Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 02:35 am BST

PDB ID	:	5V1D
Title	:	Complex structure of the bovine PERK luminal domain and its substrate peptide
Authors	:	Wang, P.; Li, J.; Sha, B.
Deposited on	:	2017-03-02
Resolution	:	2.80 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:

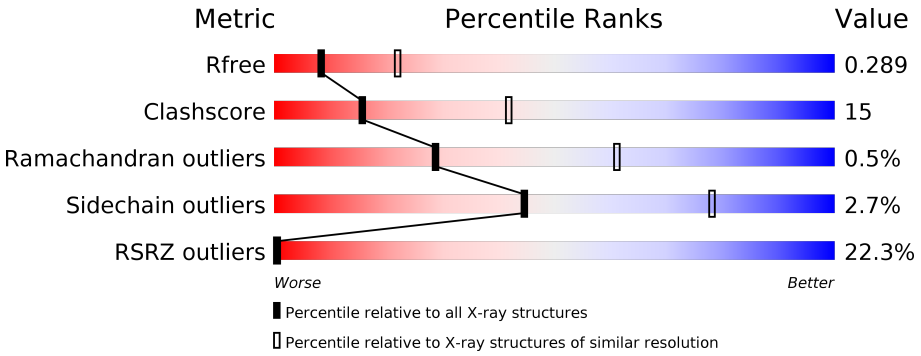
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	326	13% 39% 19% • 41%
1	B	326	15% 36% 22% 42%
1	C	326	14% 53% 21% • 25%
1	D	326	15% 53% 22% • 24%
2	E	12	50% 58% 17% 25%
2	F	12	42% 17% 42% 17% 25%

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Mol	Chain	Length	Quality of chain
2	G	12	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7270 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 eIF2AK3 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	0	0	0
			1511	975	254	277	5			
1	B	190	Total	C	N	O	S	0	0	0
			1477	949	251	272	5			
1	C	244	Total	C	N	O	S	0	0	0
			1916	1219	321	368	8			
1	D	247	Total	C	N	O	S	0	0	0
			1944	1237	328	371	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	337	SER	CYS	engineered mutation	UNP A5D791
B	337	SER	CYS	engineered mutation	UNP A5D791
C	337	SER	CYS	engineered mutation	UNP A5D791
D	337	SER	CYS	engineered mutation	UNP A5D791

- Molecule 2 is a protein called 12-mer peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	9	Total	C	N	O	0	0	0
			83	58	14	11			
2	F	9	Total	C	N	O	0	0	0
			83	58	14	11			
2	G	9	Total	C	N	O	0	0	0
			83	58	14	11			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	43	Total	O	0	0
			43	43		

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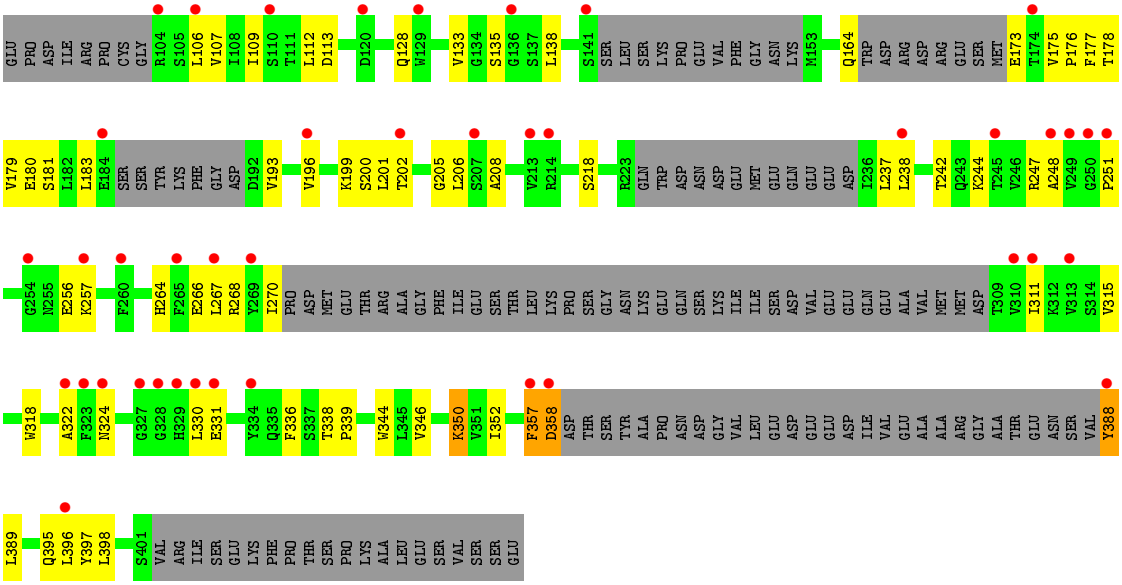
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	2	Total O 2 2	0	0
3	B	24	Total O 24 24	0	0
3	C	53	Total O 53 53	0	0
3	F	1	Total O 1 1	0	0
3	D	46	Total O 46 46	0	0
3	G	4	Total O 4 4	0	0

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.

