Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2022 – 11:43 am BST

PDB ID	:	7QG4
Title	:	Apo crystal structure of a mutant of SN243 (D415N)
Authors	:	Neun, S.; Brear, P.; Campbell, E.; Omari, K.; Wagner, O.; Hyvonen, M.; Hollfelder, F.
Deposited on	:	2021-12-07
Resolution	:	2.08 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:

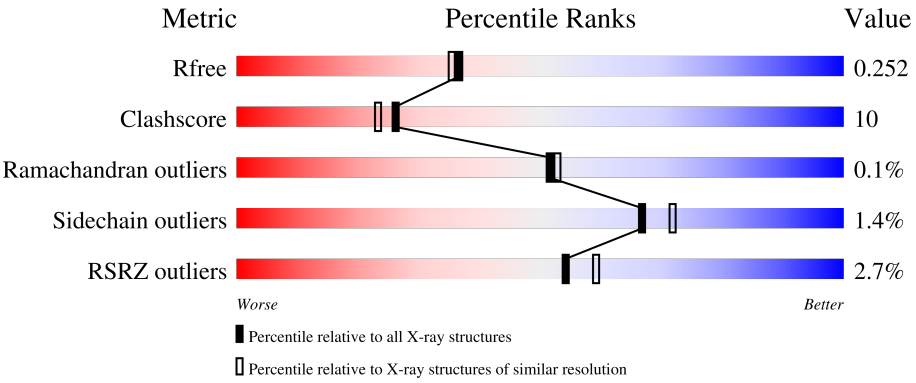
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.08 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	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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	2% 79% 19%
1	B	759	3% 74% 23%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11826 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.

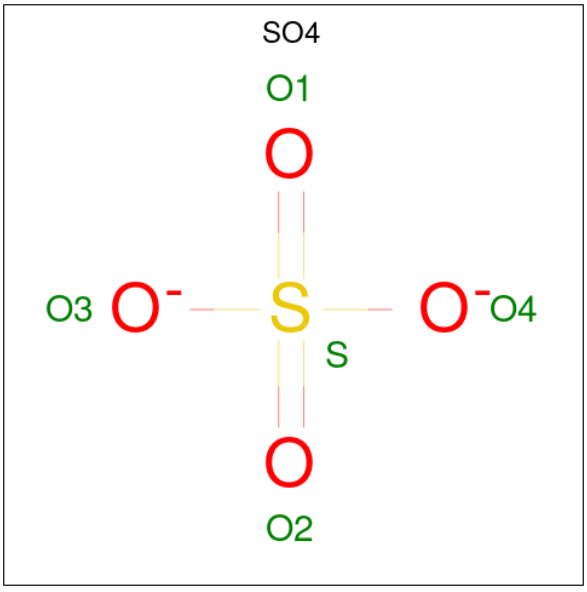
- Molecule 1 is a protein called SN243.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	746	Total	C	N	O	S	0	2	0
			5691	3564	937	1170	20			
1	B	746	Total	C	N	O	S	0	4	0
			5710	3575	941	1174	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	12	Total	Zn	0	0
			12	12		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

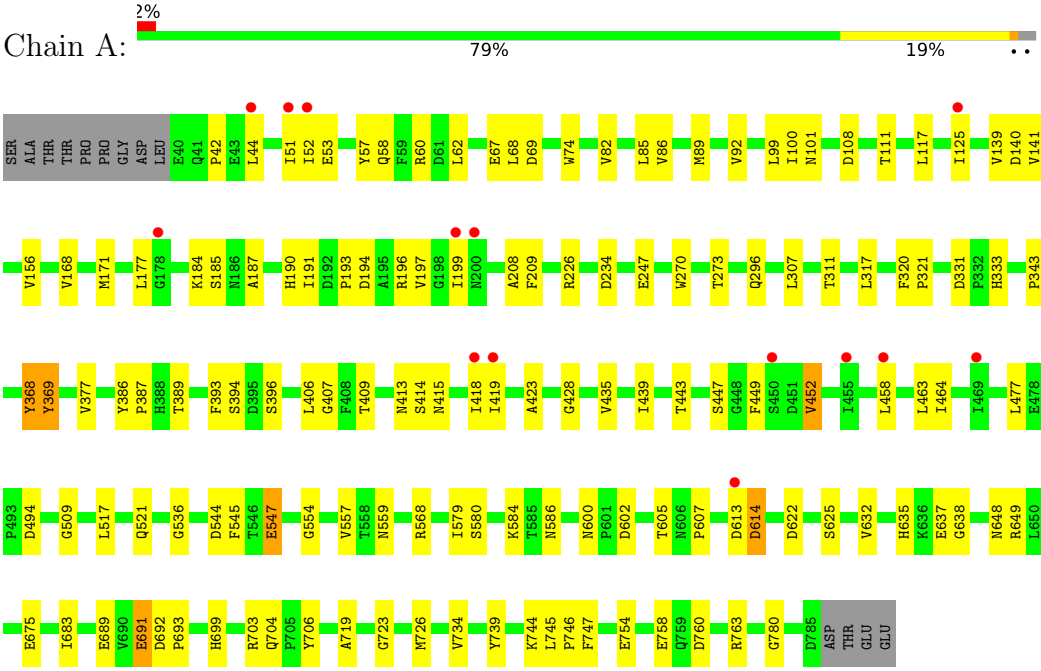
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	238	Total O 238 238	0	0
4	B	156	Total O 156 156	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

