



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 29, 2024 – 12:16 PM EDT

PDB ID : 3VAC
Title : Crystal Structure of the CFA/I Enterotoxigenic E. coli adhesin CfaE mutant G168D
Authors : Liu, Y.; Esser, L.; Xia, D.
Deposited on : 2011-12-29
Resolution : 2.60 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	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

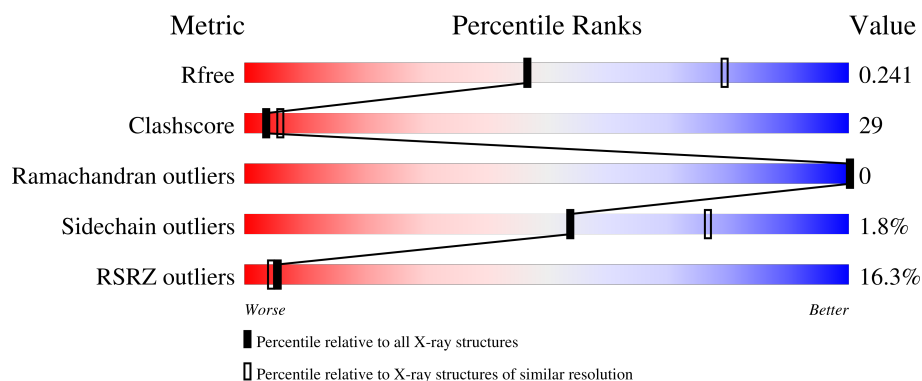
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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 $\leq 5\%$. 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	356	<div> <div>16%</div> <div>70%</div> <div>29%</div> </div>
1	B	356	<div> <div>16%</div> <div>62%</div> <div>37%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5785 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 CFA/I fimbrial subunit E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	0	0
			2768	1733	479	545	11			
1	B	356	Total	C	N	O	S	0	0	0
			2768	1733	479	545	11			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	168	ASP	GLY	engineered mutation	UNP P25734
A	361	ASP	-	expression tag	UNP P25734
A	362	ASN	-	expression tag	UNP P25734
A	363	LYS	-	expression tag	UNP P25734
A	364	GLN	-	expression tag	UNP P25734
A	365	VAL	-	expression tag	UNP P25734
A	366	GLU	-	expression tag	UNP P25734
A	367	LYS	-	expression tag	UNP P25734
A	368	ASN	-	expression tag	UNP P25734
A	369	ILE	-	expression tag	UNP P25734
A	370	THR	-	expression tag	UNP P25734
A	371	VAL	-	expression tag	UNP P25734
A	372	THR	-	expression tag	UNP P25734
A	373	ALA	-	expression tag	UNP P25734
A	374	SER	-	expression tag	UNP P25734
A	375	VAL	-	expression tag	UNP P25734
A	376	ASP	-	expression tag	UNP P25734
A	377	PRO	-	expression tag	UNP P25734
A	378	VAL	-	expression tag	UNP P25734
B	168	ASP	GLY	engineered mutation	UNP P25734
B	361	ASP	-	expression tag	UNP P25734
B	362	ASN	-	expression tag	UNP P25734
B	363	LYS	-	expression tag	UNP P25734
B	364	GLN	-	expression tag	UNP P25734
B	365	VAL	-	expression tag	UNP P25734

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	366	GLU	-	expression tag	UNP P25734
B	367	LYS	-	expression tag	UNP P25734
B	368	ASN	-	expression tag	UNP P25734
B	369	ILE	-	expression tag	UNP P25734
B	370	THR	-	expression tag	UNP P25734
B	371	VAL	-	expression tag	UNP P25734
B	372	THR	-	expression tag	UNP P25734
B	373	ALA	-	expression tag	UNP P25734
B	374	SER	-	expression tag	UNP P25734
B	375	VAL	-	expression tag	UNP P25734
B	376	ASP	-	expression tag	UNP P25734
B	377	PRO	-	expression tag	UNP P25734
B	378	VAL	-	expression tag	UNP P25734

