Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 08:07 AM EDT

PDB ID	:	5MZ4
Title	:	Crystal Structure of full-lengh CSFV NS3/4A
Authors	:	Tortorici, M.A.; Rey, F.A.
Deposited on	:	2017-01-30
Resolution	:	3.05 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:

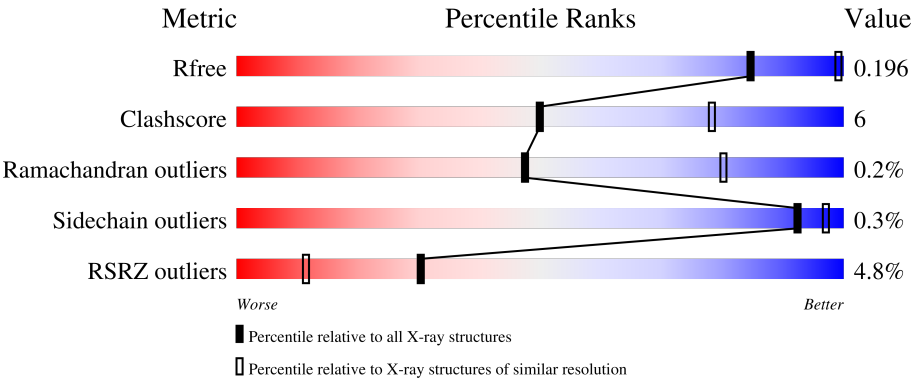
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.05 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	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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	752	3% 79% 14% 6%
1	B	752	6% 78% 12% 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10798 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 Genome polyprotein,Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	704	Total	C	N	O	S	0	0	0
			5480	3453	947	1045	35			
1	B	679	Total	C	N	O	S	0	0	0
			5308	3349	915	1008	36			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P19712
A	-18	ALA	-	expression tag	UNP P19712
A	-17	SER	-	expression tag	UNP P19712
A	-16	HIS	-	expression tag	UNP P19712
A	-15	HIS	-	expression tag	UNP P19712
A	-14	HIS	-	expression tag	UNP P19712
A	-13	HIS	-	expression tag	UNP P19712
A	-12	HIS	-	expression tag	UNP P19712
A	-11	HIS	-	expression tag	UNP P19712
A	-10	HIS	-	expression tag	UNP P19712
A	-9	HIS	-	expression tag	UNP P19712
A	-8	HIS	-	expression tag	UNP P19712
A	-7	HIS	-	expression tag	UNP P19712
A	-6	GLU	-	expression tag	UNP P19712
A	-5	ASN	-	expression tag	UNP P19712
A	-4	LEU	-	expression tag	UNP P19712
A	-3	TYR	-	expression tag	UNP P19712
A	-2	PHE	-	expression tag	UNP P19712
A	-1	GLN	-	expression tag	UNP P19712
A	0	GLY	-	expression tag	UNP P19712
A	38	GLY	-	linker	UNP P19712
A	39	SER	-	linker	UNP P19712
A	40	GLY	-	linker	UNP P19712
A	41	SER	-	linker	UNP P19712
A	204	ALA	SER	engineered mutation	UNP P19712

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP P19712
B	-18	ALA	-	expression tag	UNP P19712
B	-17	SER	-	expression tag	UNP P19712
B	-16	HIS	-	expression tag	UNP P19712
B	-15	HIS	-	expression tag	UNP P19712
B	-14	HIS	-	expression tag	UNP P19712
B	-13	HIS	-	expression tag	UNP P19712
B	-12	HIS	-	expression tag	UNP P19712
B	-11	HIS	-	expression tag	UNP P19712
B	-10	HIS	-	expression tag	UNP P19712
B	-9	HIS	-	expression tag	UNP P19712
B	-8	HIS	-	expression tag	UNP P19712
B	-7	HIS	-	expression tag	UNP P19712
B	-6	GLU	-	expression tag	UNP P19712
B	-5	ASN	-	expression tag	UNP P19712
B	-4	LEU	-	expression tag	UNP P19712
B	-3	TYR	-	expression tag	UNP P19712
B	-2	PHE	-	expression tag	UNP P19712
B	-1	GLN	-	expression tag	UNP P19712
B	0	GLY	-	expression tag	UNP P19712
B	38	GLY	-	linker	UNP P19712
B	39	SER	-	linker	UNP P19712
B	40	GLY	-	linker	UNP P19712
B	41	SER	-	linker	UNP P19712
B	204	ALA	SER	engineered mutation	UNP P19712

- Molecule 2 is water.