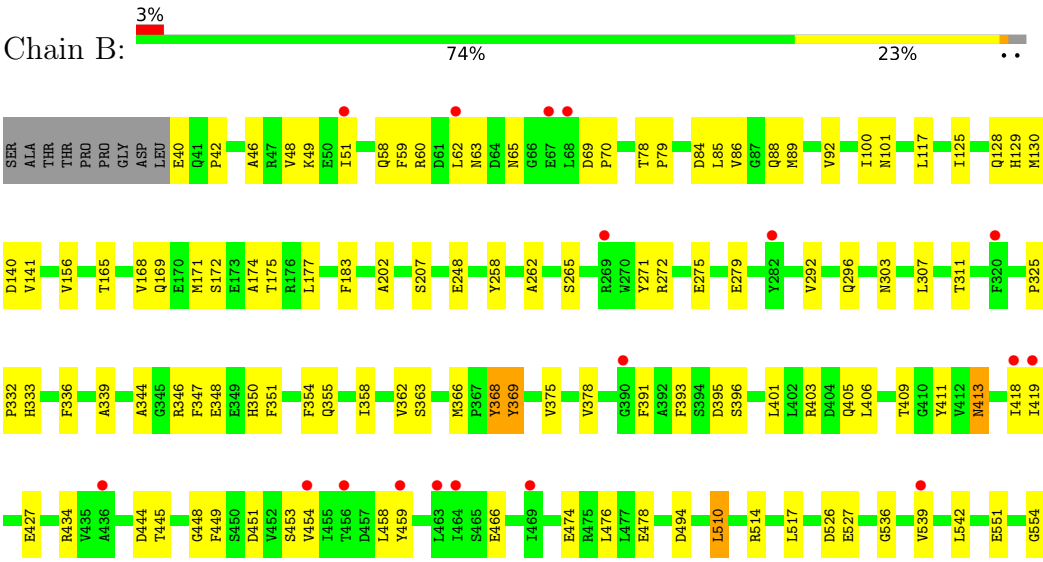
• Molecule 1: SN243

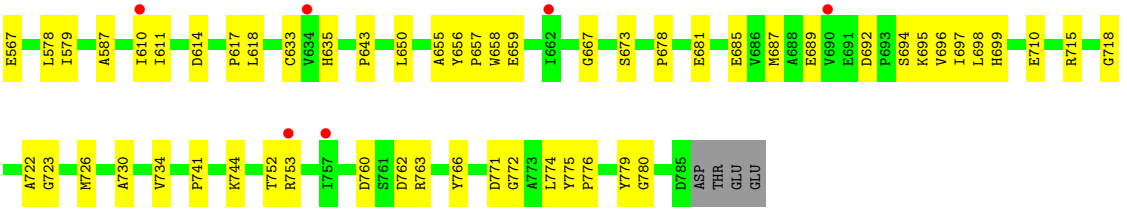
Chain A:



• Molecule 1: SN243

Chain B:




E567
L578
I579
A587
I610
I611
D614
P617
L618
C633
V634
H635
P643
L650
A655
Y656
P657
W658
E659
I662
G667
S673
P678
E681
E685
V686
M687
A688
E689
V690
E691
D692
P693
S694
K695
V696
I697
L698
H699
E710
R715
G718
A722
G723
M726
A730
V734
P741
K744
T752
R753
I757
D760
S761
D762
R763
Y766
D771
G772
A773
L774
Y775
P776
Y779
G780
D785
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	62.40Å 82.41Å 92.08Å 113.33° 90.43° 90.94°	Depositor
Resolution (Å)	75.77 – 2.08 75.66 – 2.05	Depositor EDS
% Data completeness (in resolution range)	91.5 (75.77-2.08) 91.5 (75.66-2.05)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.249 , 0.251 0.250 , 0.252	Depositor DCC
R_{free} test set	4934 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	46.6	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.007 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11826	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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: SO4, 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	0.53	0/5817	0.65	1/7932 (0.0%)
1	B	0.51	0/5837	0.63	2/7959 (0.0%)
All	All	0.52	0/11654	0.64	3/15891 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	739	TYR	C-N-CA	-5.87	107.03	121.70
1	B	395	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	510	LEU	CB-CG-CD1	5.26	119.94	111.00

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	5691	0	5354	98	1
1	B	5710	0	5366	132	1
2	A	14	0	0	0	0
2	B	12	0	0	0	0
3	A	5	0	0	1	0
4	A	238	0	0	5	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	156	0	0	3	1
All	All	11826	0	10720	230	2

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 10.