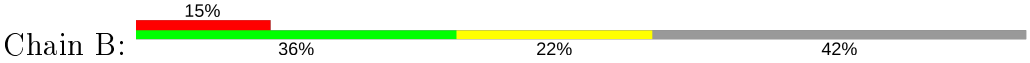
- Molecule 1: eIF2AK3 protein

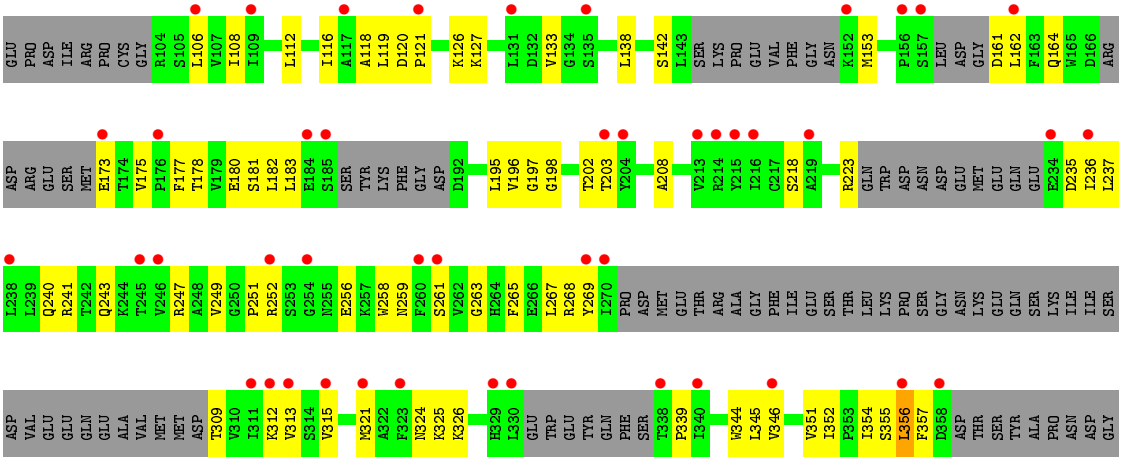
Chain A:

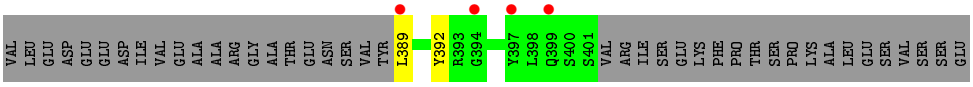


- Molecule 1: eIF2AK3 protein

Chain B:

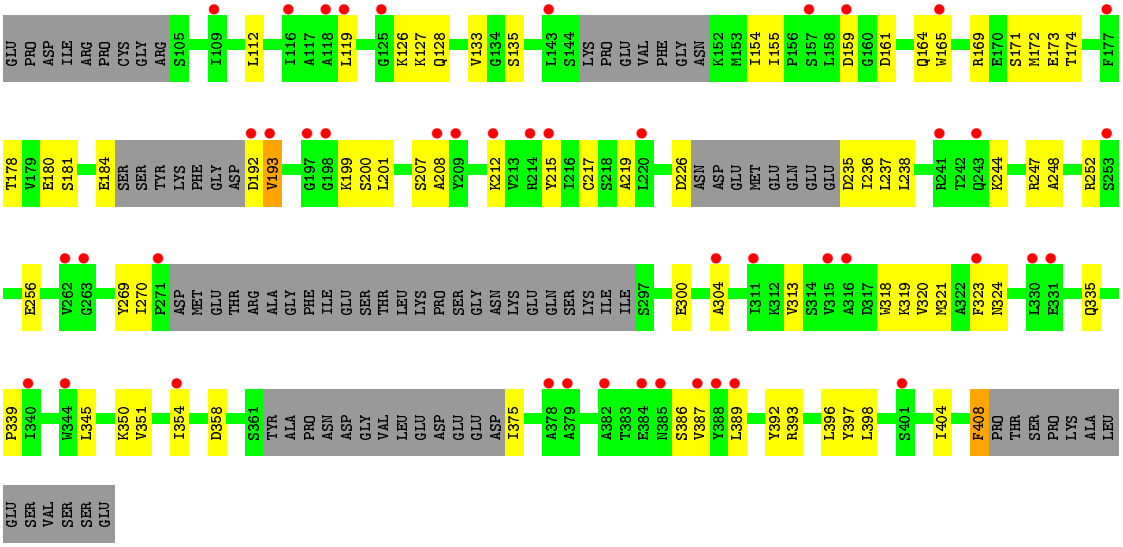






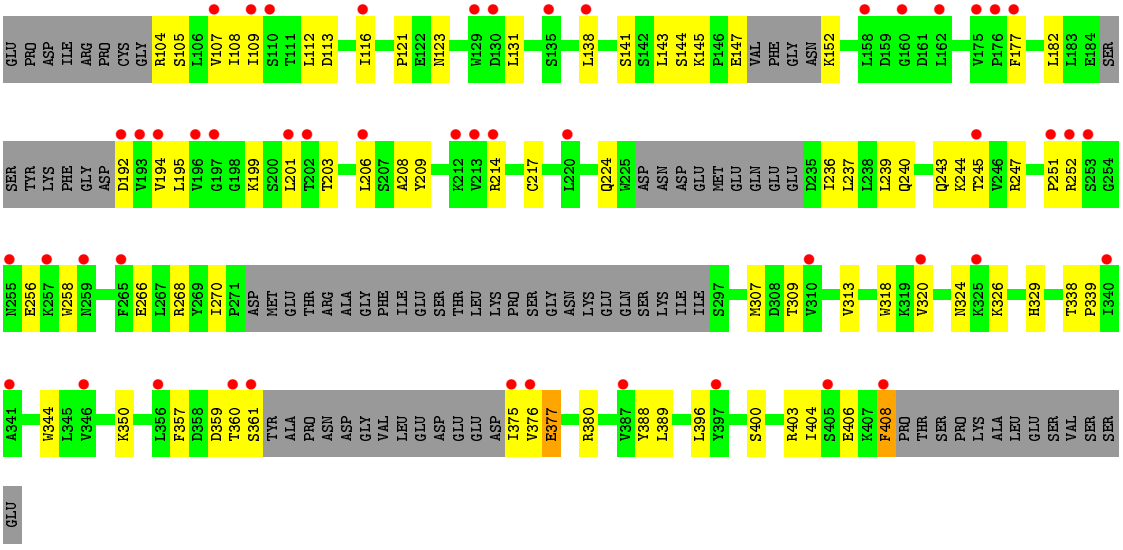
- Molecule 1: eIF2AK3 protein

Chain C:



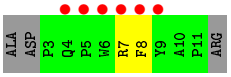
- Molecule 1: eIF2AK3 protein

Chain D:



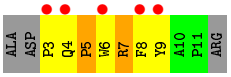
- Molecule 2: 12-mer peptide

Chain E:



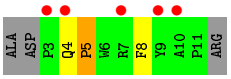
- Molecule 2: 12-mer peptide

Chain F:



- Molecule 2: 12-mer peptide

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.75Å 161.55Å 104.78Å 90.00° 106.84° 90.00°	Depositor
Resolution (Å)	47.89 – 2.80 47.89 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.4 (47.89-2.80) 91.4 (47.89-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	124.80 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.240 , 0.291 0.241 , 0.289	Depositor DCC
R_{free} test set	2024 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å^2)	59.7	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 33.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.419 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	7270	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% 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	0.31	0/1538	0.52	0/2073
1	B	0.31	0/1499	0.51	0/2016
1	C	0.31	0/1950	0.48	0/2632
1	D	0.34	0/1979	0.50	0/2670
2	E	0.40	0/89	0.50	0/122
2	F	0.35	0/89	0.58	0/122
2	G	0.35	0/89	0.56	0/122
All	All	0.32	0/7233	0.51	0/9757

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	1511	0	1528	49	0
1	B	1477	0	1504	54	0
1	C	1916	0	1899	51	0
1	D	1944	0	1934	57	0
2	E	83	0	75	4	0
2	F	83	0	75	8	0
2	G	83	0	75	3	0
3	A	43	0	0	7	0
3	B	24	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	53	0	0	3	0
3	D	46	0	0	10	0
3	E	2	0	0	1	0
3	F	1	0	0	0	0
3	G	4	0	0	0	0
All	All	7270	0	7090	208	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 15.

