Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 02:06 AM EDT

PDB ID	:	4CBH
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	:	2.51 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:

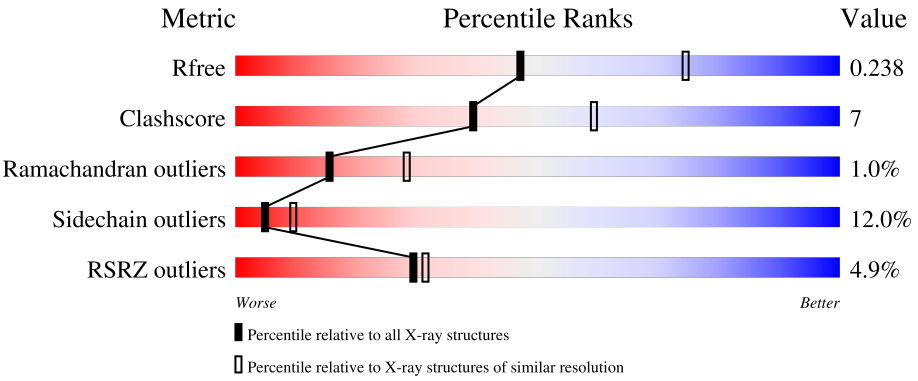
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.51 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	516	3%, 49%, 12%, ·, 35%
1	B	516	49%, 12%, ·, 36%
1	C	516	3%, 48%, 13%, ·, 36%
1	D	516	7%, 56%, 15%, ·, 25%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11813 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	333	Total	C	N	O	S	0	0	0
			2664	1693	451	502	18			
1	B	330	Total	C	N	O	S	0	0	0
			2652	1688	448	498	18			
1	C	330	Total	C	N	O	S	0	1	1
			2654	1687	452	497	18			
1	D	385	Total	C	N	O	S	0	1	1
			3075	1948	530	579	18			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	176	MET	-	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	MET	-	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

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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	MET	-	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	MET	-	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

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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 water.

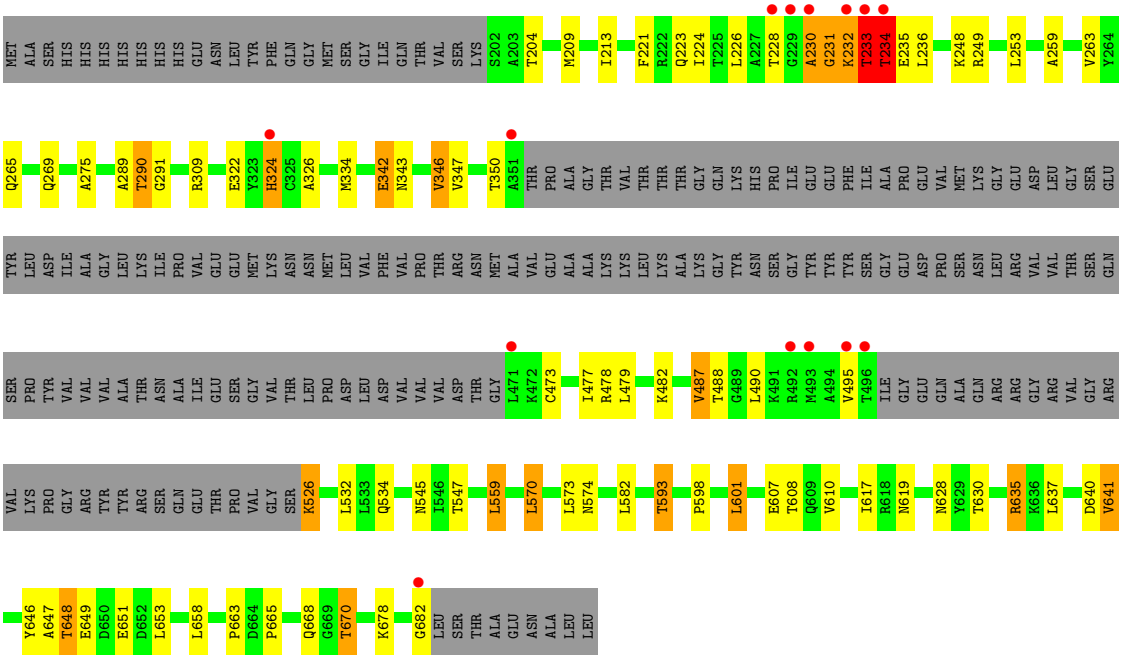
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	197	Total O 197 197	0	0
2	B	187	Total O 187 187	0	0
2	C	154	Total O 154 154	0	0
2	D	230	Total O 230 230	0	0

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.