All (230) 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:A:317:LEU:HD23	1:A:354:PHE:CD1	2.05	0.91
1:A:92:VAL:HG23	1:A:452:VAL:HG11	1.56	0.87
1:A:247:GLU:OE1	4:A:901:HOH:O	1.96	0.83
1:B:418:ILE:HG22	1:B:422:ARG:HD2	1.63	0.80
1:B:419:ILE:H	1:B:419:ILE:HD12	1.45	0.79
1:B:65:ASN:HD21	1:B:69:ASP:CG	1.89	0.75
1:B:710:GLU:HG3	1:B:715:ARG:HH11	1.52	0.75
1:A:387:PRO:HB2	1:A:389:THR:HG22	1.70	0.74
1:B:687:MET:HG2	1:B:696:VAL:HG21	1.70	0.72
1:B:63:ASN:ND2	1:B:88:GLN:HE22	1.88	0.71
1:B:65:ASN:ND2	1:B:69:ASP:OD1	2.23	0.71
1:B:419:ILE:HD13	1:B:449:PHE:HE1	1.56	0.70
1:B:451:ASP:O	1:B:454:VAL:HG12	1.92	0.69
1:A:651:ARG:NH1	4:A:903:HOH:O	2.26	0.69
1:A:317:LEU:HD23	1:A:354:PHE:HD1	1.55	0.68
1:A:317:LEU:CD2	1:A:354:PHE:CD1	2.77	0.68
1:B:715:ARG:HH21	1:B:774:LEU:HD22	1.60	0.67
1:A:492:ASP:OD1	1:A:494:ASP:OD1	2.13	0.66
1:B:526:ASP:HB2	1:B:527:GLU:OE2	1.95	0.66
1:B:418:ILE:HB	1:B:422:ARG:HB2	1.78	0.65
1:B:65:ASN:ND2	1:B:69:ASP:OD2	2.29	0.65
1:B:744:LYS:NZ	1:B:780:GLY:O	2.27	0.64
1:B:344:ALA:HB1	1:B:346:ARG:HH11	1.62	0.63
1:A:100:ILE:HG23	1:A:447:SER:HA	1.79	0.62
1:B:427:GLU:OE1	1:B:427:GLU:N	2.31	0.62
1:B:307:LEU:HD21	1:B:363:SER:HB2	1.80	0.62
1:B:65:ASN:ND2	1:B:69:ASP:CG	2.53	0.62
1:B:296:GLN:HA	1:B:311:THR:HG23	1.82	0.61
1:B:578:LEU:HD23	1:B:697:ILE:HB	1.82	0.61
1:A:418:ILE:HG13	1:A:419:ILE:HD12	1.83	0.60
1:B:63:ASN:HD22	1:B:88:GLN:HE22	1.50	0.60
1:B:330:LEU:HD13	1:B:336:PHE:HD1	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:ILE:HD13	1:A:683:ILE:HG23	1.84	0.59
1:A:419:ILE:HG21	1:A:435:VAL:HG22	1.85	0.59
1:B:48:VAL:HG11	1:B:174:ALA:HA	1.85	0.59
1:B:344:ALA:HB3	1:B:346:ARG:HD2	1.86	0.58
1:B:766:TYR:O	1:B:772:GLY:HA2	2.03	0.58
1:B:49:LYS:NZ	1:B:62:LEU:O	2.35	0.58
1:B:100:ILE:HD12	1:B:132:ARG:HB3	1.85	0.58
1:A:44:LEU:HD13	1:A:60:ARG:HG3	1.86	0.58
1:A:125:ILE:HD11	1:A:168:VAL:HG13	1.85	0.57
1:A:226:ARG:NH1	1:A:234:ASP:OD2	2.36	0.57
1:B:339:ALA:HB2	1:B:610:ILE:HD11	1.86	0.57
1:B:92:VAL:HG22	1:B:129[B]:HIS:HD2	1.70	0.56
1:B:393:PHE:CE1	1:B:423:ALA:HA	2.40	0.56
1:B:272:ARG:NE	1:B:275:GLU:OE2	2.33	0.56
1:A:85:LEU:HD23	1:A:477:LEU:HD13	1.87	0.55
1:B:172:SER:HA	1:B:175:THR:HG23	1.88	0.55
1:A:191:ILE:O	1:A:193:PRO:HD3	2.07	0.55
1:A:389:THR:HG23	1:A:394:SER:OG	2.07	0.55
1:A:270:TRP:O	1:A:273:THR:HG23	2.06	0.55
1:A:52:ILE:HD11	1:A:68:LEU:HB2	1.90	0.54
1:A:414:SER:HB3	1:A:443:THR:HG21	1.89	0.54
1:B:685:GLU:O	1:B:689:GLU:HG3	2.09	0.53
1:A:85:LEU:O	1:A:89:MET:HG3	2.09	0.52
1:A:333:HIS:CE1	1:A:369:TYR:OH	2.61	0.52
1:B:403:ARG:NH2	1:B:444:ASP:OD2	2.42	0.52
