Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 04:50 am BST

PDB ID	:	4CBG
Title	:	Pestivirus NS3 helicase
Authors	:	Tortorici, M.A.; Duquerroy, S.; Kwok, J.; Vonrhein, C.; Perez, J.; Lamp, B.; Bricogne, G.; Rumenapf, T.; Vachette, P.; Rey, F.A.
Deposited on	:	2013-10-14
Resolution	:	2.82 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 following versions of software and data (see references ⓘ) were used in the production of this report:

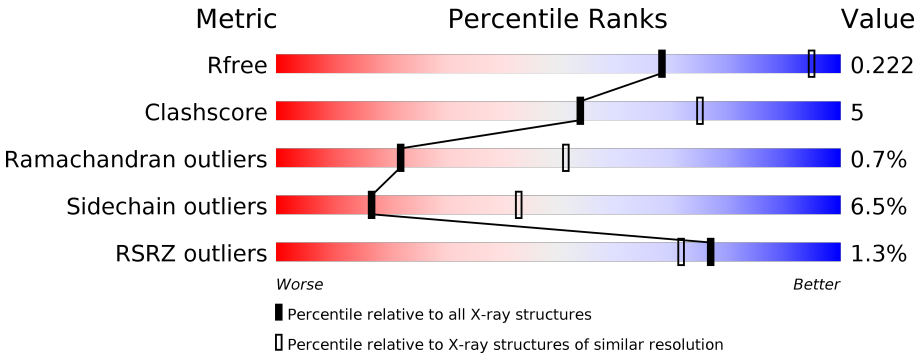
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.82 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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 on 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	516	% 75% 13% • 11%
1	B	516	% 75% 13% • 11%
1	C	516	% 74% 15% • 10%
1	D	516	% 72% 17% • 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14861 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 SERINE PROTEASE NS3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	Se	0	0	1
			3648	2316	624	686	3	19			
1	B	461	Total	C	N	O	S	Se	0	0	1
			3655	2321	625	687	3	19			
1	C	466	Total	C	N	O	S	Se	0	0	1
			3700	2348	630	700	3	19			
1	D	470	Total	C	N	O	S	Se	0	0	0
			3728	2364	634	708	3	19			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	176	MSE	-	expression tag	UNP P19712
A	177	ALA	-	expression tag	UNP P19712
A	178	SER	-	expression tag	UNP P19712
A	179	HIS	-	expression tag	UNP P19712
A	180	HIS	-	expression tag	UNP P19712
A	181	HIS	-	expression tag	UNP P19712
A	182	HIS	-	expression tag	UNP P19712
A	183	HIS	-	expression tag	UNP P19712
A	184	HIS	-	expression tag	UNP P19712
A	185	HIS	-	expression tag	UNP P19712
A	186	GLU	-	expression tag	UNP P19712
A	187	ASN	-	expression tag	UNP P19712
A	188	LEU	-	expression tag	UNP P19712
A	189	TYR	-	expression tag	UNP P19712
A	190	PHE	-	expression tag	UNP P19712
A	191	GLN	-	expression tag	UNP P19712
A	192	GLY	-	expression tag	UNP P19712
B	176	MSE	-	expression tag	UNP P19712
B	177	ALA	-	expression tag	UNP P19712
B	178	SER	-	expression tag	UNP P19712
B	179	HIS	-	expression tag	UNP P19712

Continued on next page...

Continued from previous page...

