Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2022 – 09:34 pm BST

PDB ID	:	7QE1
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:

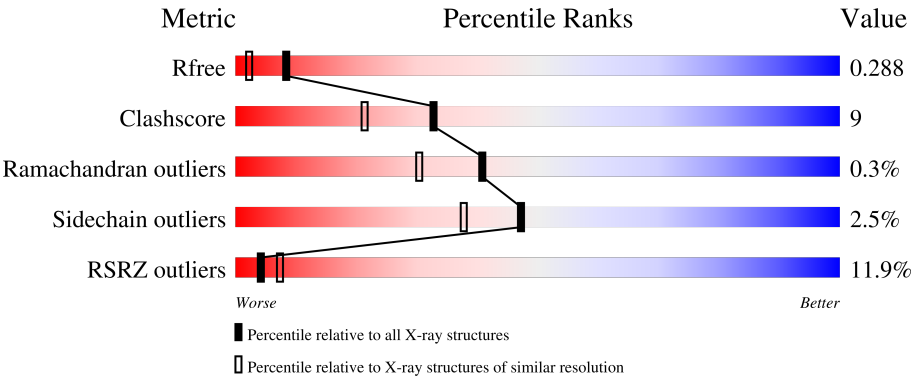
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (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 <=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	14% 76% 21%
1	B	759	9% 82% 13%

2 Entry composition (i)

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 (three-letter code: 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.

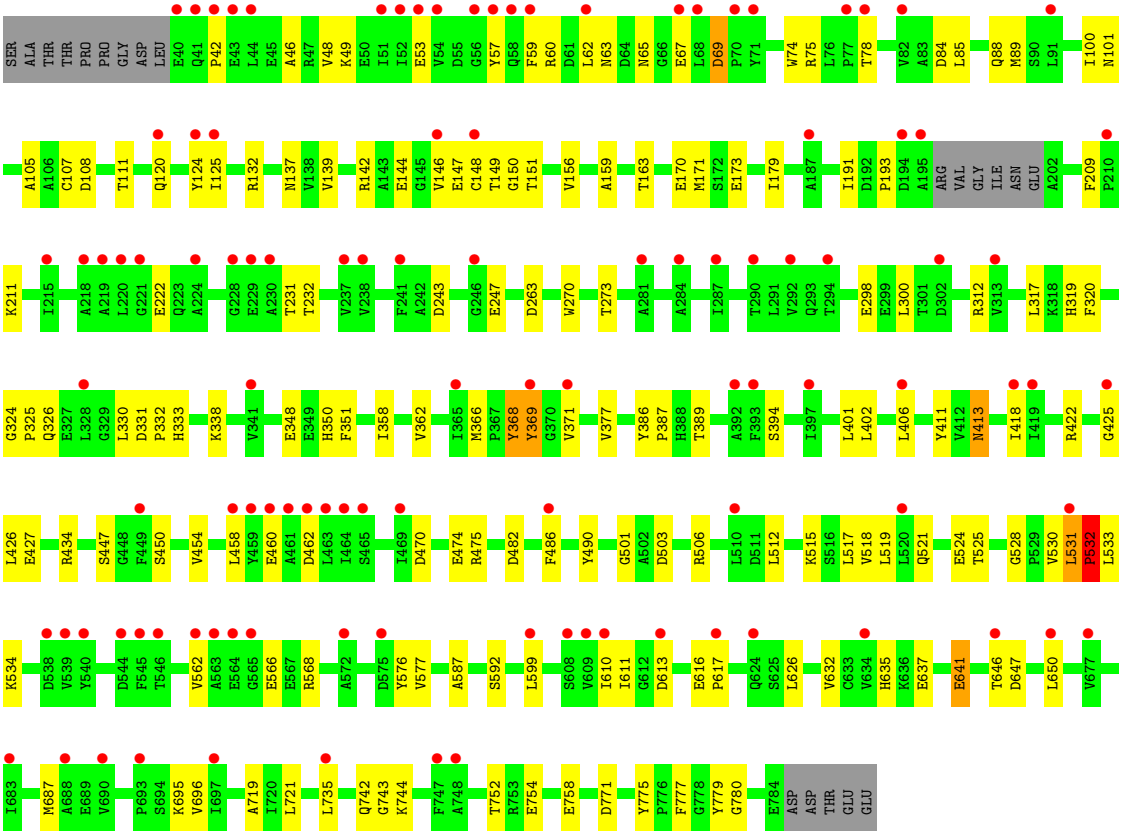
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total	O	0	0
			24	24		
3	B	67	Total	O	0	0
			67	67		

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.