All (208) 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:C:389:LEU:HD23	2:F:5:PRO:HA	1.62	0.81
1:A:112:LEU:HD12	1:A:339:PRO:HB2	1.65	0.79
1:D:266:GLU:HB3	1:D:268:ARG:HH22	1.49	0.77
1:D:359:ASP:HA	1:D:404:ILE:HG23	1.66	0.76
1:C:386:SER:HB3	2:F:8:PHE:HB3	1.68	0.74
1:D:408:PHE:HD1	3:D:507:HOH:O	1.72	0.71
1:D:357:PHE:HB3	1:D:404:ILE:HG21	1.72	0.70
1:D:152:LYS:NZ	3:D:502:HOH:O	2.22	0.70
1:A:202:THR:HG23	1:A:218:SER:HB3	1.73	0.69
1:C:155:ILE:HD12	1:C:396:LEU:HB2	1.74	0.69
1:B:178:THR:H	1:B:181:SER:HB2	1.57	0.68
1:C:236:ILE:HD11	1:C:270:ILE:HD12	1.73	0.68
1:A:178:THR:H	1:A:181:SER:HB2	1.59	0.67
1:B:202:THR:HG23	1:B:218:SER:HB3	1.78	0.66
1:D:192:ASP:N	3:D:505:HOH:O	2.27	0.66
1:D:377:GLU:HG2	1:D:404:ILE:HD11	1.77	0.66
1:B:119:LEU:HD22	1:B:127:LYS:HA	1.79	0.64
1:C:192:ASP:N	3:C:504:HOH:O	2.31	0.64
1:C:208:ALA:HA	1:C:237:LEU:HG	1.80	0.63
2:F:6:TRP:O	2:F:7:ARG:NH1	2.33	0.62
1:B:112:LEU:HD22	1:B:339:PRO:HB2	1.81	0.62
1:B:197:GLY:HA2	1:C:219:ALA:HB2	1.80	0.62
1:B:249:VAL:HG12	1:B:256:GLU:HA	1.81	0.62
1:B:252:ARG:HH21	1:C:235:ASP:N	1.99	0.60
1:A:389:LEU:HD11	1:A:396:LEU:HB3	1.83	0.60
1:A:196:VAL:HG23	1:A:247:ARG:HB2	1.84	0.60
1:B:183:LEU:HB3	1:C:201:LEU:HD13	1.83	0.60
1:D:104:ARG:NE	1:D:104:ARG:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ILE:HG23	1:B:116:ILE:HD11	1.83	0.59
1:B:256:GLU:OE1	1:B:259:ASN:ND2	2.36	0.59
1:C:392:TYR:OH	1:C:393:ARG:NH1	2.35	0.59
1:C:319:LYS:HG2	1:C:335:GLN:HA	1.85	0.59
1:D:113:ASP:H	1:D:338:THR:HG21	1.68	0.59
1:D:375:ILE:HA	1:D:408:PHE:HE1	1.68	0.58
1:A:205:GLY:N	3:A:510:HOH:O	2.36	0.58
1:B:345:LEU:N	1:B:352:ILE:O	2.30	0.58
1:D:109:ILE:HD13	1:D:320:VAL:HG21	1.84	0.58
1:B:196:VAL:HG21	1:C:217:CYS:HB3	1.86	0.58
1:B:175:VAL:HG12	1:B:177:PHE:H	1.68	0.58
1:C:159:ASP:O	1:C:244:LYS:NZ	2.37	0.58
1:B:138:LEU:O	1:B:263:GLY:N	2.35	0.57
1:D:361:SER:HB2	1:D:406:GLU:H	1.69	0.57
1:A:176:PRO:HB2	3:A:523:HOH:O	2.03	0.57
1:B:309:THR:N	3:B:505:HOH:O	2.37	0.57
1:B:153:MET:N	1:B:153:MET:SD	2.76	0.57
1:A:133:VAL:HG23	1:A:135:SER:H	1.68	0.56
1:C:375:ILE:HA	1:C:408:PHE:HB3	1.87	0.56
1:C:126:LYS:NZ	1:C:128:GLN:OE1	2.39	0.55
1:B:389:LEU:N	3:B:506:HOH:O	2.39	0.54
1:B:180:GLU:HA	1:B:183:LEU:HD12	1.89	0.54
1:D:247:ARG:NE	1:D:256:GLU:OE2	2.38	0.54
1:C:119:LEU:HD23	1:C:127:LYS:HA	1.88	0.54
1:A:208:ALA:HA	1:A:237:LEU:HD22	1.90	0.54
1:B:309:THR:N	3:B:507:HOH:O	2.40	0.54
1:D:208:ALA:HA	1:D:237:LEU:HG	1.89	0.54
1:A:106:LEU:HD21	1:A:128:GLN:HG3	1.90	0.54
1:A:264:HIS:NE2	1:A:266:GLU:OE1	2.38	0.54
1:A:193:VAL:HG21	1:A:248:ALA:HB1	1.90	0.53
1:A:388:TYR:HB3	2:E:8:PHE:HA	1.90	0.53
1:C:173:GLU:HG2	1:C:174:THR:H	1.74	0.53
1:C:199:LYS:HG3	1:C:244:LYS:HG2	1.91	0.53
1:B:161:ASP:OD1	1:B:162:LEU:N	2.39	0.52
1:A:388:TYR:O	1:A:398:LEU:HA	2.09	0.52
1:C:350:LYS:NZ	3:C:501:HOH:O	2.22	0.52
2:F:4:GLN:O	2:F:9:TYR:OH	2.28	0.52
1:A:175:VAL:HG23	1:A:177:PHE:H	1.74	0.52
1:D:194:VAL:HG13	1:D:251:PRO:HA	1.91	0.52
1:B:120:ASP:HB3	1:B:126:LYS:HG2	1.91	0.52
1:C:193:VAL:HG21	1:C:248:ALA:HB1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:ARG:NH1	1:C:171:SER:HB3	2.25	0.51
1:A:112:LEU:HD23	1:A:138:LEU:HB2	1.91	0.51
1:C:235:ASP:N	3:C:515:HOH:O	2.43	0.51