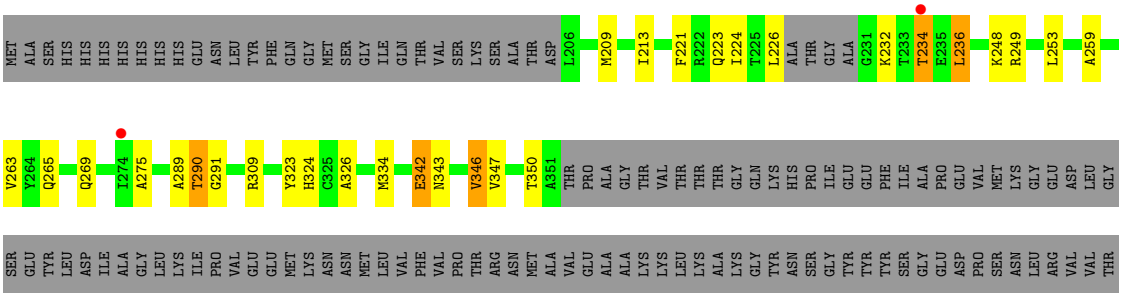
• Molecule 1: SERINE PROTEASE NS3

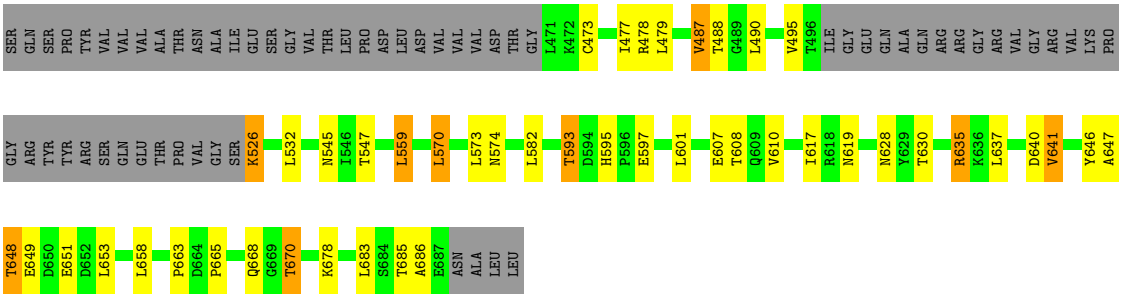
Chain A:



• Molecule 1: SERINE PROTEASE NS3

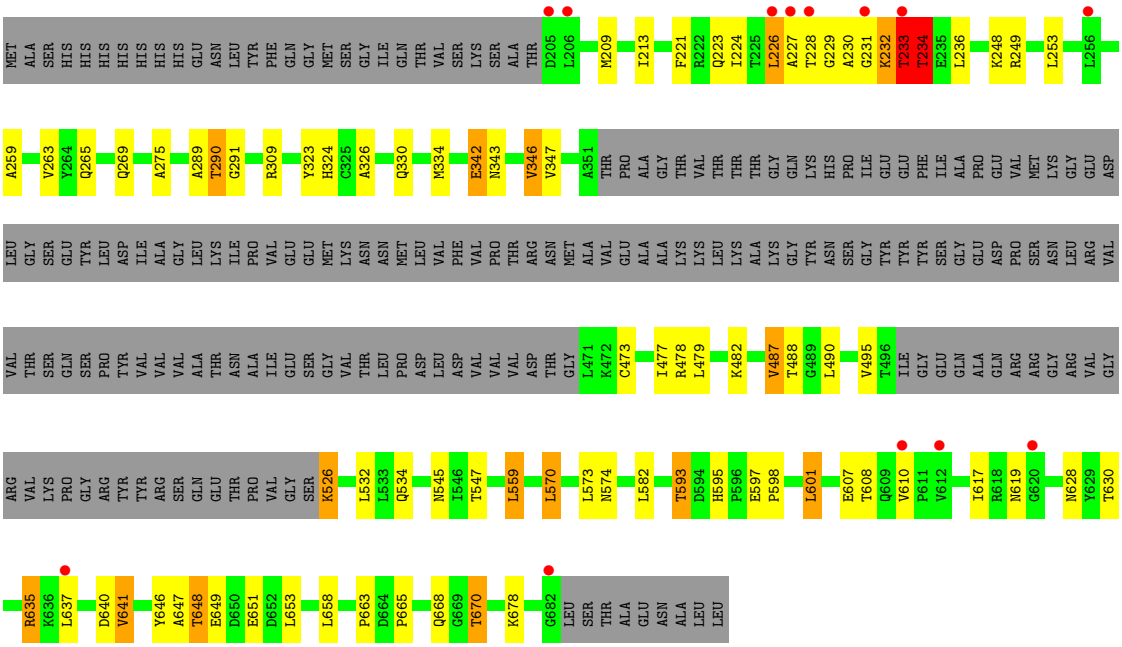
Chain B:





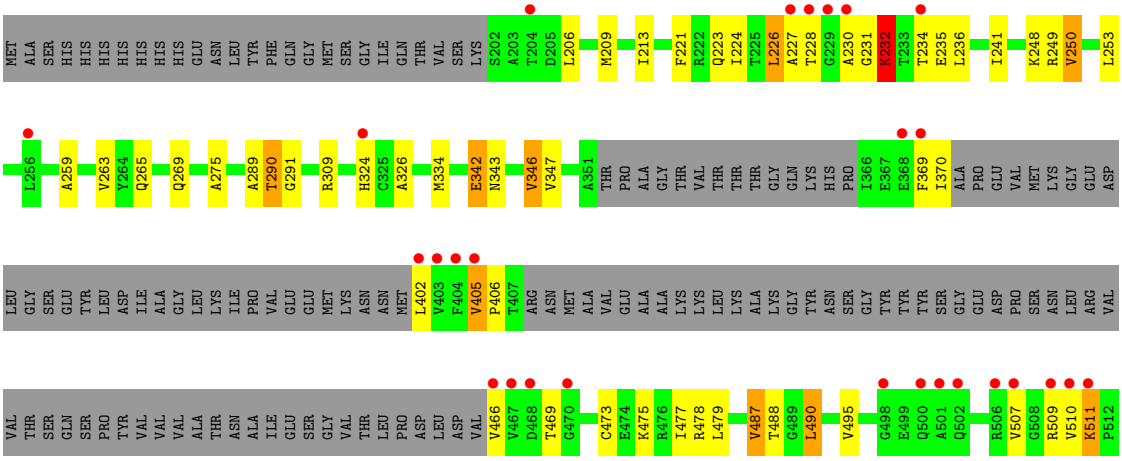
• Molecule 1: SERINE PROTEASE NS3

Chain C:



• Molecule 1: SERINE PROTEASE NS3

Chain D:




G513 R514 Y515 Y516 R517 S518 Q519 E520 V523 G524 S525 K526 L532 N545 I546 T547 L559 L570 L573 N574 L582 T593 D594 H595 P596 E597 L601 E607 T608 Q609 V610 K616 N619 N628 Y629 T630 R635 K636 L637 D640 V641 Y646 A647 T648
E649 D650 E651 L658 P663 D664 P665 Q668 Q669 T670 K678 A689 LEU LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.07Å 144.44Å 118.69Å 90.00° 92.94° 90.00°	Depositor
Resolution (Å)	72.22 – 2.51 72.22 – 2.51	Depositor EDS
% Data completeness (in resolution range)	88.6 (72.22-2.51) 88.7 (72.22-2.51)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.13.0	Depositor
R, R_{free}	0.203 , 0.232 0.215 , 0.238	Depositor DCC
R_{free} test set	3572 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	49.1	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 64.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11813	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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	0.53	0/2715	0.81	3/3671 (0.1%)
1	B	0.52	0/2702	0.77	2/3651 (0.1%)
1	C	0.54	0/2705	0.81	4/3657 (0.1%)
1	D	0.55	0/3132	0.78	1/4234 (0.0%)
All	All	0.53	0/11254	0.79	10/15213 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
All	All	0	4

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	233	THR	C-N-CA	9.71	145.98	121.70
1	C	233	THR	C-N-CA	9.48	145.40	121.70
1	A	231	GLY	C-N-CA	6.41	137.72	121.70
1	C	229	GLY	C-N-CA	5.94	136.56	121.70
1	A	290	THR	N-CA-C	5.81	126.67	111.00
1	D	290	THR	N-CA-C	5.66	126.28	111.00
1	C	290	THR	N-CA-C	5.64	126.23	111.00
1	B	290	THR	N-CA-C	5.55	125.98	111.00
1	C	234	THR	N-CA-CB	5.40	120.56	110.30
1	B	234	THR	CB-CA-C	5.32	125.97	111.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	233	THR	Peptide,Mainchain
1	C	233	THR	Peptide,Mainchain

5.2 Too-close contacts (i)

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	2664	0	2666	43	0
1	B	2652	0	2658	41	0
1	C	2654	0	2658	46	0
1	D	3075	0	3078	46	0
2	A	197	0	0	3	0
2	B	187	0	0	1	0
2	C	154	0	0	3	0
2	D	230	0	0	2	0
All	All	11813	0	11060	164	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 7.