1:B:536:GLY:HA2	1:B:554:GLY:O	2.09	0.52
1:A:369:TYR:CD1	1:A:418:ILE:HG21	2.45	0.52
1:B:348:GLU:HA	1:B:351:PHE:CE2	2.44	0.52
1:A:307:LEU:HD13	1:A:479:PRO:HA	1.92	0.52
1:B:125:ILE:HD12	1:B:171:MET:HE3	1.91	0.52
1:B:542:LEU:HG	1:B:678:PRO:HG3	1.90	0.52
1:A:51:ILE:HD13	1:A:60:ARG:HG2	1.91	0.52
1:A:622:ASP:OD1	1:A:625:SER:OG	2.28	0.52
1:B:459:TYR:HE1	1:B:466:GLU:HB2	1.75	0.52
1:A:754:GLU:O	1:A:758:GLU:HG3	2.10	0.51
1:B:401:LEU:HD12	1:B:405:GLN:HB2	1.92	0.51
1:A:209:PHE:CE2	1:A:509:GLY:HA2	2.45	0.51
1:B:326:GLN:OE1	1:B:332:PRO:HD3	2.10	0.51
1:B:699:HIS:NE2	1:B:723:GLY:HA3	2.26	0.51
1:A:296:GLN:HA	1:A:311:THR:HG23	1.92	0.51
1:A:547:GLU:OE1	1:A:559:ASN:HB2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:THR:O	1:A:607:PRO:HD3	2.10	0.51
1:B:63:ASN:HD21	1:B:69:ASP:CG	2.14	0.51
1:B:125:ILE:HD12	1:B:171:MET:CE	2.41	0.51
1:B:336:PHE:CE2	1:B:657:PRO:HG3	2.45	0.51
1:B:459:TYR:CE1	1:B:466:GLU:HB2	2.46	0.51
1:A:51:ILE:CD1	1:A:60:ARG:HG2	2.39	0.50
1:B:78:THR:HG21	1:B:478:GLU:HG3	1.93	0.50
1:B:330:LEU:HD22	1:B:336:PHE:CE1	2.46	0.50
1:B:358:ILE:HA	1:B:362:VAL:HG12	1.92	0.50
1:A:699:HIS:NE2	1:A:723:GLY:HA3	2.25	0.50
1:B:140:ASP:OD1	1:B:141:VAL:N	2.41	0.50
1:B:710:GLU:HG3	1:B:715:ARG:HD2	1.94	0.50
1:B:587:ALA:HB1	1:B:650:LEU:HD12	1.92	0.50
1:B:346:ARG:HD3	1:B:762:ASP:O	2.12	0.50
1:A:320:PHE:CD1	1:A:321:PRO:HA	2.47	0.50
1:B:633:CYS:HA	1:B:643:PRO:HG2	1.94	0.49
1:B:330:LEU:HD22	1:B:336:PHE:HE1	1.77	0.49
1:A:458:LEU:HD23	1:A:463:LEU:HD12	1.94	0.49
1:A:614:ASP:OD1	1:A:614:ASP:N	2.46	0.49
1:A:692:ASP:OD1	1:A:693:PRO:HD2	2.12	0.49
1:B:454:VAL:O	1:B:458:LEU:HG	2.13	0.49
1:B:89:MET:HG2	1:B:177:LEU:CD1	2.43	0.49
1:A:331:ASP:OD2	1:A:333:HIS:ND1	2.42	0.49
1:B:355[A]:GLN:HA	1:B:358:ILE:HD12	1.95	0.49
1:B:566:GLU:HG2	1:B:567:GLU:H	1.77	0.49
1:A:125:ILE:HG21	1:A:171:MET:HG2	1.95	0.48
1:B:117:LEU:HD13	1:B:171:MET:HE1	1.94	0.48
1:B:325:PRO:HD3	1:B:350:HIS:CE1	2.47	0.48
1:B:348:GLU:HA	1:B:351:PHE:CD2	2.48	0.48
1:A:579:ILE:CD1	1:A:683:ILE:HG23	2.44	0.48
1:B:566:GLU:HG2	1:B:567:GLU:N	2.28	0.48
1:A:545:PHE:CE2	1:A:580:SER:HB2	2.49	0.48
1:B:86:VAL:HG21	1:B:474:GLU:HG3	1.95	0.48
1:B:331:ASP:OD1	1:B:368:TYR:OH	2.31	0.48
1:B:445:THR:HB	1:B:476:LEU:HD21	1.95	0.48
1:B:635:HIS:HB3	4:B:944:HOH:O	2.14	0.48
1:B:418:ILE:CB	1:B:422:ARG:HB2	2.44	0.48
1:B:579:ILE:HB	1:B:698:LEU:HD23	1.96	0.48
1:B:774:LEU:HG	1:B:775:TYR:CD2	2.49	0.48
1:A:393:PHE:CE2	1:A:423:ALA:HA	2.48	0.47
1:A:651:ARG:HG2	4:A:993:HOH:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:LYS:NZ	1:A:413:ASN:HD22	2.12	0.47