1:D:240:GLN:HE22	1:D:268:ARG:HE	1.58	0.51
1:D:199:LYS:HG3	1:D:244:LYS:HG2	1.92	0.51
2:G:4:GLN:HB3	2:G:5:PRO:HD2	1.91	0.51
1:B:235:ASP:N	1:B:235:ASP:OD2	2.43	0.51
1:C:207:SER:HG	1:C:212:LYS:H	1.58	0.51
1:D:112:LEU:HA	1:D:138:LEU:HD12	1.92	0.51
1:A:206:LEU:HB2	1:A:237:LEU:HD21	1.93	0.51
1:A:200:SER:O	1:A:242:THR:HA	2.11	0.51
1:C:133:VAL:HG23	1:C:135:SER:H	1.75	0.51
1:C:178:THR:N	1:C:181:SER:OG	2.43	0.50
1:C:313:VAL:HG12	1:C:354:ILE:HG22	1.92	0.50
1:C:247:ARG:NH1	1:C:256:GLU:OE1	2.45	0.50
1:A:107:VAL:HG12	1:A:109:ILE:HD11	1.92	0.50
1:B:344:TRP:HA	1:B:354:ILE:H	1.76	0.50
1:A:350:LYS:NZ	1:A:352:ILE:HD11	2.28	0.49
1:B:325:LYS:NZ	3:B:510:HOH:O	2.45	0.49
1:B:236:ILE:HG13	1:C:252:ARG:HG3	1.93	0.49
1:A:344:TRP:N	3:A:507:HOH:O	2.46	0.49
1:B:312:LYS:HE3	1:B:357:PHE:CE2	2.48	0.49
1:D:116:ILE:O	1:D:131:LEU:N	2.45	0.49
1:B:198:GLY:HA3	1:C:200:SER:HA	1.95	0.49
1:D:182:LEU:HD23	1:D:195:LEU:HD13	1.93	0.48
1:B:106:LEU:HD13	1:B:118:ALA:HB1	1.95	0.48
1:B:112:LEU:HD23	1:B:392:TYR:HB2	1.95	0.48
1:D:240:GLN:CD	1:D:268:ARG:HH21	2.17	0.48
1:C:300:GLU:N	1:C:300:GLU:OE2	2.47	0.48
1:D:375:ILE:HG13	1:D:408:PHE:HE1	1.79	0.48
2:G:4:GLN:HB3	2:G:5:PRO:CD	2.44	0.47
1:B:106:LEU:HA	1:B:121:PRO:HD3	1.97	0.47
1:A:395:GLN:NE2	1:A:396:LEU:O	2.48	0.47
1:D:318:TRP:CG	1:D:339:PRO:HA	2.49	0.47
2:F:7:ARG:HG3	2:F:8:PHE:H	1.79	0.47
1:B:315:VAL:HG12	1:B:357:PHE:O	2.14	0.47
1:A:180:GLU:HA	1:A:183:LEU:HD12	1.96	0.47
1:C:387:VAL:O	2:F:8:PHE:HA	2.15	0.47
1:D:105:SER:N	3:D:509:HOH:O	2.47	0.47
1:A:315:VAL:HG12	1:A:357:PHE:O	2.14	0.47
1:B:182:LEU:HB3	1:B:195:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ILE:HD13	1:A:336:PHE:CZ	2.50	0.47
1:D:243:GLN:NE2	3:D:511:HOH:O	2.47	0.47
1:D:224:GLN:N	1:D:224:GLN:OE1	2.48	0.46
1:C:180:GLU:OE2	1:C:244:LYS:NZ	2.43	0.46
1:D:375:ILE:HA	1:D:408:PHE:CE1	2.50	0.46
1:B:268:ARG:HH11	1:B:351:VAL:HB	1.80	0.46
1:A:237:LEU:H	1:A:237:LEU:HD23	1.80	0.46
1:D:107:VAL:HG23	1:D:121:PRO:HD3	1.96	0.46
1:D:236:ILE:HB	1:D:270:ILE:HB	1.97	0.46
1:A:350:LYS:NZ	3:A:514:HOH:O	2.46	0.46
1:C:165:TRP:HE3	1:C:172:MET:HB2	1.79	0.46
1:D:307:MET:O	1:D:309:THR:HG23	2.16	0.46
1:C:165:TRP:HE1	2:F:3:PRO:HD3	1.81	0.46
1:A:238:LEU:HD12	1:A:268:ARG:HB2	1.97	0.46
1:B:344:TRP:CE2	3:B:504:HOH:O	2.69	0.46
1:C:318:TRP:CE2	1:C:339:PRO:HG3	2.51	0.46
1:C:387:VAL:HG13	1:C:398:LEU:HD22	1.98	0.46
1:D:206:LEU:HD11	1:D:239:LEU:HD12	1.98	0.46
1:D:375:ILE:HG13	1:D:408:PHE:CE1	2.51	0.45
1:C:226:ASP:N	1:C:226:ASP:OD2	2.47	0.45
1:D:240:GLN:NE2	1:D:268:ARG:HH21	2.14	0.45
1:D:113:ASP:N	1:D:338:THR:HG21	2.30	0.45
1:D:400:SER:O	1:D:400:SER:OG	2.32	0.45
1:B:251:PRO:O	1:C:215:TYR:OH	2.21	0.45
1:A:247:ARG:NH1	1:A:256:GLU:OE2	2.49	0.45
1:A:318:TRP:CE2	1:A:339:PRO:HG3	2.51	0.45
1:A:389:LEU:HD11	1:A:396:LEU:HD23	1.99	0.45
1:D:141:SER:OG	1:D:141:SER:O	2.35	0.45
1:A:358:ASP:HB3	2:E:8:PHE:CE2	2.52	0.45
1:B:346:VAL:HG12	1:B:351:VAL:HG22	1.99	0.45
1:D:313:VAL:HG22	1:D:320:VAL:HG22	1.98	0.45
1:A:267:LEU:O	3:A:501:HOH:O	2.21	0.45
1:C:321:MET:HE3	1:C:323:PHE:HZ	1.83	0.45
1:B:241:ARG:HG3	1:B:265:PHE:CZ	2.52	0.44
1:D:123:ASN:O	3:D:501:HOH:O	2.20	0.44
1:A:358:ASP:HB3	2:E:8:PHE:HE2	1.82	0.44
1:D:357:PHE:HB3	1:D:404:ILE:CG2	2.43	0.44