All (164) 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:682:GLY:O	1:B:685:THR:CG2	1.75	1.35
1:A:324:HIS:CD2	1:A:350:THR:OG1	2.02	1.11
1:A:682:GLY:O	1:B:685:THR:HG22	0.93	1.09
1:A:324:HIS:HD2	1:A:350:THR:OG1	1.53	0.91
1:B:234:THR:HG21	1:B:263:VAL:HG11	1.55	0.88
1:C:227:ALA:HA	1:C:228:THR:CG2	2.03	0.87
1:D:607:GLU:OE2	1:D:670:THR:HG21	1.74	0.87
1:B:607:GLU:OE2	1:B:670:THR:HG21	1.76	0.85
1:A:665:PRO:HB3	1:A:670:THR:HG23	1.59	0.84
1:D:665:PRO:HB3	1:D:670:THR:HG23	1.60	0.84
1:B:665:PRO:HB3	1:B:670:THR:HG23	1.60	0.82
1:A:607:GLU:OE2	1:A:670:THR:HG21	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:665:PRO:HB3	1:C:670:THR:HG23	1.61	0.81
1:C:607:GLU:OE2	1:C:670:THR:HG21	1.79	0.80
1:D:226:LEU:HG	1:D:231:GLY:HA3	1.66	0.77
1:B:593:THR:HG23	1:B:630:THR:O	1.86	0.75
1:C:593:THR:HG23	1:C:630:THR:O	1.86	0.75
1:C:227:ALA:HA	1:C:228:THR:HG23	1.68	0.74
1:A:593:THR:HG23	1:A:630:THR:O	1.88	0.74
1:D:593:THR:HG23	1:D:630:THR:O	1.87	0.74
1:C:227:ALA:HA	1:C:228:THR:HG22	1.69	0.73
1:C:226:LEU:O	1:C:228:THR:HG22	1.89	0.72
1:B:213:ILE:HD11	1:B:224:ILE:HD11	1.76	0.68
1:C:309:ARG:HH21	1:C:343:ASN:HD21	1.43	0.67
1:C:213:ILE:HD11	1:C:224:ILE:HD11	1.76	0.67
1:A:309:ARG:HH21	1:A:343:ASN:HD21	1.43	0.67
2:A:2180:HOH:O	1:B:686:ALA:O	2.12	0.66
1:A:648:THR:HG21	2:A:2134:HOH:O	1.95	0.66
1:B:309:ARG:HH21	1:B:343:ASN:HD21	1.44	0.66
1:A:213:ILE:HD11	1:A:224:ILE:HD11	1.79	0.65
1:D:213:ILE:HD11	1:D:224:ILE:HD11	1.79	0.64
1:B:547:THR:HG21	1:B:570:LEU:HB3	1.81	0.63
1:C:231:GLY:O	1:C:232:LYS:HB3	1.99	0.63
1:D:309:ARG:HH21	1:D:343:ASN:HD21	1.47	0.62
1:D:547:THR:HG21	1:D:570:LEU:HB3	1.81	0.62
1:D:275:ALA:O	1:D:291:GLY:HA3	2.00	0.62
1:C:595:HIS:HD2	1:C:597:GLU:H	1.48	0.61
1:D:641:VAL:HG22	1:D:663:PRO:HD3	1.81	0.61
1:B:635:ARG:NH2	1:B:640:ASP:O	2.30	0.61
1:C:259:ALA:O	1:C:263:VAL:HG23	2.01	0.61
1:B:641:VAL:HG22	1:B:663:PRO:HD3	1.83	0.61
1:C:547:THR:HG21	1:C:570:LEU:HB3	1.83	0.61
1:C:635:ARG:NH2	1:C:640:ASP:O	2.32	0.60
1:C:326:ALA:HB3	1:C:526:LYS:HE2	1.82	0.60
1:D:259:ALA:O	1:D:263:VAL:HG23	2.02	0.60
1:D:595:HIS:HD2	1:D:597:GLU:H	1.49	0.60
1:B:275:ALA:O	1:B:291:GLY:HA3	2.01	0.60
1:C:641:VAL:HG22	1:C:663:PRO:HD3	1.84	0.60
1:A:547:THR:HG21	1:A:570:LEU:HB3	1.84	0.60
1:B:259:ALA:O	1:B:263:VAL:HG23	2.02	0.59
1:B:595:HIS:HD2	1:B:597:GLU:H	1.51	0.59
1:A:259:ALA:O	1:A:263:VAL:HG23	2.03	0.59
1:A:641:VAL:HG22	1:A:663:PRO:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:GLN:O	1:D:269:GLN:HG2	2.02	0.59
1:D:466:VAL:HG23	1:D:507:VAL:HG13	1.86	0.57