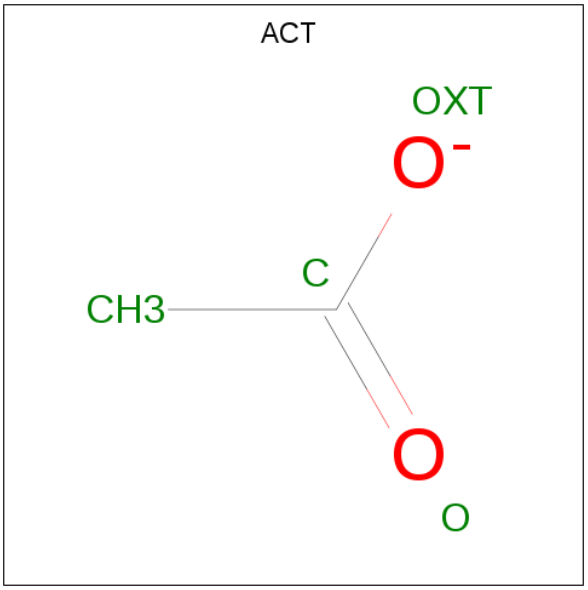
Chain	Residue	Modelled	Actual	Comment	Reference
B	180	HIS	-	expression tag	UNP P19712
B	181	HIS	-	expression tag	UNP P19712
B	182	HIS	-	expression tag	UNP P19712
B	183	HIS	-	expression tag	UNP P19712
B	184	HIS	-	expression tag	UNP P19712
B	185	HIS	-	expression tag	UNP P19712
B	186	GLU	-	expression tag	UNP P19712
B	187	ASN	-	expression tag	UNP P19712
B	188	LEU	-	expression tag	UNP P19712
B	189	TYR	-	expression tag	UNP P19712
B	190	PHE	-	expression tag	UNP P19712
B	191	GLN	-	expression tag	UNP P19712
B	192	GLY	-	expression tag	UNP P19712
C	176	MSE	-	expression tag	UNP P19712
C	177	ALA	-	expression tag	UNP P19712
C	178	SER	-	expression tag	UNP P19712
C	179	HIS	-	expression tag	UNP P19712
C	180	HIS	-	expression tag	UNP P19712
C	181	HIS	-	expression tag	UNP P19712
C	182	HIS	-	expression tag	UNP P19712
C	183	HIS	-	expression tag	UNP P19712
C	184	HIS	-	expression tag	UNP P19712
C	185	HIS	-	expression tag	UNP P19712
C	186	GLU	-	expression tag	UNP P19712
C	187	ASN	-	expression tag	UNP P19712
C	188	LEU	-	expression tag	UNP P19712
C	189	TYR	-	expression tag	UNP P19712
C	190	PHE	-	expression tag	UNP P19712
C	191	GLN	-	expression tag	UNP P19712
C	192	GLY	-	expression tag	UNP P19712
D	176	MSE	-	expression tag	UNP P19712
D	177	ALA	-	expression tag	UNP P19712
D	178	SER	-	expression tag	UNP P19712
D	179	HIS	-	expression tag	UNP P19712
D	180	HIS	-	expression tag	UNP P19712
D	181	HIS	-	expression tag	UNP P19712
D	182	HIS	-	expression tag	UNP P19712
D	183	HIS	-	expression tag	UNP P19712
D	184	HIS	-	expression tag	UNP P19712
D	185	HIS	-	expression tag	UNP P19712
D	186	GLU	-	expression tag	UNP P19712
D	187	ASN	-	expression tag	UNP P19712

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	188	LEU	-	expression tag	UNP P19712
D	189	TYR	-	expression tag	UNP P19712
D	190	PHE	-	expression tag	UNP P19712
D	191	GLN	-	expression tag	UNP P19712
D	192	GLY	-	expression tag	UNP P19712

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is water.

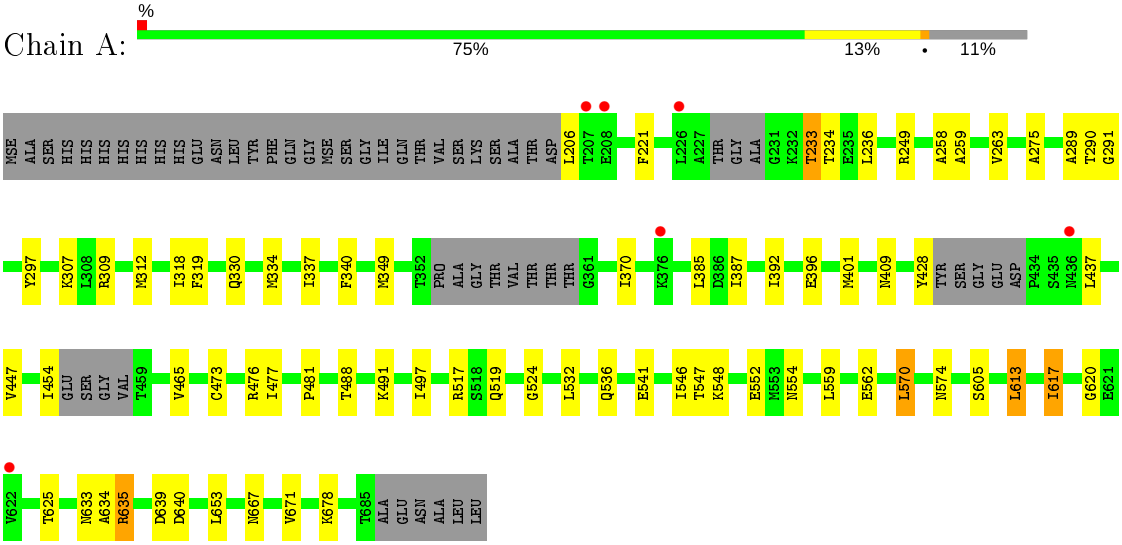
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	39	Total O 39 39	0	0
3	B	33	Total O 33 33	0	0
3	C	18	Total O 18 18	0	0
3	D	32	Total O 32 32	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