1:B:223:ARG:HD2	1:B:223:ARG:HA	1.90	0.44
1:D:318:TRP:CD1	1:D:318:TRP:N	2.84	0.44
1:B:108:ILE:HG21	1:B:267:LEU:HD13	1.99	0.44
1:A:238:LEU:HD13	1:D:194:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:LEU:HD11	1:D:396:LEU:HD22	1.99	0.44
1:A:109:ILE:HD13	1:A:336:PHE:HZ	1.83	0.43
1:D:214:ARG:HD3	1:D:214:ARG:HA	1.73	0.43
1:B:313:VAL:HG12	1:B:356:LEU:HA	2.01	0.43
1:B:313:VAL:HG11	1:B:356:LEU:HD22	1.99	0.43
1:C:304:ALA:HB1	1:C:345:LEU:HD23	2.00	0.43
1:D:324:ASN:ND2	1:D:326:LYS:O	2.47	0.43
1:B:344:TRP:NE1	3:B:504:HOH:O	2.36	0.43
1:A:199:LYS:HD3	1:A:201:LEU:HD11	1.99	0.43
1:C:269:TYR:HB2	1:C:351:VAL:HG13	2.01	0.43
1:C:313:VAL:HB	1:C:320:VAL:HG22	2.00	0.43
1:A:251:PRO:HB2	1:D:270:ILE:HG21	2.01	0.43
1:D:403:ARG:HD3	1:D:404:ILE:N	2.34	0.43
1:B:142:SER:O	1:B:258:TRP:HA	2.19	0.42
1:B:355:SER:HB2	1:B:357:PHE:CZ	2.54	0.42
1:C:387:VAL:HG22	1:C:398:LEU:HB3	2.00	0.42
1:A:331:GLU:OE1	3:A:503:HOH:O	2.21	0.42
1:C:389:LEU:HD12	1:C:397:TYR:O	2.19	0.42
1:D:147:GLU:N	3:D:502:HOH:O	2.52	0.42
1:D:143:LEU:HD23	1:D:144:SER:N	2.34	0.42
1:D:177:PHE:CD1	1:D:182:LEU:HD11	2.53	0.42
1:D:258:TRP:HB2	3:D:503:HOH:O	2.18	0.42
1:A:112:LEU:HD11	1:A:397:TYR:CZ	2.54	0.42
1:D:203:THR:HG22	1:D:217:CYS:HB2	2.02	0.42
1:D:388:TYR:HB2	2:G:8:PHE:CE1	2.54	0.42
1:A:257:LYS:NZ	3:A:517:HOH:O	2.52	0.42
1:C:112:LEU:HD11	1:C:397:TYR:CZ	2.54	0.42
1:C:161:ASP:OD1	1:C:161:ASP:N	2.52	0.42
1:C:207:SER:OG	1:C:212:LYS:N	2.47	0.42
1:D:408:PHE:N	3:D:507:HOH:O	2.50	0.42
1:A:238:LEU:HD11	1:A:270:ILE:HD11	2.01	0.42
1:A:311:ILE:HA	1:A:322:ALA:HA	2.02	0.42
1:B:133:VAL:HG21	1:B:265:PHE:HZ	1.84	0.42
1:B:106:LEU:O	1:B:346:VAL:HG22	2.19	0.42
1:B:203:THR:OG1	1:B:240:GLN:OE1	2.34	0.41
1:B:324:ASN:OD1	1:B:326:LYS:N	2.48	0.41
1:D:240:GLN:OE1	1:D:240:GLN:N	2.52	0.41
1:D:108:ILE:N	1:D:344:TRP:O	2.53	0.41
1:B:164:GLN:O	1:B:173:GLU:HG3	2.21	0.41
2:F:4:GLN:HA	2:F:5:PRO:HD3	1.82	0.41
1:B:243:GLN:NE2	1:B:261:SER:OG	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:VAL:O	1:B:247:ARG:N	2.52	0.41
1:B:235:ASP:OD1	1:B:269:TYR:OH	2.25	0.41
1:C:238:LEU:HA	1:C:238:LEU:HD23	1.79	0.41
1:D:104:ARG:N	3:D:509:HOH:O	2.53	0.41
1:B:208:ALA:HA	1:B:237:LEU:HD12	2.02	0.41
1:B:252:ARG:NH2	1:C:235:ASP:OD2	2.54	0.41
1:A:238:LEU:HD12	1:A:268:ARG:HE	1.86	0.41
1:C:154:ILE:HD13	1:C:164:GLN:HB2	2.02	0.41
1:C:358:ASP:O	1:C:404:ILE:HG22	2.21	0.41
1:A:164:GLN:HG2	1:A:173:GLU:O	2.21	0.41
1:A:179:VAL:HG11	1:A:244:LYS:HB3	2.02	0.41
1:A:324:ASN:HB2	1:A:331:GLU:HG2	2.03	0.41
1:A:113:ASP:H	1:A:338:THR:HG21	1.87	0.40
1:A:346:VAL:HA	1:A:350:LYS:O	2.21	0.40
2:E:7:ARG:NH2	3:E:101:HOH:O	2.40	0.40
1:D:360:THR:HG22	1:D:404:ILE:O	2.22	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	179/326 (55%)	168 (94%)	11 (6%)	0	100 100
1	B	172/326 (53%)	163 (95%)	9 (5%)	0	100 100
1	C	232/326 (71%)	217 (94%)	15 (6%)	0	100 100
1	D	235/326 (72%)	210 (89%)	23 (10%)	2 (1%)	17 46
2	E	7/12 (58%)	4 (57%)	3 (43%)	0	100 100
2	F	7/12 (58%)	5 (71%)	1 (14%)	1 (14%)	0 0
2	G	7/12 (58%)	4 (57%)	2 (29%)	1 (14%)	0 0
All	All	839/1340 (63%)	771 (92%)	64 (8%)	4 (0%)	29 61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	5	PRO
2	F	5	PRO
1	D	145	LYS
1	D	376	VAL