1:B:681:GLU:O	1:B:685:GLU:HG3	2.13	0.47
1:A:99:LEU:HD22	1:A:449:PHE:HB3	1.95	0.47
1:A:632:VAL:HG23	1:A:635:HIS:CE1	2.49	0.47
1:A:744:LYS:NZ	1:A:780:GLY:O	2.46	0.47
1:B:168:VAL:HG21	1:B:183:PHE:HZ	1.80	0.47
1:B:466:GLU:O	1:B:466:GLU:HG2	2.13	0.47
1:B:62:LEU:HB3	1:B:177:LEU:O	2.14	0.47
1:A:191:ILE:HG13	1:A:208:ALA:HB1	1.97	0.47
1:A:320:PHE:CG	1:A:321:PRO:HA	2.50	0.47
1:B:271:TYR:CE1	1:B:272:ARG:HG2	2.49	0.47
1:B:347:PHE:CD1	1:B:375:VAL:HG11	2.50	0.47
1:A:139:VAL:HA	1:A:156:VAL:O	2.15	0.47
1:A:517:LEU:HD22	1:A:726:MET:HE1	1.97	0.47
1:B:333:HIS:NE2	1:B:369:TYR:OH	2.48	0.47
1:B:344:ALA:HB2	1:B:763:ARG:NH2	2.29	0.47
1:A:428:GLY:HA2	1:A:638:GLY:HA2	1.96	0.46
1:B:330:LEU:HD13	1:B:336:PHE:CD1	2.46	0.46
1:A:53:GLU:HA	1:A:57:TYR:O	2.15	0.46
1:B:51:ILE:HG23	1:B:59:PHE:O	2.16	0.46
1:A:439:ILE:HD12	1:A:464:ILE:HD11	1.98	0.46
1:A:51:ILE:CG2	1:A:58:GLN:HB3	2.46	0.46
1:B:332:PRO:HB2	1:B:369:TYR:HD1	1.81	0.46
1:B:40:GLU:O	1:B:42:PRO:HD3	2.16	0.46
1:B:517:LEU:HD22	1:B:726:MET:HE1	1.98	0.46
1:B:262:ALA:HB3	1:B:354:PHE:CZ	2.50	0.46
1:B:265:SER:HB2	1:B:279:GLU:HB3	1.98	0.46
1:B:694:SER:O	1:B:718:GLY:HA3	2.16	0.46
1:B:89:MET:HG2	1:B:177:LEU:HD12	1.98	0.45
1:A:209:PHE:CD2	1:A:509:GLY:HA2	2.51	0.45
1:A:317:LEU:HD23	1:A:354:PHE:CE1	2.51	0.45
1:A:635:HIS:ND1	1:A:637:GLU:HG3	2.30	0.45
1:A:351:PHE:CE1	1:A:406:LEU:HD21	2.51	0.45
1:B:655:ALA:O	4:B:901:HOH:O	2.21	0.45
1:A:149:THR:C	1:A:151:THR:H	2.20	0.45
1:A:632:VAL:HA	1:A:635:HIS:NE2	2.31	0.45
1:B:656:TYR:CD2	1:B:673:SER:HB3	2.51	0.45
1:A:600:ASN:OD1	1:A:602:ASP:HB2	2.17	0.45
1:A:117:LEU:N	4:A:917:HOH:O	2.44	0.45
1:A:377:VAL:HA	1:A:386:TYR:CE2	2.52	0.45
1:A:415:ASN:HB3	3:A:815:SO4:O4	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:PRO:HD2	1:B:84:ASP:OD2	2.18	0.45
1:A:196:ARG:HA	1:A:199:ILE:HG13	1.99	0.44
1:A:584:LYS:HE2	1:A:675:GLU:OE1	2.17	0.44
1:B:336:PHE:CZ	1:B:657:PRO:HG3	2.52	0.44
1:A:547:GLU:HG2	1:A:557:VAL:HG11	1.99	0.44
1:A:658:TRP:CD1	1:A:659:GLU:HG3	2.53	0.44
1:B:510:LEU:CD2	1:B:730:ALA:HB2	2.47	0.44
1:A:187:ALA:HB1	1:A:190:HIS:HD2	1.83	0.44
1:A:418:ILE:HG13	1:A:419:ILE:N	2.32	0.44
1:B:369:TYR:CD2	1:B:418:ILE:HG12	2.53	0.44
1:B:419:ILE:H	1:B:419:ILE:CD1	2.16	0.44
1:A:194:ASP:OD2	1:A:703:ARG:NH2	2.42	0.43
1:B:128:GLN:OE1	1:B:451:ASP:HA	2.19	0.43
1:B:292:VAL:O	1:B:296:GLN:HB2	2.18	0.43
1:B:355[B]:GLN:OE1	1:B:406:LEU:HD22	2.18	0.43
1:B:760:ASP:OD2	1:B:763:ARG:NH2	2.50	0.43
1:A:568:ARG:NH2	1:A:689:GLU:OE2	2.40	0.43
1:B:614:ASP:OD1	1:B:614:ASP:N	2.46	0.43
1:A:648:ASN:O	1:A:649:ARG:HB2	2.18	0.43
