wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 07:51 AM EDT

PDB ID	:	1SLQ
Title	:	Crystal structure of the trimeric state of the rhesus rotavirus VP4 membrane interaction domain, VP5CT
Authors	:	Dormitzer, P.R.; Nason, E.B.; Prasad, B.V.V.; Harrison, S.C.
Deposited on	:	2004-03-06
Resolution	:	3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

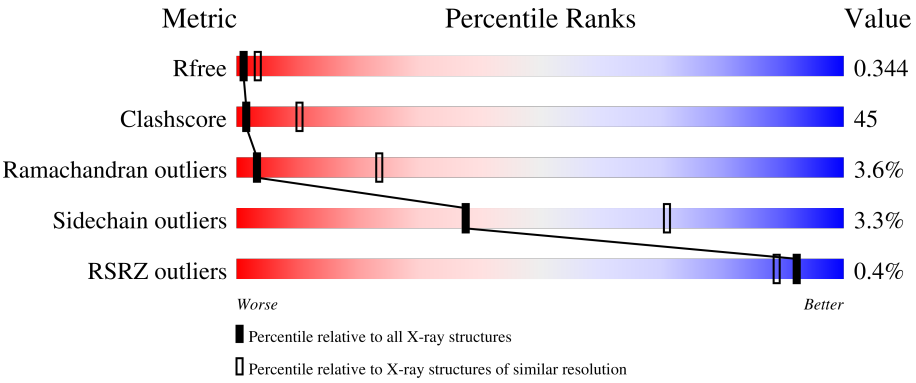
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	278	37% 58%
1	B	278	35% 57% 5%
1	C	278	41% 51%
1	D	278	% 37% 55%
1	E	278	39% 50% 6%

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Mol	Chain	Length	Quality of chain
1	F	278	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 12772 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 VP4.

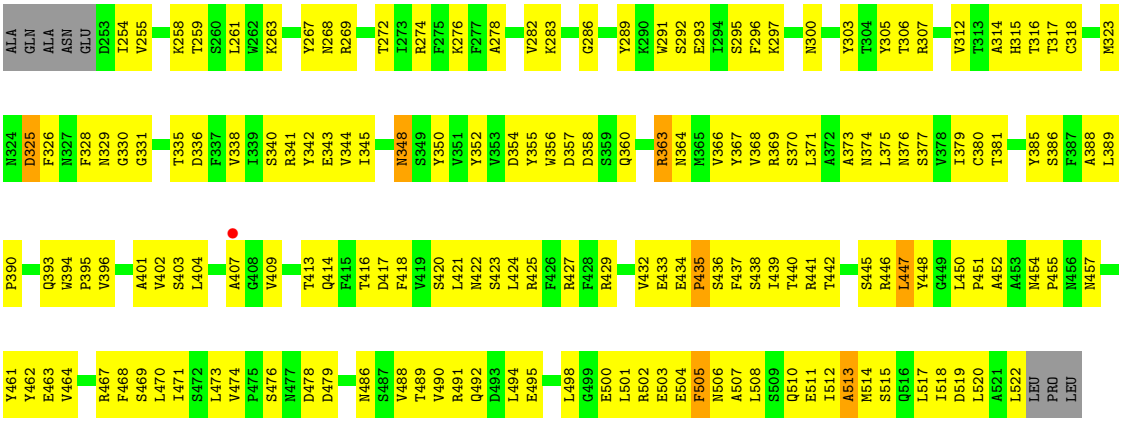
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	13	0	0
			2148	1362	361	418	7			
1	B	269	Total	C	N	O	S	0	0	0
			2140	1358	360	415	7			
1	C	266	Total	C	N	O	S	0	0	0
			2120	1342	357	414	7			
1	D	267	Total	C	N	O	S	26	0	0
			2127	1349	358	413	7			
1	E	267	Total	C	N	O	S	0	0	0
			2126	1348	358	413	7			
1	F	265	Total	C	N	O	S	98	0	0
			2111	1337	356	411	7			

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.