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	166/285 (58%)	161 (97%)	5 (3%)	41 75
1	B	164/285 (58%)	162 (99%)	2 (1%)	71 92
1	C	212/285 (74%)	208 (98%)	4 (2%)	57 85
1	D	215/285 (75%)	206 (96%)	9 (4%)	30 63
2	E	8/10 (80%)	8 (100%)	0	100 100
2	F	8/10 (80%)	7 (88%)	1 (12%)	4 14
2	G	8/10 (80%)	8 (100%)	0	100 100
All	All	781/1170 (67%)	760 (97%)	21 (3%)	44 78

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	330	LEU
1	A	350	LYS
1	A	357	PHE
1	A	358	ASP
1	A	388	TYR
1	B	321	MET
1	B	356	LEU
1	C	184	GLU
1	C	193	VAL
1	C	324	ASN
1	C	408	PHE
2	F	7	ARG

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Mol	Chain	Res	Type
1	D	201	LEU
1	D	209	TYR
1	D	245	THR
1	D	252	ARG
1	D	329	HIS
1	D	350	LYS
1	D	377	GLU
1	D	380	ARG
1	D	408	PHE

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

Mol	Chain	Res	Type
2	G	4	GLN

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 carbohydrates 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	193/326 (59%)	1.32	42 (21%)	0 0	43, 58, 70, 83	0
1	B	190/326 (58%)	1.47	49 (25%)	0 0	43, 61, 79, 100	0
1	C	244/326 (74%)	1.26	45 (18%)	1 1	34, 50, 65, 71	0
1	D	247/326 (75%)	1.25	49 (19%)	1 0	37, 49, 64, 79	0
2	E	9/12 (75%)	2.95	6 (66%)	0 0	71, 76, 82, 84	0
2	F	9/12 (75%)	2.59	5 (55%)	0 0	63, 68, 77, 87	0
2	G	9/12 (75%)	3.06	5 (55%)	0 0	51, 59, 70, 73	0
All	All	901/1340 (67%)	1.36	201 (22%)	0 0	34, 54, 73, 100	0