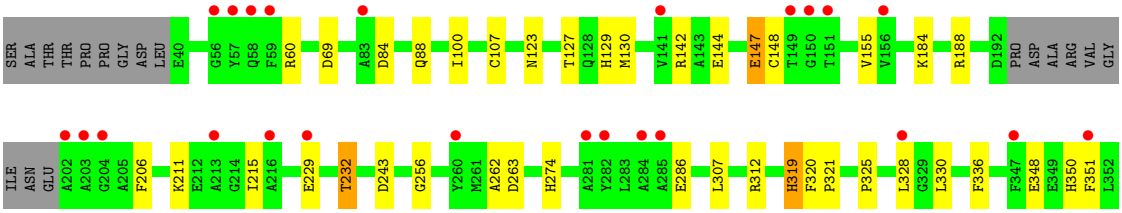
- Molecule 1: SN243

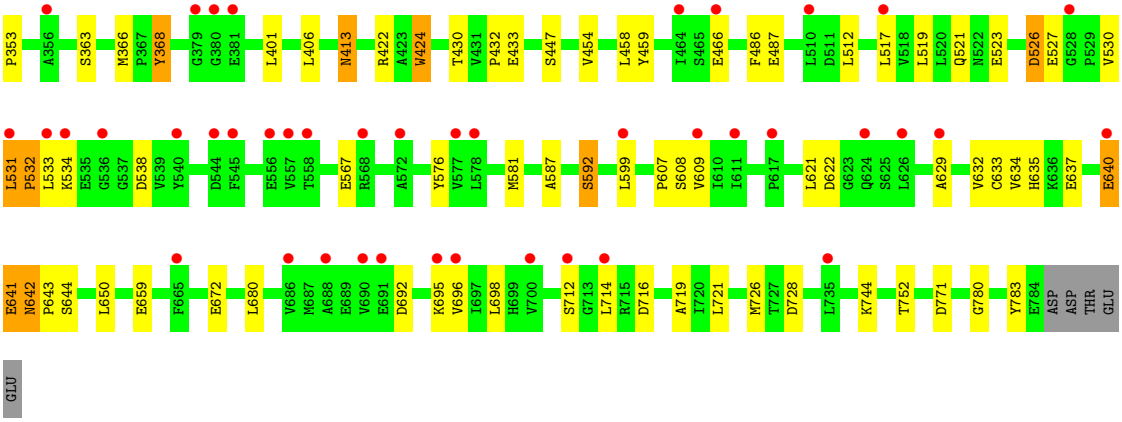
Chain A:



- Molecule 1: SN243

Chain B:




P353 A356 S363 M366 P367 Y368 G379 G380 E381 L401 L406 N413 R422 A423 W424 T430 V431 P432 E433 S447 V454 L458 Y459 I464 S465 E466 F486 E487 L510 D511 L512 L517 V518 L519 L520 Q521 N522 E523 D526 E527 G528 P529 V530
L531 P532 L533 K534 E535 G536 G537 D538 V539 Y540 D544 F545 E556 V557 T558 E567 R568 A572 Y576 V577 L578 M581 A587 S592 L599 P607 S608 V609 I610 I611 P617 L621 D622 G623 Q624 S625 L626 A629 V632 C633 V634 H635 K636 E637 E640
E641 N642 P643 S644 L650 E659 F665 E672 L680 V686 M687 A688 E689 V690 E691 D692 K695 V696 I697 L698 H699 V700 S712 G713 L714 R715 D716 A719 I720 L721 M726 T727 D728 L735 K744 T752 D771 G780 Y783 E784 ASP ASP THR GLU
GLU