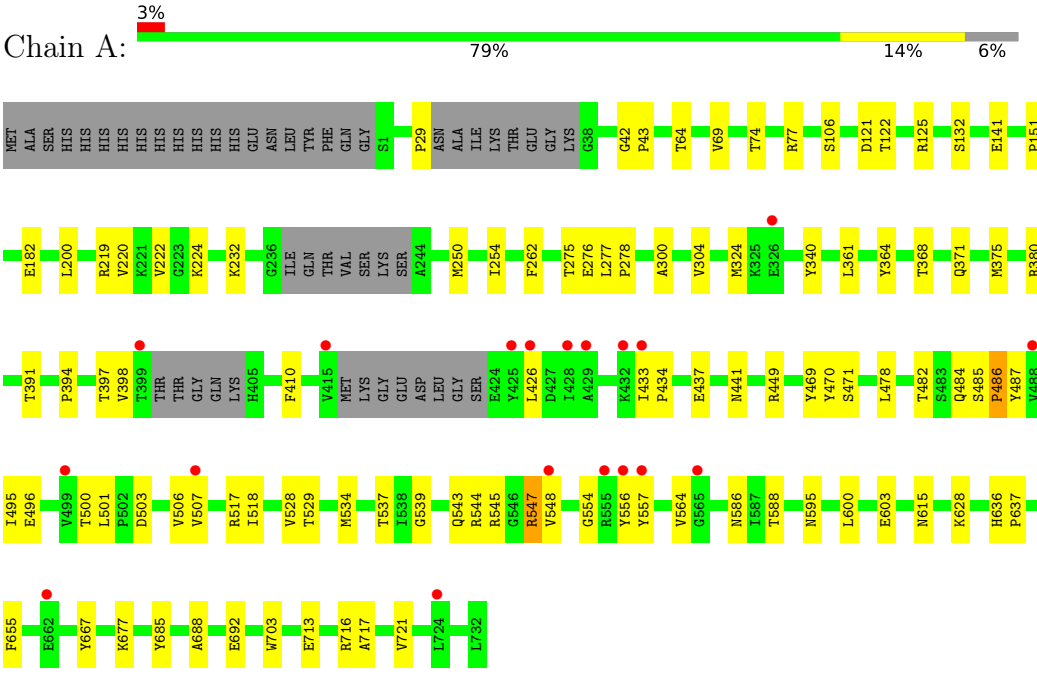
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	7	Total O 7 7	0	0
2	B	3	Total O 3 3	0	0

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.

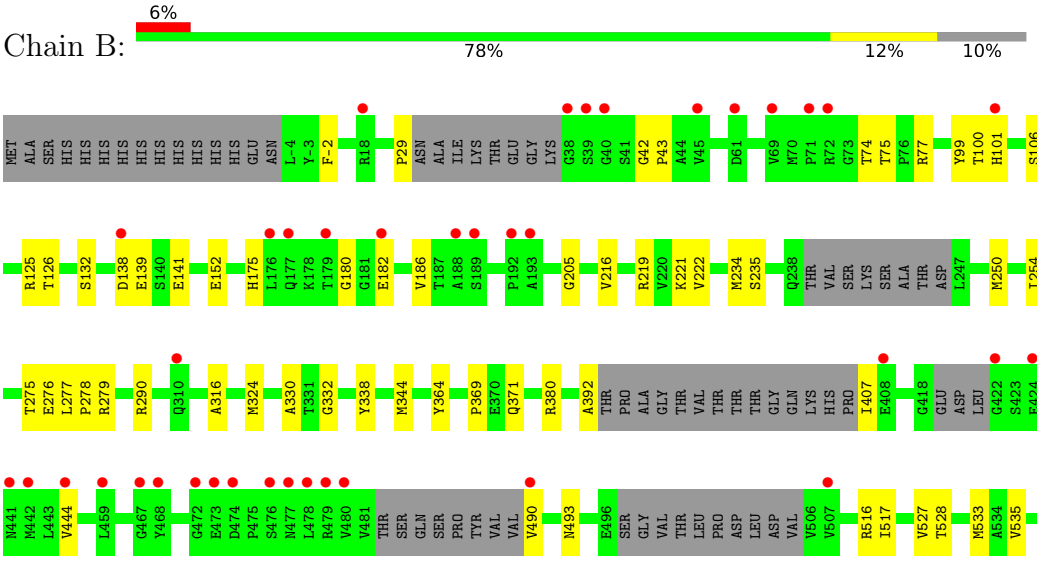
• Molecule 1: Genome polyprotein,Genome polyprotein