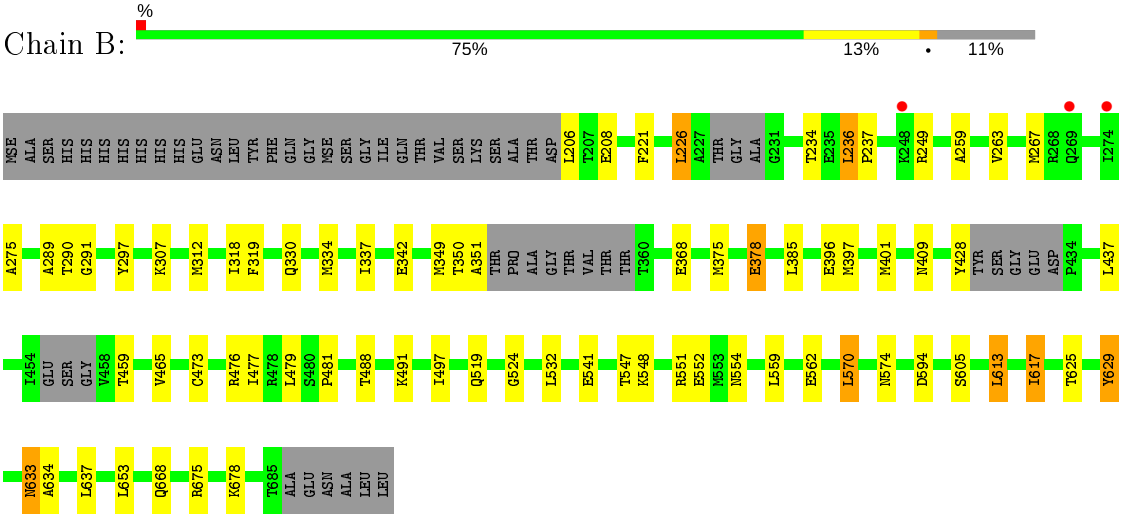
- Molecule 1: SERINE PROTEASE NS3

Chain A:



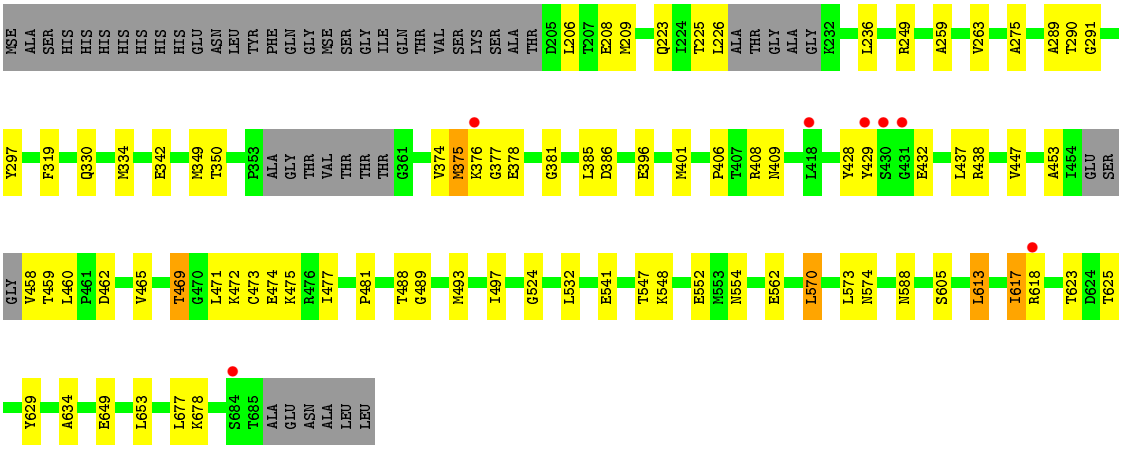
- Molecule 1: SERINE PROTEASE NS3

Chain B:



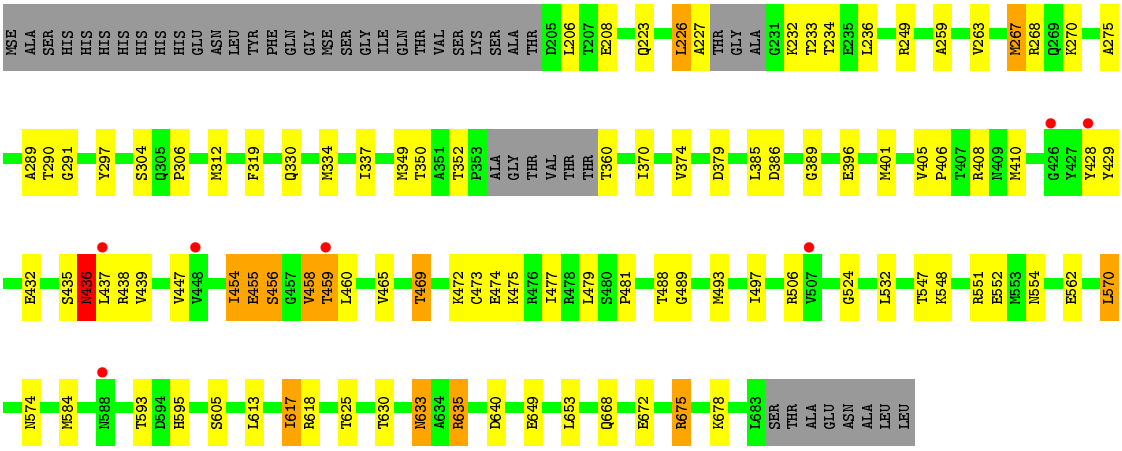
- Molecule 1: SERINE PROTEASE NS3

Chain C:



- Molecule 1: SERINE PROTEASE NS3

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.55Å 168.36Å 98.80Å 90.00° 98.52° 90.00°	Depositor
Resolution (Å)	49.52 – 2.82 49.52 – 2.82	Depositor EDS
% Data completeness (in resolution range)	90.7 (49.52-2.82) 91.1 (49.52-2.82)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.13.0	Depositor
R, R_{free}	0.166 , 0.205 0.185 , 0.222	Depositor DCC
R_{free} test set	2532 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	41.2	Xtriage
Anisotropy	1.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 66.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14861	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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: ACT

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	0/3697	0.71	1/4966 (0.0%)
1	B	0.52	0/3704	0.71	1/4976 (0.0%)
1	C	0.50	0/3752	0.74	1/5045 (0.0%)
1	D	0.50	0/3781	0.74	2/5085 (0.0%)
All	All	0.51	0/14934	0.73	5/20072 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	290	THR	N-CA-C	5.34	125.42	111.00
1	C	290	THR	N-CA-C	5.26	125.19	111.00
1	D	290	THR	N-CA-C	5.23	125.13	111.00
1	D	454	ILE	C-N-CA	5.14	134.54	121.70
1	B	290	THR	N-CA-C	5.04	124.62	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	3648	0	3672	32	0
1	B	3655	0	3681	33	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3700	0	3711	35	0
1	D	3728	0	3736	57	0
2	C	4	0	3	0	0
2	D	4	0	3	0	0
3	A	39	0	0	0	0
3	B	33	0	0	1	0
3	C	18	0	0	0	0
3	D	32	0	0	1	0
All	All	14861	0	14806	155	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 5.

