42:PRO:HD2	1:A:74:TRP:CE2	2.57	0.40
1:A:63:ASN:ND2	1:A:69:ASP:OD2	2.55	0.40
1:B:320:PHE:CD1	1:B:321:PRO:HA	2.57	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	735/759 (97%)	703 (96%)	29 (4%)	3 (0%)	30	21
1	B	732/759 (96%)	708 (97%)	22 (3%)	2 (0%)	36	28
All	All	1467/1518 (97%)	1411 (96%)	51 (4%)	5 (0%)	36	28

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	641	GLU
1	A	150	GLY
1	B	532	PRO
1	A	532	PRO
1	A	48	VAL

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	590/607 (97%)	579 (98%)	11 (2%)	50	45
1	B	588/607 (97%)	578 (98%)	10 (2%)	53	49
All	All	1178/1214 (97%)	1157 (98%)	21 (2%)	51	47

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	VAL
1	A	54	VAL
1	A	144	GLU
1	A	317	LEU
1	A	368	TYR
1	A	369	TYR
1	A	530	VAL
1	A	531	LEU
1	A	566	GLU
1	A	641	GLU
1	A	777	PHE
1	B	147	GLU
1	B	229	GLU
1	B	232	THR
1	B	317	LEU
1	B	526	ASP
1	B	531	LEU
1	B	538	ASP

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Mol	Chain	Res	Type
1	B	640	GLU
1	B	642	ASN
1	B	644	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	ASN
1	A	319	HIS
1	A	340	GLN
1	A	350	HIS
1	A	355	GLN
1	A	635	HIS
1	B	355	GLN
1	B	635	HIS
1	B	642	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 27 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

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	739/759 (97%)	1.77	253 (34%)	1 0	52, 73, 101, 122	0
1	B	736/759 (96%)	1.42	157 (21%)	2 2	50, 68, 93, 119	0
All	All	1475/1518 (97%)	1.59	410 (27%)	1 1	50, 71, 99, 122	0