1:B:234:THR:HG21	1:B:263:VAL:CG1	2.32	0.57
1:A:249:ARG:HD2	1:A:289:ALA:O	2.05	0.56
1:A:322:GLU:HA	1:A:324:HIS:NE2	2.19	0.56
1:C:275:ALA:O	1:C:291:GLY:HA3	2.04	0.56
1:A:275:ALA:O	1:A:291:GLY:HA3	2.05	0.56
1:A:334:MET:CE	1:A:559:LEU:HD23	2.36	0.56
1:B:265:GLN:O	1:B:269:GLN:HG3	2.06	0.55
1:C:648:THR:HG22	1:C:651:GLU:H	1.71	0.55
1:D:249:ARG:HD2	1:D:289:ALA:O	2.07	0.54
1:A:648:THR:HG22	1:A:651:GLU:H	1.72	0.54
1:B:648:THR:HG22	1:B:651:GLU:H	1.73	0.54
1:D:648:THR:HG22	1:D:651:GLU:H	1.73	0.54
1:A:232:LYS:HA	1:A:233:THR:C	2.28	0.54
1:B:249:ARG:HD2	1:B:289:ALA:O	2.07	0.54
1:C:334:MET:CE	1:C:559:LEU:HD23	2.38	0.54
1:A:635:ARG:NH2	1:A:640:ASP:O	2.33	0.53
1:D:510:VAL:HG13	1:D:511:LYS:HD2	1.90	0.53
1:C:249:ARG:HD2	1:C:289:ALA:O	2.08	0.53
1:C:265:GLN:O	1:C:269:GLN:HG3	2.07	0.53
1:A:265:GLN:O	1:A:269:GLN:HG3	2.09	0.53
1:D:334:MET:CE	1:D:559:LEU:HD23	2.39	0.52
1:B:487:VAL:HA	1:B:647:ALA:O	2.10	0.52
1:B:545:ASN:CB	1:C:342:GLU:HG2	2.40	0.52
1:D:487:VAL:HA	1:D:647:ALA:O	2.09	0.52
1:C:324:HIS:HB2	2:C:2052:HOH:O	2.10	0.52
1:A:234:THR:HG22	1:A:235:GLU:N	2.25	0.51
1:D:221:PHE:HD1	1:D:346:VAL:HG22	1.75	0.51
1:B:342:GLU:HG2	1:C:545:ASN:CB	2.40	0.51
1:D:241:ILE:HD12	1:D:250:VAL:HG13	1.92	0.51
1:A:545:ASN:CB	1:D:342:GLU:HG2	2.40	0.51
1:B:334:MET:CE	1:B:559:LEU:HD23	2.41	0.51
1:B:221:PHE:HD1	1:B:346:VAL:HG22	1.75	0.51
1:A:487:VAL:HA	1:A:647:ALA:O	2.11	0.51
1:A:545:ASN:HB3	1:D:342:GLU:HG2	1.93	0.50
1:C:648:THR:HG21	2:C:2088:HOH:O	2.10	0.50
1:A:234:THR:HG22	1:A:235:GLU:HG2	1.94	0.50
1:C:477:ILE:HG22	1:C:488:THR:HG22	1.93	0.50
1:C:487:VAL:HA	1:C:647:ALA:O	2.12	0.50
1:A:477:ILE:HG22	1:A:488:THR:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:ILE:HG22	1:B:488:THR:HG22	1.93	0.49
1:B:648:THR:HG21	2:B:2116:HOH:O	2.12	0.49
1:C:221:PHE:HD1	1:C:346:VAL:HG22	1.76	0.49
1:C:228:THR:H	1:C:230:ALA:HB3	1.77	0.49
1:C:595:HIS:CD2	1:C:597:GLU:H	2.28	0.49
1:A:221:PHE:HD1	1:A:346:VAL:HG22	1.76	0.49
1:D:547:THR:H	1:D:574:ASN:ND2	2.10	0.49
1:A:547:THR:H	1:A:574:ASN:ND2	2.10	0.48
1:D:477:ILE:HG22	1:D:488:THR:HG22	1.94	0.48
1:D:635:ARG:NH2	1:D:640:ASP:O	2.33	0.48
1:D:595:HIS:CD2	1:D:597:GLU:H	2.28	0.48
1:C:547:THR:H	1:C:574:ASN:ND2	2.10	0.48
1:B:593:THR:CG2	1:B:630:THR:O	2.60	0.48
1:A:593:THR:CG2	1:A:630:THR:O	2.60	0.48
1:D:234:THR:HG22	1:D:235:GLU:HG2	1.96	0.48
1:C:232:LYS:HA	1:C:233:THR:C	2.34	0.48
1:B:323:TYR:CE2	1:B:350:THR:HB	2.49	0.47
1:B:342:GLU:HG2	1:C:545:ASN:HB3	1.95	0.47
1:B:595:HIS:CD2	1:B:597:GLU:H	2.29	0.47