All (155) 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:D:593:THR:HG22	1:D:595:HIS:H	1.29	0.96
1:B:477:ILE:HG22	1:B:488:THR:HG22	1.49	0.91
1:D:477:ILE:HG22	1:D:488:THR:HG22	1.63	0.79
1:B:312:MSE:HE2	1:B:337:ILE:HG21	1.69	0.73
1:A:330:GLN:HG2	1:A:334:MSE:HE3	1.71	0.73
1:D:454:ILE:HA	1:D:455:GLU:HB2	1.72	0.72
1:A:387:ILE:HB	1:A:392:ILE:HD13	1.71	0.72
1:C:330:GLN:HG2	1:C:334:MSE:HE3	1.72	0.69
1:D:406:PRO:HD3	1:D:469:THR:HG21	1.73	0.69
1:D:330:GLN:HG2	1:D:334:MSE:HE3	1.74	0.69
1:A:312:MSE:HE2	1:A:337:ILE:HG21	1.74	0.69
1:C:406:PRO:HD3	1:C:469:THR:HG21	1.74	0.69
1:D:408:ARG:HG2	1:D:429:TYR:HB2	1.75	0.69
1:B:330:GLN:HG2	1:B:334:MSE:HE3	1.74	0.69
1:C:489:GLY:HA3	1:C:649:GLU:CG	2.26	0.66
1:D:635:ARG:NH2	1:D:640:ASP:O	2.29	0.66
1:C:408:ARG:HG2	1:C:429:TYR:HB2	1.78	0.66
1:D:593:THR:HG23	1:D:630:THR:O	1.97	0.64
1:A:635:ARG:NH2	1:A:640:ASP:O	2.31	0.64
1:D:267:MSE:HA	1:D:267:MSE:HE2	1.79	0.64
1:D:405:VAL:HG21	1:D:410:MSE:HB3	1.80	0.63
1:C:489:GLY:HA3	1:C:649:GLU:HG3	1.80	0.63
1:D:436:ASN:O	1:D:439:VAL:HG12	2.00	0.62
1:C:374:VAL:HG21	1:C:386:ASP:OD2	1.99	0.62
1:A:312:MSE:HE3	1:A:318:ILE:HD13	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:MSE:CE	1:D:267:MSE:HA	2.31	0.60
1:B:312:MSE:HE3	1:B:318:ILE:HD13	1.84	0.60
1:D:405:VAL:HG22	1:D:406:PRO:HD2	1.84	0.59
1:C:618:ARG:HB2	1:C:623:THR:HG21	1.85	0.58
1:A:233:THR:HG23	1:A:234:THR:HG23	1.87	0.57
1:B:275:ALA:O	1:B:291:GLY:HA3	2.04	0.57
1:D:226:LEU:HD23	1:D:233:THR:HG22	1.87	0.57
1:A:401:MSE:HE2	1:A:447:VAL:HG21	1.86	0.56
1:C:477:ILE:HG22	1:C:488:THR:HG22	1.86	0.56
1:D:493:MSE:HE2	3:D:2017:HOH:O	2.04	0.56
1:D:551:ARG:HH11	1:D:551:ARG:HG2	1.69	0.56
1:D:489:GLY:HA3	1:D:649:GLU:CG	2.36	0.56
1:B:249:ARG:HD2	1:B:289:ALA:O	2.05	0.56
1:B:397:MSE:HE1	1:B:401:MSE:HE1	1.87	0.56
1:D:249:ARG:HD2	1:D:289:ALA:O	2.05	0.56
1:D:593:THR:CG2	1:D:595:HIS:HB2	2.35	0.56
1:C:472:LYS:HE3	1:C:493:MSE:HG3	1.88	0.55
1:C:249:ARG:HD2	1:C:289:ALA:O	2.07	0.55
1:B:259:ALA:O	1:B:263:VAL:HG23	2.07	0.54
1:A:249:ARG:HD2	1:A:289:ALA:O	2.07	0.54
1:A:477:ILE:HG22	1:A:488:THR:HG22	1.89	0.54
1:B:375:MSE:O	1:B:378:GLU:HB2	2.08	0.54
1:A:481:PRO:HB2	1:A:678:LYS:HE2	1.90	0.53
1:C:489:GLY:HA3	1:C:649:GLU:HG2	1.90	0.53
1:D:304:SER:OG	1:D:306:PRO:HD2	2.09	0.52
1:A:428:TYR:HB2	1:A:437:LEU:HD11	1.92	0.52
1:D:428:TYR:HB2	1:D:437:LEU:HD11	1.91	0.52
1:C:481:PRO:HB2	1:C:678:LYS:HE2	1.92	0.52