All (410) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	461	ALA	8.9
1	A	418	ILE	7.3
1	A	531	LEU	6.7
1	B	531	LEU	6.0
1	A	369	TYR	5.7
1	B	204	GLY	5.5
1	A	419	ILE	5.0
1	A	195	ALA	5.0
1	A	463	LEU	5.0
1	A	76	LEU	4.7
1	A	224	ALA	4.6
1	A	68	LEU	4.6
1	B	686	VAL	4.4
1	A	610	ILE	4.4
1	A	563	ALA	4.4
1	A	459	TYR	4.3
1	B	328	LEU	4.3
1	B	203	ALA	4.2
1	B	282	TYR	4.2
1	A	148	CYS	4.1
1	A	237	VAL	4.1
1	A	639	HIS	4.0
1	B	150	GLY	4.0
1	A	469	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	532	PRO	4.0
1	A	143	ALA	4.0
1	A	238	VAL	3.9
1	A	462	ASP	3.9
1	A	57	TYR	3.9
1	A	318	LYS	3.9
1	A	297	GLY	3.9
1	A	425	GLY	3.9
1	A	193	PRO	3.8
1	B	92	VAL	3.8
1	B	284	ALA	3.8
1	B	151	THR	3.7
1	A	393	PHE	3.7
1	A	368	TYR	3.7
1	A	194	ASP	3.6
1	A	607	PRO	3.6
1	A	106	ALA	3.6
1	A	211	LYS	3.6
1	A	634	VAL	3.6
1	A	544	ASP	3.6
1	A	765	GLY	3.6
1	A	82	VAL	3.6
1	A	416	THR	3.6
1	A	436	ALA	3.5
1	B	532	PRO	3.5
1	A	229	GLU	3.5
1	A	392	ALA	3.5
1	A	228	GLY	3.5
1	B	536	GLY	3.5
1	A	609	VAL	3.5
1	B	690	VAL	3.5
1	A	150	GLY	3.5
1	A	191	ILE	3.4
1	A	464	ILE	3.4
1	B	707	VAL	3.4
1	A	397	ILE	3.4
1	A	458	LEU	3.4
1	A	271	TYR	3.4
1	A	378	VAL	3.4
1	B	750	ALA	3.4
1	A	707	VAL	3.3
1	B	696	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	328	LEU	3.3
1	A	319	HIS	3.3
1	A	59	PHE	3.3
1	B	149	THR	3.3
1	A	42	PRO	3.3
1	B	152	GLY	3.3
1	A	52	ILE	3.3
1	A	219	ALA	3.3
1	B	202	ALA	3.3
1	B	557	VAL	3.3
1	B	615	GLY	3.3
1	A	613	ASP	3.2
1	A	44	LEU	3.2
1	A	221	GLY	3.2
1	B	540	TYR	3.2
1	B	688	ALA	3.2
1	B	109	PRO	3.2
1	B	146	VAL	3.2
1	B	396	SER	3.2
1	A	421	ASP	3.2
1	B	544	ASP	3.2
1	B	141	VAL	3.2
1	A	62	LEU	3.2
1	B	691	GLU	3.2
1	A	218	ALA	3.1
1	B	611	ILE	3.1
1	B	609	VAL	3.1
1	B	380	GLY	3.1
1	B	319	HIS	3.1
1	B	378	VAL	3.1
1	A	481	PHE	3.1
1	A	230	ALA	3.1
1	A	417	GLY	3.1
1	A	748	ALA	3.1
1	B	572	ALA	3.1
1	A	386	TYR	3.0
1	B	54	VAL	3.0
1	B	347	PHE	3.0
1	A	465	SER	3.0
1	A	409	THR	3.0
1	B	221	GLY	3.0
1	A	264	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	517	LEU	3.0
1	A	438	ALA	3.0
1	B	563	ALA	3.0
1	A	300	LEU	2.9
1	A	708	LEU	2.9
1	A	78	THR	2.9
1	B	727	THR	2.9
1	A	545	PHE	2.9
1	A	317	LEU	2.9
1	A	485	LEU	2.9
1	A	146	VAL	2.9
1	A	778	GLY	2.9
1	B	556	GLU	2.9
1	B	219	ALA	2.9
1	B	318	LYS	2.9
1	A	753	ARG	2.9
1	A	86	VAL	2.9
1	B	115	GLY	2.9
1	A	391	PHE	2.9
1	A	174	ALA	2.9
1	A	262	ALA	2.9
1	A	688	ALA	2.9
1	B	599	LEU	2.9
1	A	56	GLY	2.9
1	B	297	GLY	2.9
1	B	537	GLY	2.9
1	A	530	VAL	2.8
1	A	769	THR	2.8
1	B	452	VAL	2.8
1	B	530	VAL	2.8
1	A	284	ALA	2.8
1	B	351	PHE	2.8
1	A	460	GLU	2.8
1	A	470	ASP	2.8
1	B	482	ASP	2.8
1	A	307	LEU	2.8
1	B	220	LEU	2.8
1	A	55	ASP	2.8
1	B	264	LEU	2.8
1	B	624	GLN	2.8
1	A	424	TRP	2.8
1	B	529	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	395	ASP	2.8
1	B	205	ALA	2.8
1	A	449	PHE	2.8
1	B	114	PHE	2.8
1	A	107	CYS	2.8
1	A	383	GLY	2.8
1	A	151	THR	2.8
1	A	327	GLU	2.8
1	A	443	THR	2.8
1	A	782	THR	2.8
1	B	254	LEU	2.8
1	A	432	PRO	2.8
1	B	309	PRO	2.8
1	A	428	GLY	2.7
1	A	471	LEU	2.7
1	A	520	LEU	2.7
1	A	599	LEU	2.7
1	A	621	LEU	2.7
1	A	745	LEU	2.7
1	A	781	LEU	2.7
1	B	510	LEU	2.7
1	B	397	ILE	2.7
1	B	565	GLY	2.7
1	B	117	LEU	2.7
1	B	471	LEU	2.7
1	A	112	GLY	2.7
1	B	441	GLY	2.7
1	A	215	ILE	2.7
1	B	571	ALA	2.6
1	A	644	SER	2.6
1	A	330	LEU	2.6
1	A	352	LEU	2.6
1	A	51	ILE	2.6
1	B	83	ALA	2.6
1	B	728	ASP	2.6
1	A	231	THR	2.6
1	B	642	ASN	2.6
1	A	254	LEU	2.6
1	A	315	LEU	2.6
1	A	662	ILE	2.6
1	B	52	ILE	2.6
1	A	304	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	373	VAL	2.6
1	B	285	ALA	2.6
1	A	525	THR	2.6
1	A	747	PHE	2.6
1	A	74	TRP	2.6
1	A	406	LEU	2.6
1	B	621	LEU	2.6
1	B	714	LEU	2.6
1	A	455	ILE	2.6
1	A	371	VAL	2.6
1	A	282	TYR	2.5
1	B	693	PRO	2.5
1	A	777	PHE	2.5