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.09 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.240 , 0.290 0.244 , 0.288	Depositor DCC
R_{free} test set	6081 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)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.49	0/5743	0.65	1/7831 (0.0%)
1	B	0.50	2/5722 (0.0%)	0.66	1/7801 (0.0%)
All	All	0.49	2/11465 (0.0%)	0.66	2/15632 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	567	GLU	CD-OE1	5.95	1.32	1.25
1	B	567	GLU	CD-OE2	5.02	1.31	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	532	PRO	N-CA-C	-5.62	97.48	112.10
1	B	319	HIS	CB-CA-C	5.45	121.29	110.40

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	117	0
1	B	5598	0	5273	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	190	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 (190) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:GLU:H	1:B:527:GLU:CD	2.07	0.58
1:A:752:THR:HG21	1:A:771:ASP:HB3	1.84	0.58
1:A:144:GLU:HB3	1:B:144:GLU:CD	2.24	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:B:632:VAL:HA	1:B:635:HIS:NE2	2.20	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:148:CYS:SG	1:A:148:CYS:O	2.64	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:144:GLU:H	1:A:144:GLU:CD	2.11	0.54
1:A:325:PRO:HD3	1:A:350:HIS:ND1	2.23	0.54
1:B:531:LEU:O	1:B:532:PRO:C	2.44	0.54
1:B:629:ALA:HA	1:B:634:VAL:HG21	1.90	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: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
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:A:149:THR:C	1:A:151:THR:H	2.13	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:A:531:LEU:O	1:A:532:PRO:C	2.47	0.51
1:B:659:GLU:OE2	1:B:672:GLU:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:147:GLU:H	1:A:147:GLU:CD	2.15	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:100:ILE:HG23	1:A:447:SER:HA	1.96	0.48
1:A:611:ILE:HD12	1:A:611:ILE:C	2.34	0.48
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:609:VAL:HG12	1:B:622:ASP:C	2.33	0.47
1:B:130:MET:HB3	1:B:130:MET:HE2	1.69	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:B:641:GLU:O	1:B:642:ASN:C	2.51	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:358:ILE:HA	1:A:362:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:60:ARG:NH1	1:A:486:PHE:O	2.47	0.44
1:B:147:GLU:H	1:B:147:GLU:CD	2.20	0.44
1:A:411:TYR:HB3	1:A:475:ARG:HB3	2.00	0.44
1:B:680:LEU:HD11	1:B:714:LEU:HD21	2.00	0.44
1:A:518:VAL:HG22	1:A:743:GLY:C	2.38	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: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:B:430:THR:HG22	1:B:433:GLU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:GLU:OE1	1:A:742:GLN:NE2	2.49	0.42
1:A:641:GLU:H	1:A:641:GLU:CD	2.22	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:425:GLY:C	1:A:426:LEU:HD12	2.39	0.42
1:B:523:GLU:O	1:B:530:VAL:HG23	2.19	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: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: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
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:320:PHE:CE1	1:A:402:LEU:HB2	2.56	0.41
1:A:460:GLU:C	1:A:462:ASP:H	2.24	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: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%)	34	22
1	B	732/759 (96%)	708 (97%)	22 (3%)	2 (0%)	41	30
All	All	1467/1518 (97%)	1411 (96%)	51 (4%)	5 (0%)	41	30

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 (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	590/607 (97%)	577 (98%)	13 (2%)	52	44
1	B	588/607 (97%)	571 (97%)	17 (3%)	42	31
All	All	1178/1214 (97%)	1148 (98%)	30 (2%)	47	38

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ASP

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Mol	Chain	Res	Type
1	A	107	CYS
1	A	243	ASP
1	A	317	LEU
1	A	368	TYR
1	A	369	TYR
1	A	413	ASN
1	A	524	GLU
1	A	530	VAL
1	A	531	LEU
1	A	566	GLU
1	A	641	GLU
1	A	777	PHE
1	B	69	ASP
1	B	147	GLU
1	B	229	GLU
1	B	232	THR
1	B	368	TYR
1	B	413	ASN
1	B	424	TRP
1	B	526	ASP
1	B	531	LEU
1	B	538	ASP
1	B	581	MET
1	B	592	SER
1	B	640	GLU
1	B	642	ASN
1	B	644	SER
1	B	716	ASP
1	B	728	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	340	GLN
1	A	635	HIS
1	B	131	HIS
1	B	355	GLN
1	B	635	HIS
1	B	642	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