1:B:46:ALA:HB2	1:B:60:ARG:HD2	2.01	0.43
1:B:411:TYR:CD2	1:B:476:LEU:HD23	2.53	0.43
1:B:517:LEU:HD12	1:B:722:ALA:O	2.18	0.43
1:B:202:ALA:HB1	4:B:975:HOH:O	2.19	0.43
1:B:265:SER:H	1:B:279:GLU:HA	1.83	0.43
1:B:139:VAL:HA	1:B:156:VAL:O	2.18	0.43
1:B:451:ASP:OD2	1:B:453:SER:OG	2.33	0.43
1:B:85:LEU:O	1:B:89:MET:HG3	2.19	0.43
1:B:667:GLY:HA3	1:B:753:ARG:NH2	2.33	0.43
1:B:734:VAL:HG13	1:B:741:PRO:HD3	2.01	0.42
1:A:82:VAL:O	1:A:86:VAL:HG23	2.19	0.42
1:B:78:THR:HB	1:B:79:PRO:HD3	2.01	0.42
1:A:99:LEU:HD11	1:A:452:VAL:HA	2.01	0.42
1:A:760:ASP:HB2	1:A:763:ARG:HB3	2.01	0.42
1:B:128:GLN:HB2	1:B:130:MET:HG3	2.01	0.42
1:B:355[B]:GLN:HA	1:B:358:ILE:HD12	2.02	0.42
1:B:368:TYR:O	1:B:391:PHE:HB2	2.20	0.42
1:B:369:TYR:HD2	1:B:418:ILE:HG12	1.85	0.42
1:A:536:GLY:HA2	1:A:554:GLY:O	2.20	0.42
1:A:101:ASN:HB2	1:A:449:PHE:O	2.20	0.42
1:B:611:ILE:HA	1:B:617:PRO:HA	2.01	0.42
1:B:776:PRO:HD2	1:B:779:TYR:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:LEU:HB3	1:A:177:LEU:O	2.20	0.42
1:B:692:ASP:HB3	1:B:695:LYS:HD2	2.02	0.42
1:A:42:PRO:HD2	1:A:74:TRP:CE2	2.54	0.41
1:B:420:ASN:O	1:B:434:ARG:NH1	2.53	0.41
1:A:140:ASP:OD1	1:A:141:VAL:N	2.50	0.41
1:B:207:SER:OG	1:B:248:GLU:OE2	2.36	0.41
1:B:418:ILE:HG22	1:B:422:ARG:CD	2.41	0.41
1:A:746:PRO:HG2	1:A:747:PHE:CD2	2.56	0.41
1:A:177:LEU:HA	1:A:177:LEU:HD23	1.88	0.41
1:A:343:PRO:HG2	1:A:760:ASP:HB3	2.03	0.41
1:A:586:ASN:ND2	1:A:675:GLU:HB2	2.36	0.41
1:A:691:GLU:HB3	1:A:692:ASP:H	1.65	0.41
1:B:539:VAL:O	1:B:557:VAL:HA	2.20	0.41
1:B:618:LEU:HD23	1:B:618:LEU:HA	1.86	0.41
1:B:775:TYR:CD1	1:B:779:TYR:CE2	3.08	0.41
1:A:703:ARG:HD2	4:A:1022:HOH:O	2.20	0.40
1:B:368:TYR:CE1	1:B:369:TYR:CE1	3.09	0.40
1:A:517:LEU:HD23	1:A:734:VAL:HG11	2.02	0.40
1:A:745:LEU:HB3	1:A:747:PHE:O	2.22	0.40
1:B:165:THR:O	1:B:169:GLN:HG2	2.21	0.40
1:B:303:ASN:ND2	1:B:409:THR:HB	2.37	0.40
1:A:407:GLY:O	1:A:409:THR:HG23	2.21	0.40
1:B:366:MET:HA	1:B:413:ASN:O	2.21	0.40
1:A:386:TYR:HD1	1:A:396:SER:HB3	1.86	0.40
1:B:101:ASN:OD1	1:B:448:GLY:HA2	2.22	0.40
1:B:658:TRP:CD1	1:B:659:GLU:HG3	2.57	0.40
1:B:752:THR:HG21	1:B:771:ASP:OD2	2.21	0.40
1:A:108:ASP:OD2	1:A:111:THR:HG23	2.21	0.40
1:A:368:TYR:HD1	1:A:368:TYR:HA	1.80	0.40
1:A:419:ILE:HG21	1:A:435:VAL:CG2	2.51	0.40
1:A:521:GLN:O	1:A:719:ALA:HA	2.21	0.40
1:A:704:GLN:O	1:A:706:TYR:N	2.55	0.40
1:B:378:VAL:HB	1:B:401:LEU:HD13	2.03	0.40
1:B:514:ARG:HH11	1:B:514:ARG:HD3	1.68	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:ASP:OD2	1:B:551:GLU:OE1[1_655]	1.90	0.30
4:A:909:HOH:O	4:B:1042:HOH:O[1_655]	2.05	0.15