1:D:234:THR:HG22	1:D:235:GLU:N	2.29	0.47
1:B:547:THR:H	1:B:574:ASN:ND2	2.12	0.47
1:A:230:ALA:HA	1:A:231:GLY:HA3	1.64	0.47
1:D:249:ARG:NH2	2:D:2020:HOH:O	2.37	0.46
1:A:342:GLU:HG2	1:D:545:ASN:CB	2.44	0.46
1:B:326:ALA:HB3	1:B:526:LYS:HE2	1.97	0.46
1:B:545:ASN:HB3	1:C:342:GLU:HG2	1.98	0.46
1:A:326:ALA:HB3	1:A:526:LYS:HE2	1.98	0.46
1:D:523:VAL:HG13	1:D:524:GLY:H	1.81	0.46
1:B:545:ASN:HB2	1:C:342:GLU:HG2	1.98	0.46
1:D:507:VAL:HB	1:D:513:GLY:HA3	1.98	0.46
1:A:248:LYS:O	1:A:290:THR:O	2.35	0.45
1:C:479:LEU:HD11	1:C:570:LEU:HD13	1.98	0.45
1:D:326:ALA:HB3	1:D:526:LYS:HE2	1.99	0.45
1:D:593:THR:CG2	1:D:630:THR:O	2.60	0.45
1:A:342:GLU:HG2	1:D:545:ASN:HB3	1.98	0.45
1:C:248:LYS:O	1:C:290:THR:O	2.34	0.44
1:A:209:MET:O	1:A:213:ILE:HG12	2.17	0.44
1:D:209:MET:O	1:D:213:ILE:HG12	2.17	0.44
1:D:248:LYS:O	1:D:290:THR:O	2.35	0.44
1:C:209:MET:O	1:C:213:ILE:HG12	2.17	0.44
1:A:479:LEU:HD11	1:A:570:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:MET:O	1:B:213:ILE:HG12	2.18	0.44
1:D:405:VAL:HG22	1:D:406:PRO:HD2	2.00	0.44
1:B:479:LEU:HD11	1:B:570:LEU:HD13	1.99	0.44
1:D:478:ARG:HD3	1:D:649:GLU:OE2	2.19	0.43
1:A:322:GLU:HA	1:A:324:HIS:CE1	2.53	0.43
1:B:478:ARG:HD3	1:B:649:GLU:OE2	2.18	0.43
1:C:593:THR:CG2	1:C:630:THR:O	2.60	0.43
1:A:478:ARG:HD3	1:A:649:GLU:OE2	2.18	0.42
1:C:478:ARG:HD3	1:C:649:GLU:OE2	2.18	0.42
1:B:342:GLU:HG2	1:C:545:ASN:HB2	2.01	0.42
1:D:479:LEU:HD11	1:D:570:LEU:HD13	2.02	0.42
1:A:598:PRO:O	1:A:601:LEU:HB2	2.19	0.42
1:A:534:GLN:NE2	2:A:2101:HOH:O	2.52	0.42
1:B:248:LYS:O	1:B:290:THR:O	2.37	0.42
1:D:369:PHE:HB2	1:D:516:TYR:HA	2.02	0.41
1:C:309:ARG:HH21	1:C:343:ASN:ND2	2.13	0.41
1:C:617:ILE:HD13	1:C:653:LEU:HD23	2.02	0.41
1:D:616:LYS:HG2	2:D:2175:HOH:O	2.20	0.41
1:C:534:GLN:NE2	2:C:2080:HOH:O	2.52	0.41
1:A:617:ILE:HD13	1:A:653:LEU:HD23	2.03	0.41
1:D:227:ALA:HB3	1:D:230:ALA:HB3	2.02	0.41
1:A:324:HIS:HD2	1:A:350:THR:CB	2.29	0.41
1:C:323:TYR:HA	1:C:330:GLN:NE2	2.35	0.41
1:B:236:LEU:HD23	1:B:236:LEU:HA	1.96	0.41
1:D:232:LYS:H	1:D:234:THR:H	1.68	0.41
1:D:475:LYS:HG2	1:D:490:LEU:HD13	2.03	0.41
1:B:617:ILE:HD13	1:B:653:LEU:HD23	2.04	0.40
1:C:598:PRO:O	1:C:601:LEU:HB2	2.21	0.40
1:D:477:ILE:HD12	1:D:479:LEU:HD21	2.04	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	327/516 (63%)	315 (96%)	7 (2%)	5 (2%)	10 18
1	B	322/516 (62%)	316 (98%)	4 (1%)	2 (1%)	25 43
1	C	325/516 (63%)	314 (97%)	7 (2%)	4 (1%)	13 24
1	D	378/516 (73%)	364 (96%)	11 (3%)	3 (1%)	19 35
All	All	1352/2064 (66%)	1309 (97%)	29 (2%)	14 (1%)	15 28