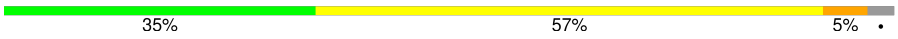
• Molecule 1: VP4

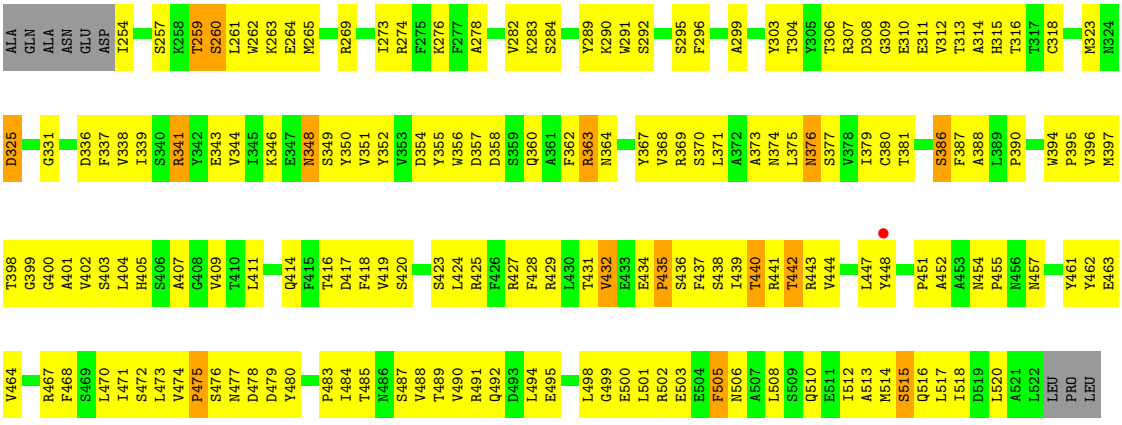
Chain A:



• Molecule 1: VP4

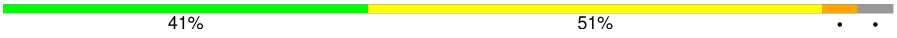
Chain B:

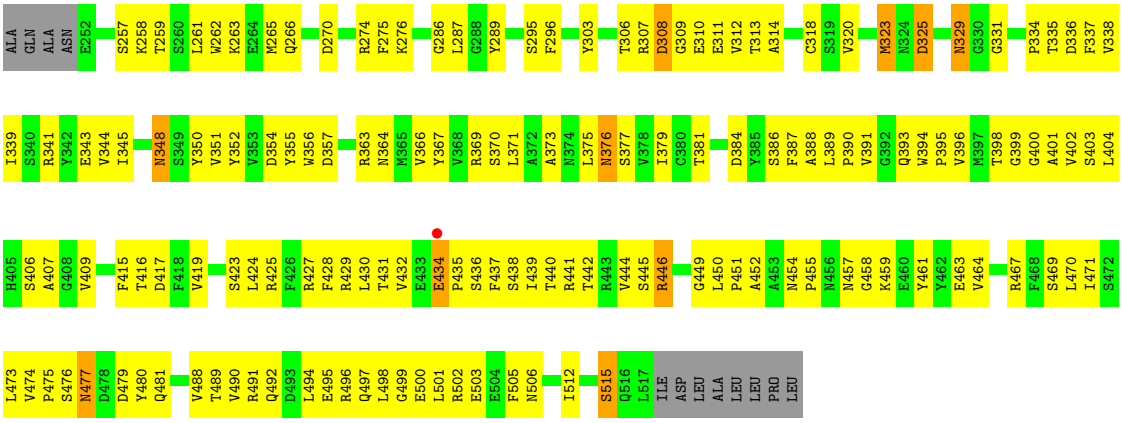




• Molecule 1: VP4

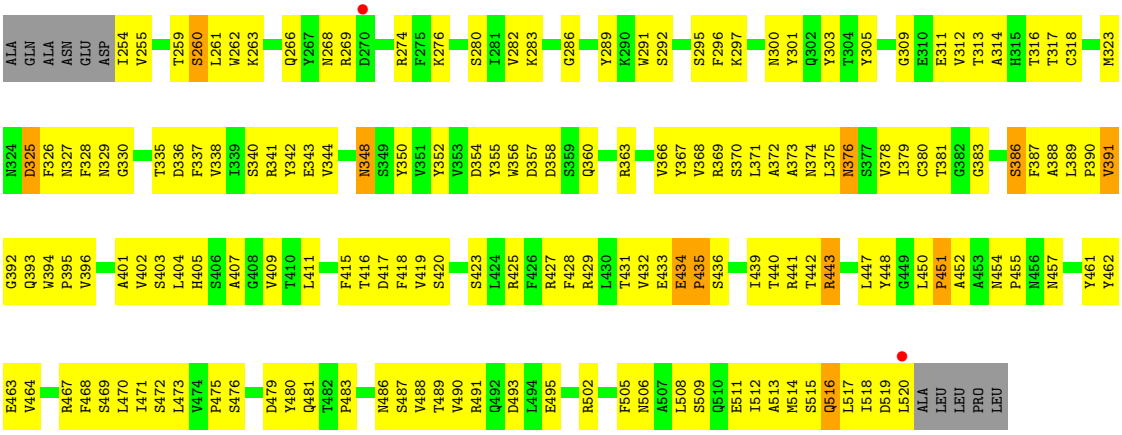
Chain C:





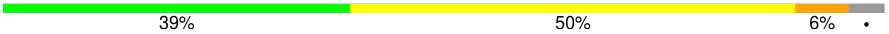
• Molecule 1: VP4

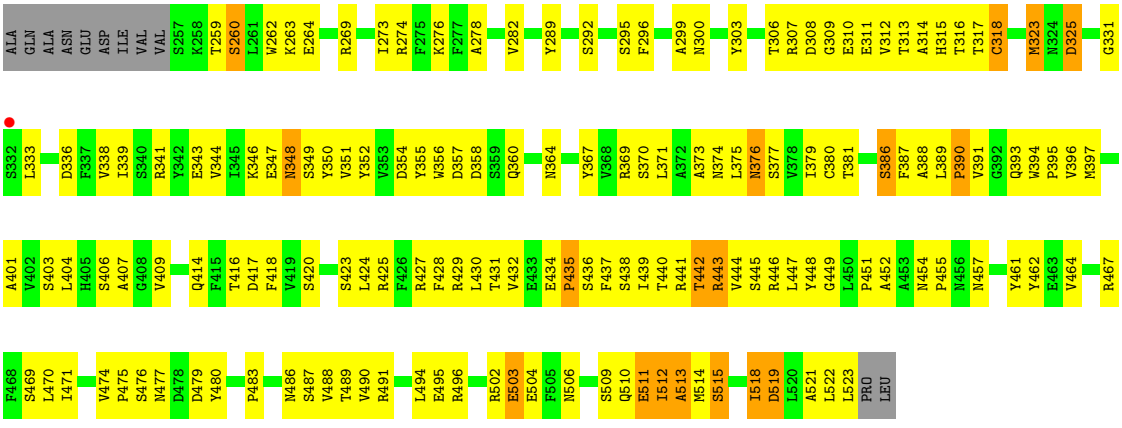
Chain D:



• Molecule 1: VP4

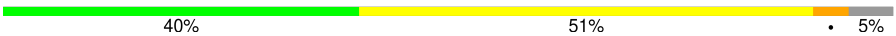
Chain E:

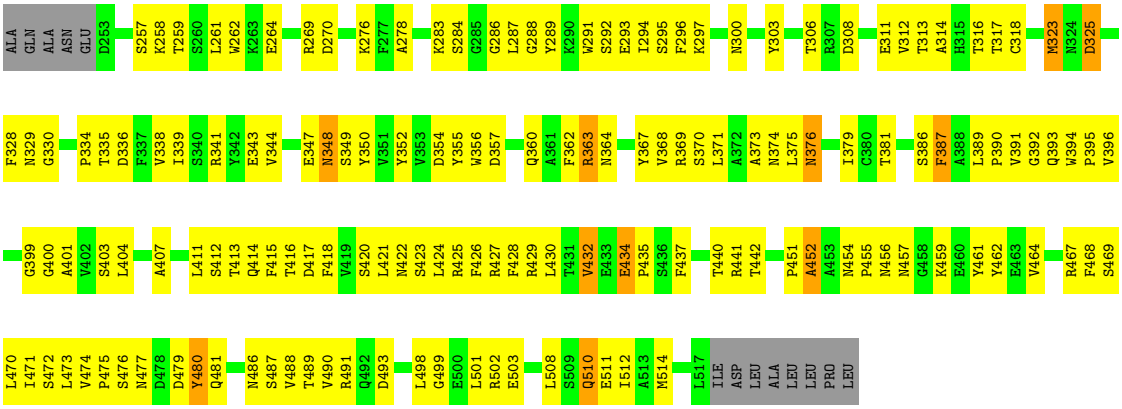




• Molecule 1: VP4

Chain F:




ALA GLN ALA ASN GLU D253
S257 K258 T259 S260 L261 W262 K263 E264 R269 D270 K276 F277 A278 K283 S284 G285 G286 L287 G288 Y289 K290 W291 S292 E293 I294 S295 F296 K297 N300 Y303 T306 R307 D308 E311 V312 T313 A314 H315 T316 T317 C318 M323 N324 D325
F328 N329 G330 P334 T335 D336 F337 V338 I339 S340 R341 Y342 E343 V344 E347 N348 S349 Y350 V351 Y352 V353 D354 Y355 W356 D357 Q360 A361 F362 R363 N364 Y367 V368 R369 S370 L371 A372 A373 N374 L375 M376 I379 C380 T381 S386 F387 A388 L389 P390 V391 G392 Q393 W394 P395 V396
G399 G400 A401 V402 S403 L404 A407 L411 S412 T413 Q414 F415 T416 D417 F418 V419 S420 L421 N422 S423 L424 R425 F426 R427 F428 R429 L430 T431 V432 E433 E434 P435 S436 F437 T440 R441 T442 P451 A452 A453 N454 P455 N456 N457 G458 K459 E460 Y461 Y462 E463 V464 R467 F468 S469
L470 I471 S472 L473 V474 P475 S476 N477 D478 D479 Y480 Q481 N486 S487 V488 T489 V490 R491 Q492 D493 L498 G499 E500 L501 R502 E503 L508 S509 Q510 E511 I512 A513 M514 L517 ILE ASP LEU ALA LEU LEU PRO LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 2 2	Depositor
Cell constants a, b, c, α, β, γ	244.84Å 244.84Å 104.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 19.98 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-3.20) 99.8 (19.98-3.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	12.30 (at 3.22Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.308 , 0.338 0.313 , 0.344	Depositor DCC
R_{free} test set	2625 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	92.3	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 78.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12772	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 70.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0016e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.55	0/2196	0.78	0/2983
1	B	0.55	0/2188	0.75	0/2972
1	C	0.55	0/2168	0.77	0/2944
1	D	0.53	0/2175	0.78	0/2954
1	E	0.54	0/2174	0.76	0/2952
1	F	0.54	0/2159	0.79	1/2932 (0.0%)
All	All	0.54	0/13060	0.77	1/17737 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	434	GLU	N-CA-C	5.42	125.65	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	2148	0	2077	224	0
1	B	2140	0	2073	213	0
1	C	2120	0	2041	213	0
1	D	2127	0	2057	225	0
1	E	2126	0	2055	205	0
1	F	2111	0	2035	194	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12772	0	12338	1118	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 45.

The worst 5 of 1118 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:286:GLY:O	1:E:510:GLN:HA	1.42	1.18
1:D:289:TYR:CD2	1:D:335:THR:HA	1.78	1.18
1:A:439:ILE:HB	1:A:442:THR:HG21	1.26	1.18
1:D:289:TYR:HD2	1:D:335:THR:HA	1.01	1.15
1:A:289:TYR:CD2	1:A:335:THR:HA	1.84	1.13

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	268/278 (96%)	223 (83%)	38 (14%)	7 (3%)	5	31
1	B	267/278 (96%)	222 (83%)	32 (12%)	13 (5%)	2	17
1	C	264/278 (95%)	225 (85%)	32 (12%)	7 (3%)	5	30
1	D	265/278 (95%)	216 (82%)	38 (14%)	11 (4%)	3	20
1	E	265/278 (95%)	219 (83%)	35 (13%)	11 (4%)	3	20
1	F	263/278 (95%)	227 (86%)	28 (11%)	8 (3%)	4	28
All	All	1592/1668 (95%)	1332 (84%)	203 (13%)	57 (4%)	3	23

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	435	PRO
1	A	513	ALA
1	B	440	THR
1	B	475	PRO
1	D	260	SER

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	238/244 (98%)	231 (97%)	7 (3%)	42	74
1	B	237/244 (97%)	230 (97%)	7 (3%)	41	73
1	C	235/244 (96%)	229 (97%)	6 (3%)	46	76
1	D	236/244 (97%)	228 (97%)	8 (3%)	37	70
1	E	235/244 (96%)	224 (95%)	11 (5%)	26	62
1	F	234/244 (96%)	227 (97%)	7 (3%)	41	73
All	All	1415/1464 (97%)	1369 (97%)	46 (3%)	38	71

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	318	CYS
1	E	442	THR
1	E	323	MET
1	E	386	SER
1	E	512	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	374	ASN
1	E	497	GLN
1	D	324	ASN
1	E	422	ASN

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Mol	Chain	Res	Type
1	F	348	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	268/278 (96%)	-0.28	1 (0%)	92	89	35, 86, 141, 172	0
1	B	269/278 (96%)	-0.39	1 (0%)	92	89	28, 87, 135, 164	0
1	C	266/278 (95%)	-0.34	1 (0%)	92	89	38, 88, 146, 189	0
1	D	264/278 (94%)	-0.30	2 (0%)	86	78	34, 90, 142, 177	0
1	E	267/278 (96%)	-0.33	1 (0%)	92	89	44, 87, 142, 175	0
1	F	253/278 (91%)	-0.37	0	100	100	33, 85, 133, 167	0
All	All	1587/1668 (95%)	-0.34	6 (0%)	92	89	28, 87, 141, 189	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	434	GLU	2.8
1	D	270	ASP	2.3
1	D	520	LEU	2.3
1	E	332	SER	2.3
1	A	407	ALA	2.2

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.