Chain A:



• Molecule 1: Genome polyprotein,Genome polyprotein

Chain B:




G545
R546
V547
GLY
ARG
VAL
LYS
PRO
GLY
ARG
Y555
Y556
Q559
A575
I580
N585
N594
E602
L617
I618
N628
R632
T648
Q649
V650
F654
I657
Y684
A687
E691
A694
W702
V720
V721
E727
L730
L731

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	127.21Å 168.84Å 98.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.95 – 3.05 38.95 – 3.05	Depositor EDS
% Data completeness (in resolution range)	97.5 (38.95-3.05) 97.6 (38.95-3.05)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 3.06Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.193 , 0.233 0.196 , 0.196	Depositor DCC
R_{free} test set	2043 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	69.8	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 58.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10798	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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

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	0.30	0/5586	0.50	0/7562
1	B	0.29	0/5406	0.49	0/7300
All	All	0.30	0/10992	0.50	0/14862

There are no bond length outliers.

There are no bond angle outliers.

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	5480	0	5481	74	0
1	B	5308	0	5305	58	0
2	A	7	0	0	0	0
2	B	3	0	0	0	0
All	All	10798	0	10786	125	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 6.

All (125) 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:496:GLU:O	1:A:547:ARG:NH2	2.12	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:ASN:HB2	1:A:544:ARG:HH21	1.47	0.80
1:B:132:SER:HB3	1:B:141:GLU:HB2	1.66	0.76
1:A:471:SER:HA	1:A:495:ILE:HD11	1.69	0.75
1:B:101:HIS:NE2	1:B:216:VAL:HG21	2.04	0.72
1:A:141:GLU:OE2	1:A:219:ARG:NH2	2.23	0.70
1:A:132:SER:HB2	1:A:141:GLU:HB2	1.73	0.69
1:B:221:LYS:HD2	1:B:235:SER:HA	1.74	0.69
1:A:106:SER:HB2	1:A:219:ARG:HH21	1.58	0.69
1:B:100:THR:O	1:B:101:HIS:ND1	2.27	0.67
1:B:-2:PHE:HB3	1:B:721:VAL:HA	1.78	0.65
1:B:74:THR:HG22	1:B:125:ARG:HB3	1.78	0.65
1:B:138:ASP:HB2	1:B:221:LYS:HD3	1.80	0.64
1:A:410:PHE:HB2	1:A:556:TYR:O	1.98	0.64
1:B:720:VAL:O	1:B:721:VAL:HG22	1.98	0.62
1:B:493:ASN:HB2	1:B:543:ARG:HH21	1.66	0.60
1:A:469:TYR:HE2	1:A:495:ILE:HG21	1.66	0.60
1:B:99:TYR:CE1	1:B:106:SER:HB3	2.37	0.60
1:A:449:ARG:NH2	1:A:471:SER:OG	2.36	0.58
1:A:74:THR:HG22	1:A:125:ARG:HB3	1.85	0.58
1:A:507:VAL:HB	1:A:556:TYR:CD1	2.39	0.58