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	322	ALA	8.5
1	A	329	HIS	7.7
1	B	216	ILE	7.3
2	G	7	ARG	6.9
2	F	4	GLN	6.7
1	B	311	ILE	6.4
2	E	8	PHE	6.1
1	D	201	LEU	5.7
1	A	323	PHE	5.2
2	G	9	TYR	5.2
1	B	313	VAL	5.1
1	B	389	LEU	5.1
1	A	330	LEU	5.1
1	D	360	THR	5.0
1	A	324	ASN	4.8
1	B	184	GLU	4.7
1	C	159	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	312	LYS	4.6
1	C	262	VAL	4.5
1	C	382	ALA	4.5
1	A	311	ILE	4.4
1	A	104	ARG	4.4
1	D	375	ILE	4.4
1	A	327	GLY	4.3
1	C	209	TYR	4.3
2	F	3	PRO	4.2
1	B	219	ALA	4.1
1	B	131	LEU	4.1
1	B	204	TYR	4.1
1	B	157	SER	4.0
1	A	388	TYR	4.0
1	B	329	HIS	3.9
1	B	397	TYR	3.8
1	D	253	SER	3.8
2	G	4	GLN	3.8
1	D	397	TYR	3.8
1	C	379	ALA	3.8
1	A	328	GLY	3.7
1	A	257	LYS	3.7
1	D	158	LEU	3.7
2	E	9	TYR	3.7
1	C	198	GLY	3.6
1	A	249	VAL	3.6
2	E	7	ARG	3.6
1	A	260	PHE	3.5
1	B	176	PRO	3.5
1	D	408	PHE	3.5
1	A	120	ASP	3.5
1	D	376	VAL	3.5
1	C	401	SER	3.5
1	D	194	VAL	3.4
1	B	152	LYS	3.4
1	D	341	ALA	3.4
1	A	265	PHE	3.4
1	B	323	PHE	3.4
1	D	192	ASP	3.3
1	B	399	GLN	3.3
1	B	260	PHE	3.3
1	C	125	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
2	E	5	PRO	3.3
1	B	358	ASP	3.3
1	B	270	ILE	3.2
1	C	109	ILE	3.2
1	B	214	ARG	3.2
1	B	238	LEU	3.1
1	D	340	ILE	3.1
1	B	356	LEU	3.1
1	D	356	LEU	3.1
2	E	6	TRP	3.1
1	C	208	ALA	3.1
2	F	6	TRP	3.1
1	D	175	VAL	3.1
1	D	257	LYS	3.0
1	B	330	LEU	3.0
1	C	304	ALA	3.0
1	C	263	GLY	2.9
2	G	3	PRO	2.9
1	C	385	ASN	2.9
1	C	214	ARG	2.9
1	C	378	ALA	2.9
1	C	192	ASP	2.9
1	A	207	SER	2.9
1	B	394	GLY	2.9
1	D	135	SER	2.9
1	B	213	VAL	2.9
1	D	197	GLY	2.9
2	F	8	PHE	2.9
1	A	357	PHE	2.9
1	D	346	VAL	2.9
1	C	271	PRO	2.9
1	A	358	ASP	2.8
1	D	220	LEU	2.8
1	C	340	ILE	2.8
1	A	251	PRO	2.8
1	A	106	LEU	2.8
1	B	246	VAL	2.8
1	C	220	LEU	2.8
1	C	311	ILE	2.8
1	A	250	GLY	2.8
1	C	243	GLN	2.7
1	D	176	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	384	GLU	2.7
1	C	165	TRP	2.7
1	B	315	VAL	2.7
1	A	141	SER	2.7
1	A	174	THR	2.7
1	D	196	VAL	2.7
1	B	162	LEU	2.7
1	C	389	LEU	2.6
1	D	206	LEU	2.6
1	D	387	VAL	2.6
1	C	197	GLY	2.6
1	D	325	LYS	2.5
1	D	138	LEU	2.5
1	D	214	ARG	2.5
1	C	344	TRP	2.5
1	A	396	LEU	2.5
1	B	261	SER	2.5
2	E	4	GLN	2.5
1	B	321	MET	2.5
1	A	184	GLU	2.5
1	A	214	ARG	2.5
1	C	316	ALA	2.5
1	B	269	TYR	2.5
1	B	106	LEU	2.5
2	F	9	TYR	2.5
1	B	203	THR	2.4
1	C	241	ARG	2.4
1	D	202	THR	2.4
2	G	10	ALA	2.4
1	D	116	ILE	2.4
1	A	110	SER	2.4
1	C	157	SER	2.4
1	C	354	ILE	2.4
1	D	129	TRP	2.4
1	A	136	GLY	2.4
1	D	107	VAL	2.4
1	C	212	LYS	2.4
1	C	315	VAL	2.4
1	B	173	GLU	2.4
1	C	118	ALA	2.4
1	D	251	PRO	2.3
1	A	334	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	245	THR	2.3
1	B	254	GLY	2.3
1	A	213	VAL	2.3
1	D	193	VAL	2.3
1	B	121	PRO	2.3
1	C	253	SER	2.3
1	C	215	TYR	2.3
1	D	213	VAL	2.3
1	D	320	VAL	2.3
1	B	185	SER	2.3
1	D	212	LYS	2.3
1	B	156	PRO	2.3
1	B	245	THR	2.3
1	A	267	LEU	2.2
1	D	245	THR	2.2
1	C	387	VAL	2.2
1	D	259	ASN	2.2
1	B	117	ALA	2.2
1	D	310	VAL	2.2
1	D	405	SER	2.2
1	C	143	LEU	2.2
1	D	162	LEU	2.2
1	A	313	VAL	2.2
1	A	238	LEU	2.2
1	D	252	ARG	2.2
1	C	331	GLU	2.1
1	B	346	VAL	2.1
1	C	388	TYR	2.1
1	A	248	ALA	2.1
1	D	255	ASN	2.1
1	D	160	GLY	2.1
1	A	196	VAL	2.1
1	A	269	TYR	2.1
1	B	236	ILE	2.1
1	B	340	ILE	2.1
1	C	323	PHE	2.1
1	D	130	ASP	2.1
1	C	116	ILE	2.1
1	B	234	GLU	2.1
1	D	110	SER	2.1
1	A	254	GLY	2.1
1	C	193	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	109	ILE	2.1
1	D	177	PHE	2.1
1	A	331	GLU	2.1
1	D	361	SER	2.1
1	C	119	LEU	2.0
1	C	330	LEU	2.0
1	A	310	VAL	2.0
1	B	215	TYR	2.0
1	A	202	THR	2.0
1	B	135	SER	2.0
1	A	129	TRP	2.0
1	C	177	PHE	2.0
1	B	109	ILE	2.0
1	B	338	THR	2.0
1	D	265	PHE	2.0
1	B	252	ARG	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 carbohydrates 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.