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, 95^{th} 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%)	1.09	109 (14%) 2 3	52, 73, 101, 122	0
1	B	736/759 (96%)	0.74	66 (8%) 9 15	50, 68, 93, 119	0
All	All	1475/1518 (97%)	0.91	175 (11%) 4 7	50, 71, 99, 122	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	ALA	6.3
1	A	418	ILE	5.6
1	B	531	LEU	5.4
1	A	531	LEU	5.3
1	A	44	LEU	4.9
1	A	610	ILE	4.8
1	A	463	LEU	4.6
1	A	68	LEU	4.6
1	A	52	ILE	4.4
1	A	57	TYR	4.3
1	A	693	PRO	4.3
1	A	224	ALA	4.3
1	A	62	LEU	4.3
1	A	458	LEU	4.2
1	B	572	ALA	4.2
1	A	77	PRO	4.1
1	B	202	ALA	4.1
1	A	462	ASP	4.0
1	A	58	GLN	4.0
1	A	461	ALA	3.9
1	A	369	TYR	3.9
1	A	146	VAL	3.9
1	A	397	ILE	3.9
1	A	572	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	690	VAL	3.8
1	B	695	LYS	3.8
1	A	194	ASP	3.7
1	A	59	PHE	3.7
1	A	609	VAL	3.7
1	B	380	GLY	3.6
1	A	460	GLU	3.6
1	A	688	ALA	3.5
1	B	150	GLY	3.5
1	B	691	GLU	3.5
1	A	544	ASP	3.5
1	A	545	PHE	3.5
1	A	465	SER	3.4
1	A	42	PRO	3.4
1	B	577	VAL	3.3
1	B	686	VAL	3.3
1	A	54	VAL	3.2
1	B	151	THR	3.2
1	B	213	ALA	3.2
1	A	219	ALA	3.2
1	A	419	ILE	3.1
1	B	700	VAL	3.1
1	A	82	VAL	3.0
1	B	540	TYR	3.0
1	A	238	VAL	3.0
1	A	464	ILE	3.0
1	A	229	GLU	3.0
1	B	534	LYS	3.0
1	B	557	VAL	3.0
1	B	510	LEU	3.0
1	B	58	GLN	3.0
1	B	229	GLU	2.9
1	B	696	VAL	2.9
1	A	510	LEU	2.9
1	B	533	LEU	2.9
1	B	204	GLY	2.9
1	B	149	THR	2.9
1	A	599	LEU	2.9
1	A	221	GLY	2.9
1	B	83	ALA	2.9
1	A	294	THR	2.8
1	A	237	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	624	GLN	2.8
1	A	51	ILE	2.8
1	B	282	TYR	2.8
1	B	284	ALA	2.8
1	A	41	GLN	2.8
1	B	517	LEU	2.8
1	B	558	THR	2.7
1	B	599	LEU	2.7
1	A	617	PRO	2.7
1	A	735	LEU	2.7
1	B	556	GLU	2.7
1	B	379	GLY	2.7
1	A	290	THR	2.7
1	B	544	ASP	2.6
1	A	228	GLY	2.6
1	A	540	TYR	2.6
1	A	91	LEU	2.6
1	A	613	ASP	2.6
1	B	203	ALA	2.6
1	B	381	GLU	2.6
1	A	546	THR	2.6
1	B	57	TYR	2.6
1	B	528	GLY	2.5
1	A	148	CYS	2.5
1	A	650	LEU	2.5
1	B	56	GLY	2.5
1	A	697	ILE	2.5
1	B	629	ALA	2.5
1	A	40	GLU	2.5
1	B	640	GLU	2.5
1	A	393	PHE	2.5
1	A	747	PHE	2.5
1	B	536	GLY	2.5
1	A	328	LEU	2.5
1	B	624	GLN	2.5
1	A	67	GLU	2.5
1	B	617	PRO	2.5
1	A	486	PHE	2.5
1	A	575	ASP	2.5
1	A	565	GLY	2.4
1	B	59	PHE	2.4
1	A	392	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	328	LEU	2.4
1	A	218	ALA	2.4
1	A	563	ALA	2.4
1	A	287	ILE	2.4
1	A	70	PRO	2.4
1	A	246	GLY	2.4
1	B	714	LEU	2.4
1	B	688	ALA	2.4
1	A	365	ILE	2.4