1:B:234:THR:HB	1:B:267:MSE:SE	2.61	0.51
1:A:258:ALA:CB	1:B:459:THR:HB	2.40	0.51
1:D:259:ALA:O	1:D:263:VAL:HG23	2.11	0.51
1:D:275:ALA:O	1:D:291:GLY:HA3	2.11	0.51
1:B:481:PRO:HB2	1:B:678:LYS:HE2	1.91	0.51
1:C:259:ALA:O	1:C:263:VAL:HG23	2.11	0.51
1:D:401:MSE:HE2	1:D:447:VAL:HG21	1.91	0.51
1:D:319:PHE:HB3	1:D:349:MSE:HE2	1.93	0.51
1:D:489:GLY:HA3	1:D:649:GLU:HG3	1.91	0.51
1:A:319:PHE:HB3	1:A:349:MSE:HE2	1.94	0.50
1:B:548:LYS:HG3	1:B:551:ARG:HH21	1.76	0.50
1:C:547:THR:HG21	1:C:570:LEU:HB3	1.93	0.50
1:D:472:LYS:HE3	1:D:493:MSE:HG3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:401:MSE:HE2	1:C:447:VAL:HG21	1.91	0.50
1:B:547:THR:HG21	1:B:570:LEU:HB3	1.93	0.50
1:C:497:ILE:HD12	1:C:524:GLY:HA2	1.93	0.50
1:B:368:GLU:OE1	1:D:370:ILE:HD11	2.11	0.50
1:D:396:GLU:HG3	1:D:465:VAL:HG11	1.94	0.50
1:D:547:THR:HG21	1:D:570:LEU:HB3	1.92	0.50
1:B:594:ASP:OD1	1:B:629:TYR:HA	2.11	0.50
1:A:275:ALA:O	1:A:291:GLY:HA3	2.12	0.50
1:D:374:VAL:HG22	1:D:389:GLY:O	2.12	0.50
1:C:475:LYS:HA	1:C:489:GLY:O	2.12	0.49
1:A:259:ALA:O	1:A:263:VAL:HG23	2.12	0.49
1:A:312:MSE:HE1	1:A:318:ILE:HG21	1.94	0.49
1:B:396:GLU:HG3	1:B:465:VAL:HG11	1.95	0.49
1:D:481:PRO:HB2	1:D:678:LYS:HE2	1.95	0.49
1:C:319:PHE:HB3	1:C:349:MSE:HE2	1.94	0.48
1:B:226:LEU:O	1:B:351:ALA:HA	2.14	0.48
1:D:593:THR:HG21	1:D:595:HIS:HB2	1.95	0.48
1:A:297:TYR:CZ	1:A:330:GLN:HG3	2.49	0.48
1:D:497:ILE:HD12	1:D:524:GLY:HA2	1.96	0.48
1:C:428:TYR:HB2	1:C:437:LEU:HD11	1.95	0.47
1:D:227:ALA:HA	1:D:352:THR:OG1	2.13	0.47
1:B:319:PHE:HB3	1:B:349:MSE:HE2	1.96	0.47
1:A:613:LEU:HD13	1:A:634:ALA:CB	2.45	0.47
1:A:370:ILE:HD13	1:A:517:ARG:HG3	1.96	0.47
1:B:221:PHE:HZ	1:B:559:LEU:HD21	1.78	0.47
1:B:617:ILE:HG21	1:B:653:LEU:HD23	1.96	0.47
1:C:548:LYS:O	1:C:552:GLU:HG3	2.14	0.47
1:D:617:ILE:HG21	1:D:653:LEU:HD23	1.96	0.47
1:C:489:GLY:CA	1:C:649:GLU:HG2	2.45	0.47
1:A:330:GLN:HG2	1:A:334:MSE:CE	2.43	0.47
1:A:396:GLU:HG3	1:A:465:VAL:HG11	1.97	0.47
1:B:428:TYR:HB2	1:B:437:LEU:HD11	1.97	0.47
1:A:497:ILE:HD12	1:A:524:GLY:HA2	1.97	0.46
1:A:547:THR:HG21	1:A:570:LEU:HB3	1.97	0.46
1:C:275:ALA:O	1:C:291:GLY:HA3	2.16	0.46
1:D:593:THR:HG22	1:D:595:HIS:HB2	1.98	0.46
1:D:474:GLU:HB3	1:D:493:MSE:SE	2.65	0.46
1:D:668:GLN:HE22	1:D:672:GLU:HB2	1.80	0.46
1:B:312:MSE:HE1	1:B:318:ILE:HG21	1.97	0.46
1:D:267:MSE:HE1	1:D:270:LYS:HD3	1.98	0.46
1:D:454:ILE:HB	1:D:506:ARG:NH2	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:TYR:CZ	1:B:330:GLN:HG3	2.51	0.46