1:A:437:GLU:OE1	1:A:506:VAL:HG21	2.05	0.57
1:A:492:THR:HG22	1:A:494:ALA:H	1.70	0.57
1:A:484:GLN:HG2	1:A:486:PRO:HD2	1.86	0.56
1:A:121:ASP:OD1	1:A:122:THR:N	2.36	0.56
1:B:222:VAL:HB	1:B:234:MET:HB2	1.88	0.55
1:B:277:LEU:HB3	1:B:278:PRO:HD3	1.87	0.55
1:A:485:SER:HB2	1:A:486:PRO:HD3	1.89	0.54
1:B:101:HIS:CE1	1:B:216:VAL:HG21	2.44	0.53
1:B:290:ARG:HD2	1:B:330:ALA:O	2.09	0.53
1:A:277:LEU:HB3	1:A:278:PRO:HD3	1.91	0.53
1:B:139:GLU:HG2	1:B:219:ARG:NH2	2.25	0.52
1:B:628:ASN:HB3	1:B:632:ARG:NH1	2.25	0.52
1:A:383:GLU:HG2	1:B:585:ASN:CB	2.40	0.52
1:A:517:ARG:NH2	1:A:534:MET:SD	2.83	0.52
1:B:75:THR:O	1:B:126:THR:HA	2.10	0.51
1:B:547:VAL:HG23	1:B:555:TYR:CZ	2.45	0.51
1:A:250:MET:O	1:A:254:ILE:HG12	2.11	0.51
1:A:655:PHE:CG	1:A:692:GLU:HG2	2.46	0.51
1:B:152:GLU:OE1	1:B:180:GLY:N	2.43	0.50
1:B:338:TYR:CZ	1:B:371:GLN:HG3	2.47	0.50
1:B:580:ILE:HD11	1:B:617:LEU:HD21	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:THR:OG1	1:A:371:GLN:HB2	2.12	0.49
1:B:275:THR:OG1	1:B:276:GLU:N	2.44	0.49
1:A:222:VAL:HG22	1:B:730:LEU:HD23	1.93	0.49
1:B:267:LEU:O	1:B:392:ALA:HA	2.13	0.49
1:A:588:THR:H	1:A:615:ASN:HD22	1.61	0.49
1:B:684:TYR:HB2	1:B:702:TRP:CZ3	2.46	0.49
1:A:383:GLU:HG2	1:B:585:ASN:HB3	1.95	0.49
1:A:64:THR:HG22	1:A:69:VAL:O	2.14	0.48
1:A:545:ARG:HG2	1:A:556:TYR:CD2	2.48	0.48
1:A:588:THR:H	1:A:615:ASN:ND2	2.11	0.48
1:A:394:PRO:HD2	1:A:397:THR:HG21	1.95	0.47
1:A:182:GLU:HG3	1:A:232:LYS:HD3	1.96	0.47
1:B:182:GLU:HG2	1:B:234:MET:HA	1.94	0.47
1:B:516:ARG:NH2	1:B:533:MET:SD	2.88	0.47
1:B:175:HIS:HB2	1:B:186:VAL:O	2.14	0.47
1:A:713:GLU:OE1	1:A:716:ARG:HD3	2.16	0.46
1:A:434:PRO:HD2	1:A:557:TYR:CE2	2.50	0.46
1:A:300:ALA:O	1:A:304:VAL:HG23	2.15	0.46
1:A:398:VAL:HG13	1:A:539:GLY:HA2	1.96	0.46
1:A:361:LEU:HD13	1:A:375:MET:HG2	1.97	0.46
1:A:667:TYR:CZ	1:A:677:LYS:HD3	2.51	0.46
1:B:250:MET:O	1:B:254:ILE:HG12	2.15	0.46
1:B:407:ILE:HB	1:B:555:TYR:CE2	2.51	0.46
1:A:537:THR:HA	1:A:564:VAL:O	2.16	0.45
1:A:636:HIS:ND1	1:A:637:PRO:HD2	2.31	0.45
1:B:654:PHE:CG	1:B:691:GLU:HG2	2.51	0.45
1:A:713:GLU:OE2	1:A:716:ARG:NH1	2.47	0.45
1:A:586:ASN:OD1	1:A:615:ASN:ND2	2.46	0.45
1:B:77:ARG:HB2	1:B:126:THR:HB	1.98	0.45
1:A:713:GLU:HA	1:A:716:ARG:HG2	1.98	0.45
1:B:139:GLU:HG2	1:B:219:ARG:HH21	1.81	0.45
1:A:380:ARG:O	1:B:380:ARG:NH2	2.50	0.45
1:B:425:TYR:HD1	1:B:434:PRO:HA	1.81	0.45
1:B:108:VAL:HG23	1:B:205:GLY:HA2	1.99	0.44
1:A:507:VAL:HB	1:A:556:TYR:HD1	1.80	0.44