1	B	545	PHE	2.3
1	A	56	GLY	2.3
1	B	568	ARG	2.3
1	B	216	ALA	2.3
1	B	347	PHE	2.3
1	A	302	ASP	2.3
1	B	356	ALA	2.3
1	B	464	ILE	2.3
1	A	220	LEU	2.3
1	A	120	GLN	2.2
1	A	215	ILE	2.2
1	A	406	LEU	2.2
1	B	578	LEU	2.2
1	A	449	PHE	2.2
1	B	665	PHE	2.2
1	A	187	ALA	2.2
1	A	748	ALA	2.2
1	A	469	ILE	2.2
1	A	683	ILE	2.2
1	A	459	TYR	2.2
1	A	538	ASP	2.2
1	A	539	VAL	2.2
1	A	677	VAL	2.2
1	A	230	ALA	2.2
1	A	564	GLU	2.2
1	A	341	VAL	2.2
1	B	735	LEU	2.1
1	B	712	SER	2.1
1	B	156	VAL	2.1
1	A	281	ALA	2.1
1	B	281	ALA	2.1
1	B	260	TYR	2.1
1	A	292	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	313	VAL	2.1
1	A	425	GLY	2.1
1	B	285	ALA	2.1
1	A	608	SER	2.1
1	A	71	TYR	2.1
1	A	124	TYR	2.1
1	A	53	GLU	2.1
1	A	690	VAL	2.1
1	B	609	VAL	2.1
1	A	125	ILE	2.1
1	B	626	LEU	2.1
1	A	43	GLU	2.1
1	A	562	VAL	2.1
1	A	634	VAL	2.1
1	B	141	VAL	2.1
1	A	284	ALA	2.1
1	A	210	PRO	2.1
1	A	78	THR	2.0
1	A	371	VAL	2.0
1	A	520	LEU	2.0
1	B	611	ILE	2.0
1	A	241	PHE	2.0
1	B	351	PHE	2.0
1	A	646	THR	2.0
1	B	466	GLU	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 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, 95^{th} 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	808	1/1	0.25	0.06	129,129,129,129	0
2	ZN	A	805	1/1	0.59	0.08	134,134,134,134	0
2	ZN	B	807	1/1	0.79	0.07	127,127,127,127	0
2	ZN	A	807	1/1	0.81	0.12	124,124,124,124	0
2	ZN	B	813	1/1	0.82	0.21	136,136,136,136	0
2	ZN	A	810	1/1	0.83	0.31	91,91,91,91	0
2	ZN	A	813	1/1	0.83	0.16	108,108,108,108	0
2	ZN	A	809	1/1	0.84	0.07	84,84,84,84	0
2	ZN	A	811	1/1	0.85	0.06	136,136,136,136	0
2	ZN	A	804	1/1	0.86	0.04	105,105,105,105	0
2	ZN	A	814	1/1	0.88	0.07	127,127,127,127	0
2	ZN	B	812	1/1	0.88	0.04	127,127,127,127	0
2	ZN	B	806	1/1	0.88	0.12	124,124,124,124	0
2	ZN	A	802	1/1	0.90	0.04	97,97,97,97	0
2	ZN	B	802	1/1	0.93	0.03	94,94,94,94	0
2	ZN	B	803	1/1	0.93	0.16	77,77,77,77	0
2	ZN	A	803	1/1	0.94	0.11	87,87,87,87	0
2	ZN	B	805	1/1	0.94	0.10	74,74,74,74	0
2	ZN	A	812	1/1	0.95	0.03	122,122,122,122	0
2	ZN	B	808	1/1	0.95	0.10	132,132,132,132	0
2	ZN	B	801	1/1	0.95	0.07	84,84,84,84	0
2	ZN	A	806	1/1	0.95	0.15	133,133,133,133	0
2	ZN	A	801	1/1	0.96	0.10	81,81,81,81	0
2	ZN	B	804	1/1	0.97	0.06	82,82,82,82	0
2	ZN	B	810	1/1	0.97	0.10	82,82,82,82	0
2	ZN	B	809	1/1	0.98	0.05	129,129,129,129	0
2	ZN	B	811	1/1	0.98	0.27	66,66,66,66	0

6.5 Other polymers (i)

There are no such residues in this entry.