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	LYS
1	C	495	VAL
1	D	523	VAL
1	C	234	THR
1	D	524	GLY
1	A	228	THR
1	A	234	THR
1	D	232	LYS
1	A	230	ALA
1	A	619	ASN
1	B	232	LYS
1	C	232	LYS
1	C	619	ASN
1	B	619	ASN

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	289/442 (65%)	254 (88%)	35 (12%)	5 9
1	B	289/442 (65%)	256 (89%)	33 (11%)	5 11
1	C	288/442 (65%)	256 (89%)	32 (11%)	6 11
1	D	333/442 (75%)	289 (87%)	44 (13%)	4 7
All	All	1199/1768 (68%)	1055 (88%)	144 (12%)	5 9

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	THR
1	A	223	GLN
1	A	226	LEU
1	A	234	THR
1	A	236	LEU
1	A	253	LEU
1	A	324	HIS
1	A	342	GLU
1	A	346	VAL
1	A	347	VAL
1	A	473	CYS
1	A	482	LYS
1	A	487	VAL
1	A	490	LEU
1	A	495	VAL
1	A	526	LYS
1	A	532	LEU
1	A	559	LEU
1	A	570	LEU
1	A	573	LEU
1	A	582	LEU
1	A	593	THR
1	A	601	LEU
1	A	608	THR
1	A	610	VAL
1	A	628	ASN
1	A	635	ARG
1	A	637	LEU
1	A	641	VAL
1	A	646	TYR
1	A	648	THR
1	A	658	LEU
1	A	668	GLN
1	A	670	THR
1	A	678	LYS
1	B	223	GLN
1	B	226	LEU
1	B	236	LEU
1	B	253	LEU
1	B	324	HIS
1	B	342	GLU
1	B	346	VAL

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Mol	Chain	Res	Type
1	B	347	VAL
1	B	473	CYS
1	B	487	VAL
1	B	490	LEU
1	B	495	VAL
1	B	526	LYS
1	B	532	LEU
1	B	559	LEU
1	B	570	LEU
1	B	573	LEU
1	B	582	LEU
1	B	593	THR
1	B	601	LEU
1	B	608	THR
1	B	610	VAL
1	B	628	ASN
1	B	635	ARG
1	B	637	LEU
1	B	641	VAL
1	B	646	TYR
1	B	648	THR
1	B	658	LEU
1	B	668	GLN
1	B	670	THR
1	B	678	LYS
1	B	683	LEU
1	C	223	GLN
1	C	226	LEU
1	C	234	THR
1	C	236	LEU
1	C	253	LEU
1	C	342	GLU
1	C	346	VAL
1	C	347	VAL
1	C	473	CYS
1	C	482	LYS
1	C	487	VAL
1	C	490	LEU
1	C	526	LYS
1	C	532	LEU
1	C	559	LEU
1	C	570	LEU