1:A:548:VAL:HG11	1:A:554:GLY:HA3	1.97	0.44
1:A:545:ARG:O	1:A:556:TYR:OH	2.25	0.44
1:A:548:VAL:CG1	1:A:554:GLY:HA3	2.48	0.44
1:B:527:VAL:HA	1:B:687:ALA:O	2.18	0.44
1:B:324:MET:SD	1:B:344:MET:HG2	2.58	0.44
1:B:657:ILE:HD11	1:B:694:ALA:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:594:ASN:HD22	1:B:602:GLU:HG3	1.82	0.43
1:A:433:ILE:HG13	1:A:557:TYR:CD2	2.54	0.43
1:A:717:ALA:O	1:A:721:VAL:HG23	2.18	0.43
1:A:441:ASN:ND2	1:A:503:ASP:O	2.41	0.43
1:A:151:PRO:HG2	1:A:154:ALA:HB2	1.99	0.43
1:A:449:ARG:HB2	1:A:470:TYR:CD1	2.53	0.43
1:A:487:TYR:CE1	1:A:501:LEU:HD12	2.53	0.43
1:B:338:TYR:CE2	1:B:371:GLN:HG3	2.53	0.43
1:B:444:VAL:HB	1:B:490:VAL:HG22	2.00	0.43
1:B:535:VAL:HG22	1:B:539:GLU:HB2	2.01	0.43
1:A:275:THR:OG1	1:A:276:GLU:N	2.52	0.43
1:A:642:LEU:O	1:A:646:SER:HB3	2.19	0.43
1:B:316:ALA:O	1:B:332:GLY:HA3	2.19	0.43
1:A:224:LYS:HA	1:B:727:GLU:O	2.19	0.42
1:A:77:ARG:HH12	1:A:121:ASP:CB	2.32	0.42
1:A:478:LEU:O	1:A:482:THR:HG23	2.19	0.42
1:B:618:ILE:HG22	1:B:618:ILE:O	2.19	0.42
1:A:42:GLY:N	1:A:43:PRO:HD3	2.34	0.42
1:A:158:VAL:HG21	1:A:220:VAL:HG21	2.00	0.42
1:A:324:MET:HA	1:A:340:TYR:CE1	2.54	0.42
1:A:426:LEU:HD23	1:A:433:ILE:O	2.20	0.42
1:B:369:PRO:HA	1:B:575:ALA:HB2	2.02	0.42
1:B:544:ARG:HG3	1:B:555:TYR:CD1	2.56	0.41
1:A:200:LEU:HB3	1:B:731:LEU:HD13	2.02	0.41
1:A:518:ILE:HG22	1:A:529:THR:HG22	2.03	0.41
1:A:685:TYR:HB2	1:A:703:TRP:CZ3	2.55	0.41
1:B:276:GLU:OE1	1:B:279:ARG:NH2	2.50	0.41
1:A:528:VAL:HA	1:A:688:ALA:O	2.20	0.41
1:B:42:GLY:N	1:B:43:PRO:HD3	2.35	0.41
1:A:262:PHE:HA	1:A:387:VAL:O	2.20	0.41
1:B:364:TYR:HA	1:B:371:GLN:NE2	2.35	0.41
1:B:517:ILE:HG22	1:B:528:THR:HG22	2.01	0.41
1:A:383:GLU:HG2	1:B:585:ASN:HB2	2.02	0.41
1:B:648:THR:HG22	1:B:650:VAL:H	1.85	0.41
1:A:364:TYR:CZ	1:A:600:LEU:HD22	2.55	0.41
1:A:364:TYR:CE1	1:A:600:LEU:HD22	2.56	0.41
1:A:501:LEU:HD13	1:A:501:LEU:HA	1.91	0.41
1:A:539:GLY:O	1:A:543:GLN:HG3	2.21	0.41
1:A:391:THR:HG21	1:A:394:PRO:HA	2.03	0.40
1:A:595:ASN:ND2	1:A:603:GLU:HG3	2.36	0.40
1:B:99:TYR:HE2	1:B:219:ARG:HG2	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:LYS:HE3	1:A:628:LYS:HB2	1.82	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	694/752 (92%)	676 (97%)	16 (2%)	2 (0%)	41 74
1	B	663/752 (88%)	649 (98%)	13 (2%)	1 (0%)	47 80
All	All	1357/1504 (90%)	1325 (98%)	29 (2%)	3 (0%)	47 80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	500	THR
1	B	721	VAL
1	A	486	PRO