1	A	182	LEU	2.5
1	A	283	LEU	2.5
1	B	283	LEU	2.5
1	B	533	LEU	2.5
1	A	119	ALA	2.5
1	B	155	VAL	2.5
1	B	232	THR	2.5
1	A	382	PRO	2.5
1	B	758	GLU	2.5
1	A	354	PHE	2.5
1	A	305	LEU	2.5
1	B	300	LEU	2.5
1	A	611	ILE	2.5
1	A	655	ALA	2.5
1	A	48	VAL	2.5
1	A	294	THR	2.5
1	A	341	VAL	2.5
1	B	156	VAL	2.5
1	B	377	VAL	2.5
1	B	634	VAL	2.5
1	B	359	ASP	2.5
1	A	775	TYR	2.5
1	A	152	GLY	2.5
1	B	663	LEU	2.5
1	A	266	THR	2.5
1	A	54	VAL	2.5
1	A	77	PRO	2.5
1	B	66	GLY	2.4
1	B	260	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	665	PHE	2.4
1	B	171	MET	2.4
1	B	757	ILE	2.4
1	A	285	ALA	2.4
1	A	356	ALA	2.4
1	A	740	ALA	2.4
1	A	577	VAL	2.4
1	B	238	VAL	2.4
1	B	382	PRO	2.4
1	A	586	ASN	2.4
1	B	383	GLY	2.4
1	B	97	LEU	2.4
1	B	364	SER	2.4
1	A	652	PHE	2.4
1	B	777	PHE	2.4
1	A	757	ILE	2.4
1	A	306	ALA	2.4
1	B	773	ALA	2.4
1	B	48	VAL	2.4
1	B	467	GLU	2.4
1	B	352	LEU	2.4
1	A	258	TYR	2.4
1	A	83	ALA	2.4
1	B	281	ALA	2.4
1	B	381	GLU	2.4
1	B	617	PRO	2.4
1	A	377	VAL	2.4
1	A	562	VAL	2.4
1	B	554	GLY	2.4
1	A	220	LEU	2.3
1	A	295	LEU	2.3
1	A	533	LEU	2.3
1	A	656	TYR	2.3
1	A	756	ILE	2.3
1	B	216	ALA	2.3
1	B	437	ALA	2.3
1	B	112	GLY	2.3
1	A	362	VAL	2.3
1	A	626	LEU	2.3
1	A	111	THR	2.3
1	A	666	THR	2.3
1	A	408	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	57	TYR	2.3
1	A	587	ALA	2.3
1	B	215	ILE	2.3
1	A	529	PRO	2.3
1	A	379	GLY	2.3
1	A	92	VAL	2.3
1	A	116	VAL	2.3
1	A	431	VAL	2.3
1	B	341	VAL	2.3
1	B	148	CYS	2.3
1	A	650	LEU	2.3
1	A	261	MET	2.3
1	A	114	PHE	2.3
1	A	124	TYR	2.3
1	A	347	PHE	2.3
1	A	486	PHE	2.3
1	A	339	ALA	2.3
1	A	683	ILE	2.3
1	B	518	VAL	2.3
1	A	519	LEU	2.3
1	B	781	LEU	2.3
1	A	70	PRO	2.2
1	A	372	PRO	2.2
1	A	381	GLU	2.2
1	B	208	ALA	2.2
1	B	629	ALA	2.2
1	A	696	VAL	2.2
1	B	303	ASN	2.2
1	A	389	THR	2.2
1	B	370	GLY	2.2
1	A	415	ASP	2.2
1	B	502	ALA	2.2
1	A	658	TRP	2.2
1	B	249	TRP	2.2
1	B	408	PHE	2.2
1	A	287	ILE	2.2
1	A	365	ILE	2.2
1	B	699	HIS	2.2
1	A	375	VAL	2.2
1	B	373	VAL	2.2
1	B	577	VAL	2.2
1	A	163	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	290	THR	2.2
1	A	646	THR	2.2
1	A	752	THR	2.2
1	A	120	GLN	2.2
1	A	597	LEU	2.2
1	B	103	LEU	2.2
1	A	109	PRO	2.2
1	A	750	ALA	2.2
1	A	351	PHE	2.2
1	B	354	PHE	2.2
1	B	419	ILE	2.2
1	A	784	GLU	2.2
1	A	550	VAL	2.2
1	A	557	VAL	2.2
1	A	591	VAL	2.2
1	B	244	VAL	2.2
1	B	375	VAL	2.2
1	B	508	VAL	2.2
1	B	626	LEU	2.2
1	B	643	PRO	2.2
1	B	218	ALA	2.2
1	A	73	ASP	2.1
1	A	138	VAL	2.1
1	A	227	THR	2.1
1	A	244	VAL	2.1
1	B	231	THR	2.1
1	B	237	VAL	2.1
1	A	588	GLY	2.1
1	B	743	GLY	2.1
1	A	60	ARG	2.1
1	A	721	LEU	2.1
1	B	607	PRO	2.1
1	A	171	MET	2.1
1	B	639	HIS	2.1
1	A	46	ALA	2.1
1	A	496	ALA	2.1
1	A	561	ASN	2.1
1	B	494	ASP	2.1
1	A	149	THR	2.1
1	A	308	SER	2.1
1	B	666	THR	2.1
1	A	168	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	690	VAL	2.1
1	B	726	MET	2.1
1	A	85	LEU	2.1
1	B	520	LEU	2.1
1	A	405	GLN	2.1
1	A	583	ALA	2.1
1	B	213	ALA	2.1
1	B	242	ALA	2.1
1	A	125	ILE	2.1
1	A	260	TYR	2.1
1	A	342	TYR	2.1
1	B	712	SER	2.1
1	A	311	THR	2.1
1	A	758	GLU	2.1
1	B	102	THR	2.1
1	A	638	GLY	2.1
1	A	480	LEU	2.1
1	A	618	LEU	2.1
1	A	774	LEU	2.1
1	B	597	LEU	2.1
1	B	721	LEU	2.1
1	B	224	ALA	2.1
1	B	230	ALA	2.1
1	A	593	ASP	2.1
1	A	40	GLU	2.0
1	A	147	GLU	2.0
1	A	466	GLU	2.0
1	B	51	ILE	2.0
1	A	701	TYR	2.0
1	B	739	TYR	2.0
1	B	752	THR	2.0
1	A	268	PRO	2.0
1	A	700	VAL	2.0
1	A	476	LEU	2.0
1	A	731	LEU	2.0
1	A	735	LEU	2.0
1	B	356	ALA	2.0
1	B	498	ALA	2.0
1	A	711	GLU	2.0
1	A	608	SER	2.0
1	A	278	THR	2.0
1	A	65	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	323	GLY	2.0
1	A	324	GLY	2.0
1	A	620	GLY	2.0
1	B	742	GLN	2.0
1	A	617	PRO	2.0
1	A	412	VAL	2.0
1	A	454	VAL	2.0
1	A	508	VAL	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 ⓘ