1:D:312:MSE:HE3	1:D:337:ILE:HG21	1.98	0.46
1:C:613:LEU:HD13	1:C:634:ALA:CB	2.45	0.46
1:D:454:ILE:HB	1:D:506:ARG:HH22	1.80	0.46
1:A:221:PHE:HZ	1:A:559:LEU:HD21	1.81	0.45
1:C:573:LEU:HD21	1:C:677:LEU:HD11	1.98	0.45
1:D:474:GLU:HG3	1:D:475:LYS:N	2.30	0.45
1:C:330:GLN:HG2	1:C:334:MSE:CE	2.44	0.45
1:C:396:GLU:HG3	1:C:465:VAL:HG11	1.98	0.45
1:A:309:ARG:HG3	1:A:340:PHE:CD1	2.52	0.45
1:D:374:VAL:HG21	1:D:386:ASP:OD2	2.15	0.45
1:A:617:ILE:HG21	1:A:653:LEU:HD23	1.98	0.44
1:C:297:TYR:CZ	1:C:330:GLN:HG3	2.51	0.44
1:D:297:TYR:CZ	1:D:330:GLN:HG3	2.52	0.44
1:B:613:LEU:HD13	1:B:634:ALA:CB	2.47	0.44
1:C:206:LEU:HA	1:C:209:MSE:HE3	2.00	0.44
1:C:617:ILE:HG21	1:C:653:LEU:HD23	1.98	0.44
1:D:548:LYS:O	1:D:552:GLU:HG3	2.18	0.44
1:B:249:ARG:NH1	3:B:2004:HOH:O	2.47	0.44
1:B:548:LYS:O	1:B:552:GLU:HG3	2.18	0.44
1:D:554:ASN:HD22	1:D:562:GLU:HG3	1.83	0.44
1:D:479:LEU:HD11	1:D:570:LEU:HD13	1.99	0.43
1:C:375:MSE:HE2	1:C:378:GLU:HB3	2.01	0.43
1:D:438:ARG:NH2	1:D:459:THR:O	2.49	0.43
1:D:489:GLY:HA3	1:D:649:GLU:HG2	2.00	0.43
1:B:330:GLN:HG2	1:B:334:MSE:CE	2.44	0.42
1:A:401:MSE:HE2	1:A:447:VAL:CG2	2.47	0.42
1:A:667:ASN:O	1:A:671:VAL:HG23	2.20	0.42
1:B:497:ILE:HD12	1:B:524:GLY:HA2	2.01	0.42
1:C:469:THR:HG23	1:C:471:LEU:H	1.84	0.42
1:B:479:LEU:HD11	1:B:570:LEU:HD13	2.01	0.42
1:C:554:ASN:HD22	1:C:562:GLU:HG3	1.84	0.42
1:D:435:SER:HA	1:D:438:ARG:HG2	2.02	0.41
1:B:633:ASN:HD22	1:B:633:ASN:HA	1.75	0.41
1:D:456:SER:O	1:D:458:VAL:HA	2.20	0.41
1:C:474:GLU:HG3	1:C:475:LYS:N	2.36	0.41
1:B:236:LEU:HB3	1:B:237:PRO:HD3	2.02	0.41
1:B:554:ASN:HD22	1:B:562:GLU:HG3	1.86	0.41
1:D:330:GLN:HG2	1:D:334:MSE:CE	2.46	0.41
1:A:548:LYS:O	1:A:552:GLU:HG3	2.20	0.41
1:D:633:ASN:HD22	1:D:633:ASN:HA	1.75	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:401:MSE:HE2	1:C:447:VAL:CG2	2.51	0.41
1:C:437:LEU:HD23	1:C:437:LEU:HA	1.95	0.41
1:A:309:ARG:HG3	1:A:340:PHE:CG	2.56	0.41
1:D:405:VAL:CG2	1:D:410:MSE:HB3	2.50	0.40
1:A:554:ASN:HD22	1:A:562:GLU:HG3	1.86	0.40
1:D:672:GLU:OE2	1:D:675:ARG:NH1	2.54	0.40
1:A:536:GLN:HA	1:A:546:ILE:HB	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	450/516 (87%)	435 (97%)	13 (3%)	2 (0%)	34	64
1	B	451/516 (87%)	440 (98%)	10 (2%)	1 (0%)	47	76
1	C	458/516 (89%)	439 (96%)	12 (3%)	7 (2%)	10	31
1	D	464/516 (90%)	446 (96%)	15 (3%)	3 (1%)	25	54
All	All	1823/2064 (88%)	1760 (96%)	50 (3%)	13 (1%)	22	51