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	746/759 (98%)	715 (96%)	29 (4%)	2 (0%)	41 39
1	B	748/759 (99%)	715 (96%)	33 (4%)	0	100 100
All	All	1494/1518 (98%)	1430 (96%)	62 (4%)	2 (0%)	51 53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	691	GLU
1	A	544	ASP

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	598/607 (98%)	588 (98%)	10 (2%)	60 65
1	B	600/607 (99%)	593 (99%)	7 (1%)	71 76
All	All	1198/1214 (99%)	1181 (99%)	17 (1%)	67 72

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	GLU
1	A	69	ASP
1	A	185	SER
1	A	197	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	368	TYR
1	A	369	TYR
1	A	452	VAL
1	A	547	GLU
1	A	613	ASP
1	A	614	ASP
1	B	58	GLN
1	B	258	TYR
1	B	368	TYR
1	B	369	TYR
1	B	396	SER
1	B	413	ASN
1	B	494	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	413	ASN
1	A	642	ASN
1	B	88	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 26 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	A	815	-	4,4,4	0.14	0	6,6,6	0.31	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	815	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	746/759 (98%)	0.33	15 (2%)	65	68	17, 35, 61, 89	0
1	B	746/759 (98%)	0.48	26 (3%)	44	49	19, 48, 70, 94	0
All	All	1492/1518 (98%)	0.41	41 (2%)	54	59	17, 42, 67, 94	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	419	ILE	6.0
1	B	67	GLU	5.5
1	A	200	ASN	5.3
1	A	199	ILE	4.8
1	B	68	LEU	4.3
1	A	613	ASP	3.7
1	B	464	ILE	3.5
1	A	458	LEU	3.3
1	B	753	ARG	3.3
1	B	418	ILE	3.3
1	B	320	PHE	3.2
1	B	423	ALA	3.1
1	A	419	ILE	3.1
1	A	51	ILE	2.8
1	B	557	VAL	2.6
1	B	463	LEU	2.6
1	B	390	GLY	2.6
1	B	51	ILE	2.5
1	A	480	LEU	2.5
1	A	450	SER	2.5
1	B	269	ARG	2.4
1	B	459	TYR	2.4
1	B	469	ILE	2.4
1	B	662	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	539	VAL	2.3
1	A	125	ILE	2.3
1	A	44	LEU	2.2
1	B	282	TYR	2.2
1	B	436	ALA	2.2
1	B	634	VAL	2.2
1	B	456	THR	2.2
1	A	455	ILE	2.1
1	A	178	GLY	2.1
1	B	62	LEU	2.1
1	A	418	ILE	2.0
1	A	469	ILE	2.0
1	B	757	ILE	2.0
1	B	690	VAL	2.0
1	B	454	VAL	2.0
1	A	52	ILE	2.0
1	B	610	ILE	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	803	1/1	0.74	0.05	85,85,85,85	0
3	SO4	A	815	5/5	0.77	0.13	44,54,70,79	0
2	ZN	B	809	1/1	0.78	0.07	76,76,76,76	0
2	ZN	A	811	1/1	0.78	0.10	101,101,101,101	0
2	ZN	A	805	1/1	0.82	0.18	89,89,89,89	0
2	ZN	B	805	1/1	0.82	0.12	99,99,99,99	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	B	808	1/1	0.83	0.09	95,95,95,95	0
2	ZN	A	812	1/1	0.84	0.07	122,122,122,122	0
2	ZN	B	802	1/1	0.84	0.16	57,57,57,57	0
2	ZN	A	804	1/1	0.86	0.08	83,83,83,83	0
2	ZN	B	806	1/1	0.87	0.05	73,73,73,73	0
2	ZN	A	809	1/1	0.88	0.13	83,83,83,83	0
2	ZN	B	807	1/1	0.89	0.05	103,103,103,103	0
2	ZN	B	810	1/1	0.89	0.10	112,112,112,112	0
2	ZN	B	804	1/1	0.89	0.15	96,96,96,96	0
2	ZN	A	806	1/1	0.92	0.16	64,64,64,64	0
2	ZN	A	810	1/1	0.93	0.05	97,97,97,97	0
2	ZN	A	802	1/1	0.94	0.05	58,58,58,58	0
2	ZN	A	801	1/1	0.94	0.18	48,48,48,48	0
2	ZN	A	814	1/1	0.95	0.37	20,20,20,20	0
2	ZN	B	803	1/1	0.96	0.15	69,69,69,69	0
2	ZN	B	812	1/1	0.97	0.09	20,20,20,20	0
2	ZN	A	807	1/1	0.97	0.16	42,42,42,42	0
2	ZN	B	811	1/1	0.98	0.16	67,67,67,67	0
2	ZN	A	813	1/1	0.99	0.13	90,90,90,90	0
2	ZN	A	808	1/1	0.99	0.17	50,50,50,50	0
2	ZN	B	801	1/1	1.00	0.23	55,55,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.