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(Å ²)	Q<0.9
2	ZN	A	805	1/1	0.67	0.12	134,134,134,134	0
2	ZN	A	811	1/1	0.71	0.11	136,136,136,136	0
2	ZN	B	807	1/1	0.85	0.12	127,127,127,127	0
2	ZN	A	808	1/1	0.86	0.08	129,129,129,129	0
2	ZN	A	813	1/1	0.87	0.20	108,108,108,108	0
2	ZN	B	808	1/1	0.88	0.10	132,132,132,132	0
2	ZN	B	806	1/1	0.90	0.12	124,124,124,124	0
2	ZN	A	806	1/1	0.90	0.09	133,133,133,133	0
2	ZN	A	803	1/1	0.90	0.11	87,87,87,87	0
2	ZN	B	813	1/1	0.90	0.23	136,136,136,136	0
2	ZN	B	809	1/1	0.91	0.06	129,129,129,129	0
2	ZN	A	804	1/1	0.91	0.08	105,105,105,105	0
2	ZN	A	809	1/1	0.92	0.10	84,84,84,84	0
2	ZN	B	812	1/1	0.92	0.06	127,127,127,127	0
2	ZN	A	807	1/1	0.92	0.08	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	812	1/1	0.95	0.05	122,122,122,122	0
2	ZN	A	810	1/1	0.95	0.18	91,91,91,91	0
2	ZN	A	814	1/1	0.96	0.06	127,127,127,127	0
2	ZN	B	805	1/1	0.96	0.05	74,74,74,74	0
2	ZN	A	802	1/1	0.97	0.13	97,97,97,97	0
2	ZN	B	810	1/1	0.97	0.07	82,82,82,82	0
2	ZN	B	803	1/1	0.97	0.07	77,77,77,77	0
2	ZN	A	801	1/1	0.97	0.06	81,81,81,81	0
2	ZN	B	804	1/1	0.98	0.05	82,82,82,82	0
2	ZN	B	811	1/1	0.98	0.17	66,66,66,66	0
2	ZN	B	802	1/1	0.98	0.06	94,94,94,94	0
2	ZN	B	801	1/1	0.98	0.06	84,84,84,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.