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	THR
1	B	629	TYR
1	C	453	ALA
1	C	459	THR
1	C	629	TYR
1	C	376	LYS
1	C	381	GLY
1	D	436	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	377	GLY
1	C	432	GLU
1	D	432	GLU
1	D	456	SER
1	A	620	GLY

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	397/421 (94%)	376 (95%)	21 (5%)	22	52
1	B	398/421 (94%)	372 (94%)	26 (6%)	17	43
1	C	404/421 (96%)	379 (94%)	25 (6%)	18	45
1	D	406/421 (96%)	374 (92%)	32 (8%)	12	33
All	All	1605/1684 (95%)	1501 (94%)	104 (6%)	17	43

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	LEU
1	A	236	LEU
1	A	307	LYS
1	A	385	LEU
1	A	409	ASN
1	A	454	ILE
1	A	473	CYS
1	A	476	ARG
1	A	491	LYS
1	A	519	GLN
1	A	532	LEU
1	A	541	GLU
1	A	570	LEU
1	A	574	ASN
1	A	605	SER
1	A	613	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	617	ILE
1	A	625	THR
1	A	633	ASN
1	A	635	ARG
1	A	639	ASP
1	B	206	LEU
1	B	208	GLU
1	B	226	LEU
1	B	236	LEU
1	B	307	LYS
1	B	342	GLU
1	B	350	THR
1	B	378	GLU
1	B	385	LEU
1	B	409	ASN
1	B	473	CYS
1	B	476	ARG
1	B	491	LYS
1	B	519	GLN
1	B	532	LEU
1	B	541	GLU
1	B	570	LEU
1	B	574	ASN
1	B	605	SER
1	B	613	LEU
1	B	617	ILE
1	B	625	THR
1	B	633	ASN
1	B	637	LEU
1	B	668	GLN
1	B	675	ARG
1	C	208	GLU
1	C	223	GLN
1	C	225	THR
1	C	226	LEU
1	C	236	LEU
1	C	342	GLU
1	C	350	THR
1	C	375	MSE
1	C	385	LEU
1	C	409	ASN
1	C	438	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	458	VAL
1	C	460	LEU
1	C	462	ASP
1	C	469	THR
1	C	473	CYS
1	C	532	LEU
1	C	541	GLU
1	C	570	LEU
1	C	574	ASN
1	C	588	ASN
1	C	605	SER
1	C	613	LEU
1	C	617	ILE
1	C	625	THR
1	D	206	LEU
1	D	208	GLU
1	D	223	GLN
1	D	226	LEU
1	D	232	LYS
1	D	234	THR
1	D	236	LEU
1	D	267	MSE
1	D	268	ARG
1	D	350	THR
1	D	360	THR
1	D	379	ASP
1	D	385	LEU
1	D	436	ASN
1	D	455	GLU
1	D	458	VAL
1	D	459	THR
1	D	460	LEU
1	D	469	THR
1	D	473	CYS
1	D	532	LEU
1	D	570	LEU
1	D	574	ASN
1	D	584	MSE
1	D	605	SER
1	D	613	LEU
1	D	617	ILE
1	D	618	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	625	THR
1	D	633	ASN
1	D	635	ARG
1	D	675	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	GLN
1	A	534	GLN
1	A	633	ASN
1	B	265	GLN
1	B	633	ASN
1	C	269	GLN
1	D	269	GLN
1	D	271	HIS
1	D	436	ASN
1	D	569	GLN
1	D	633	ASN
1	D	668	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	ACT	C	1685	-	1,3,3	5.06	1 (100%)	0,3,3	0.00	-
2	ACT	D	1684	-	1,3,3	3.01	1 (100%)	0,3,3	0.00	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1685	ACT	CH3-C	5.06	1.55	1.48
2	D	1684	ACT	CH3-C	3.01	1.52	1.48

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	441/516 (85%)	-0.08	6 (1%)	75	69	24, 57, 98, 125	0
1	B	442/516 (85%)	-0.07	3 (0%)	87	84	26, 59, 101, 134	0
1	C	447/516 (86%)	0.01	7 (1%)	72	65	31, 68, 115, 150	0
1	D	451/516 (87%)	0.04	7 (1%)	72	65	27, 68, 117, 151	0
All	All	1781/2064 (86%)	-0.02	23 (1%)	77	72	24, 61, 111, 151	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	459	THR	3.6
1	A	207	THR	3.3
1	B	274	ILE	3.2
1	A	622	VAL	3.0
1	D	426	GLY	2.9
1	C	431	GLY	2.7
1	A	226	LEU	2.7
1	D	428	TYR	2.6
1	C	618	ARG	2.6
1	A	376	LYS	2.6
1	C	430	SER	2.6
1	C	684	SER	2.5
1	C	376	LYS	2.5
1	C	429	TYR	2.4
1	D	448	VAL	2.4
1	D	588	ASN	2.3
1	B	269	GLN	2.3
1	D	507	VAL	2.3
1	C	418	LEU	2.2
1	B	248	LYS	2.2
1	A	436	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	437	LEU	2.1
1	A	208	GLU	2.1

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 carbohydrates 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	ACT	D	1684	4/4	0.95	0.16	61,63,64,65	0
2	ACT	C	1685	4/4	0.98	0.21	60,61,63,65	0

6.5 Other polymers (i)

There are no such residues in this entry.