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Mol	Chain	Res	Type
1	C	573	LEU
1	C	582	LEU
1	C	593	THR
1	C	601	LEU
1	C	608	THR
1	C	610	VAL
1	C	628	ASN
1	C	635	ARG
1	C	637	LEU
1	C	641	VAL
1	C	646	TYR
1	C	648	THR
1	C	658	LEU
1	C	668	GLN
1	C	670	THR
1	C	678	LYS
1	D	206	LEU
1	D	223	GLN
1	D	226	LEU
1	D	228	THR
1	D	232	LYS
1	D	236	LEU
1	D	250	VAL
1	D	253	LEU
1	D	324	HIS
1	D	342	GLU
1	D	346	VAL
1	D	347	VAL
1	D	370	ILE
1	D	402	LEU
1	D	405	VAL
1	D	469	THR
1	D	473	CYS
1	D	487	VAL
1	D	490	LEU
1	D	495	VAL
1	D	509	ARG
1	D	511	LYS
1	D	517	ARG
1	D	519	GLN
1	D	526	LYS
1	D	532	LEU

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Mol	Chain	Res	Type
1	D	559	LEU
1	D	570	LEU
1	D	573	LEU
1	D	582	LEU
1	D	593	THR
1	D	601	LEU
1	D	608	THR
1	D	610	VAL
1	D	628	ASN
1	D	635	ARG
1	D	637	LEU
1	D	641	VAL
1	D	646	TYR
1	D	648	THR
1	D	658	LEU
1	D	668	GLN
1	D	670	THR
1	D	678	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	324	HIS
1	A	343	ASN
1	A	534	GLN
1	A	536	GLN
1	A	574	ASN
1	A	588	ASN
1	A	600	GLN
1	A	628	ASN
1	B	343	ASN
1	B	574	ASN
1	B	588	ASN
1	B	595	HIS
1	B	628	ASN
1	C	343	ASN
1	C	534	GLN
1	C	574	ASN
1	C	595	HIS
1	C	600	GLN
1	C	628	ASN
1	D	305	GLN

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Mol	Chain	Res	Type
1	D	343	ASN
1	D	574	ASN
1	D	588	ASN
1	D	595	HIS
1	D	600	GLN
1	D	628	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	333/516 (64%)	0.36	14 (4%) 36 39	33, 53, 112, 149	0
1	B	330/516 (63%)	0.24	2 (0%) 89 90	30, 54, 105, 125	0
1	C	330/516 (63%)	0.38	13 (3%) 39 42	33, 56, 101, 129	0
1	D	385/516 (74%)	0.58	38 (9%) 7 7	31, 54, 117, 146	0
All	All	1378/2064 (66%)	0.40	67 (4%) 29 31	30, 54, 111, 149	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	228	THR	9.4
1	D	516	TYR	8.1
1	D	515	TYR	8.0
1	D	523	VAL	7.5
1	D	227	ALA	7.5
1	C	233	THR	6.6
1	D	403	VAL	6.0
1	C	226	LEU	5.5
1	D	229	GLY	4.6
1	D	402	LEU	4.6
1	A	233	THR	4.3
1	C	227	ALA	4.3
1	D	228	THR	4.3
1	D	509	ARG	4.3
1	D	502	GLN	4.2
1	D	467	VAL	4.1
1	D	369	PHE	4.1
1	D	510	VAL	3.8
1	A	351	ALA	3.8
1	D	524	GLY	3.8
1	C	682	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	520	GLU	3.7
1	A	492	ARG	3.6
1	D	514	ARG	3.5
1	A	228	THR	3.4
1	A	682	GLY	3.4
1	D	501	ALA	3.2
1	D	506	ARG	3.1
1	D	204	THR	3.1
1	D	368	GLU	3.1
1	D	507	VAL	3.1
1	D	517	ARG	3.1
1	A	234	THR	3.0
1	D	405	VAL	3.0
1	D	404	PHE	2.9
1	D	468	ASP	2.9
1	A	229	GLY	2.9
1	B	234	THR	2.9
1	A	471	LEU	2.8
1	C	612	VAL	2.8
1	D	511	LYS	2.8
1	A	230	ALA	2.7
1	D	518	SER	2.7
1	C	637	LEU	2.7
1	D	466	VAL	2.6
1	A	496	THR	2.5
1	A	493	MET	2.5
1	A	232	LYS	2.5
1	D	513	GLY	2.5
1	D	256	LEU	2.4
1	D	498	GLY	2.4
1	D	234	THR	2.3
1	D	230	ALA	2.3
1	C	610	VAL	2.3
1	D	470	GLY	2.3
1	B	274	ILE	2.2
1	C	206	LEU	2.2
1	A	324	HIS	2.2
1	D	619	ASN	2.2
1	C	256	LEU	2.2
1	D	324	HIS	2.1
1	D	519	GLN	2.1
1	A	495	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	500	GLN	2.1
1	C	231	GLY	2.0
1	C	620	GLY	2.0
1	C	205	ASP	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.