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	599/640 (94%)	597 (100%)	2 (0%)	92 97
1	B	577/640 (90%)	576 (100%)	1 (0%)	93 98

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1176/1280 (92%)	1173 (100%)	3 (0%)	92 97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	PRO
1	A	547	ARG
1	B	29	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	615	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

There are no ligands in this entry.

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	704/752 (93%)	0.03	19 (2%) 54 26	41, 75, 140, 221	0
1	B	679/752 (90%)	0.28	47 (6%) 16 5	38, 92, 164, 220	0
All	All	1383/1504 (91%)	0.15	66 (4%) 30 11	38, 82, 154, 221	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	555	TYR	7.2
1	B	478	LEU	6.7
1	A	499	VAL	5.0
1	A	556	TYR	4.7
1	A	432	LYS	4.7
1	B	467	GLY	4.7
1	A	433	ILE	4.4
1	B	408	GLU	3.8
1	A	488	VAL	3.8
1	B	18	ARG	3.5
1	B	547	VAL	3.4
1	B	480	VAL	3.2
1	B	71	PRO	3.1
1	B	468	TYR	3.1
1	A	724	LEU	3.1
1	A	565	GLY	3.0
1	B	101	HIS	3.0
1	A	425	TYR	3.0
1	A	555	ARG	3.0
1	B	192	PRO	3.0
1	B	442	MET	2.9
1	A	429	ALA	2.9
1	B	490	VAL	2.9
1	B	193	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	177	GLN	2.8
1	B	39	SER	2.8
1	B	38	GLY	2.8
1	B	507	VAL	2.8
1	A	662	GLU	2.7
1	B	310	GLN	2.7
1	B	545	GLY	2.7
1	B	424	GLU	2.7
1	B	477	ASN	2.7
1	B	474	ASP	2.6
1	B	444	VAL	2.6
1	B	269	THR	2.6
1	B	556	TYR	2.6
1	B	176	LEU	2.4
1	B	40	GLY	2.4
1	B	189	SER	2.4
1	B	45	VAL	2.4
1	B	188	ALA	2.3
1	A	557	TYR	2.3
1	B	61	ASP	2.3
1	B	559	GLN	2.3
1	B	479	ARG	2.3
1	B	422	GLY	2.2
1	B	476	SER	2.2
1	B	138	ASP	2.2
1	A	548	VAL	2.2
1	B	473	GLU	2.2
1	A	428	ILE	2.1
1	B	72	ARG	2.1
1	A	426	LEU	2.1
1	B	118	LEU	2.1
1	B	459	LEU	2.1
1	B	546	ARG	2.1
1	A	326	GLU	2.1
1	B	179	THR	2.1
1	B	182	GLU	2.1
1	B	69	VAL	2.1
1	B	472	GLY	2.0
1	A	507	VAL	2.0
1	B	441	ASN	2.0
1	A	415	VAL	2.0
1	A	399	THR	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.