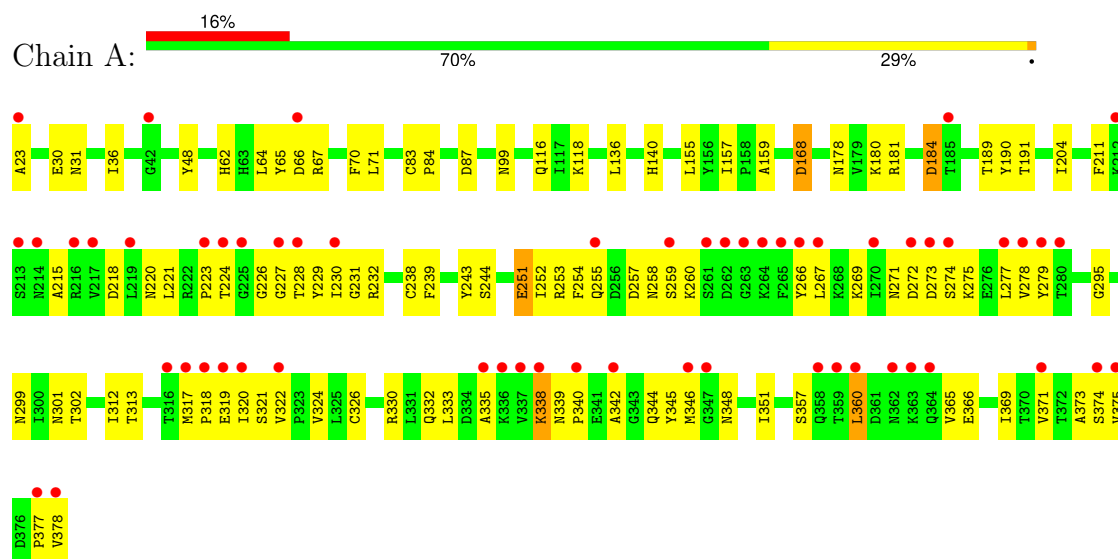
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	133	Total 133	O 133	0	0
2	B	116	Total 116	O 116	0	0

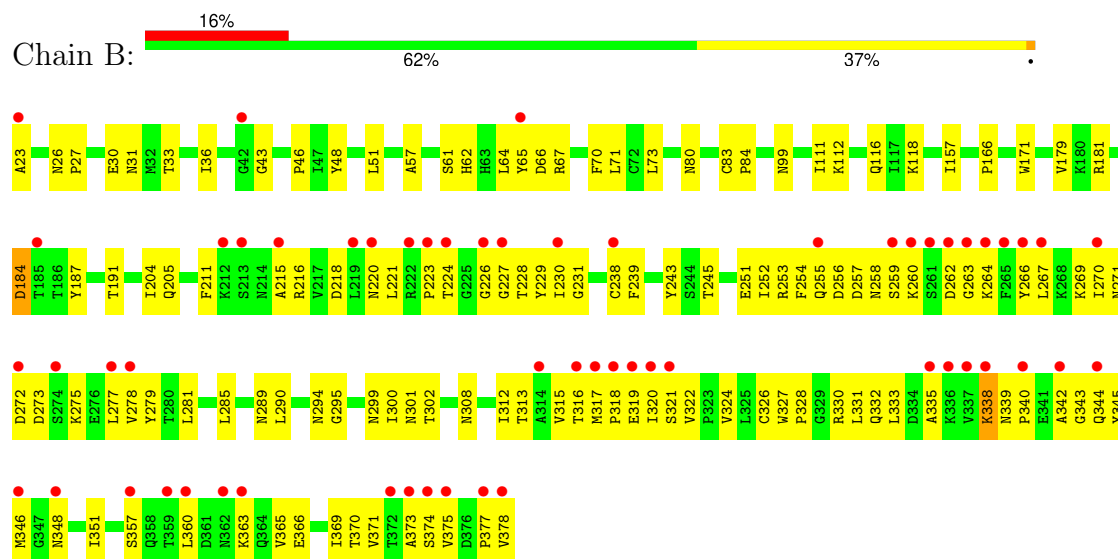
3 Residue-property plots

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: CFA/I fimbrial subunit E



• Molecule 1: CFA/I fimbrial subunit E



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	104.07Å 126.36Å 78.70Å 90.00° 100.49° 90.00°	Depositor
Resolution (Å)	46.78 – 2.60 46.78 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (46.78-2.60) 98.4 (46.78-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.184 , 0.234 0.203 , 0.241	Depositor DCC
R_{free} test set	1498 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5785	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.82	0/2822	0.82	0/3831
1	B	0.78	0/2822	0.83	0/3831
All	All	0.80	0/5644	0.83	0/7662

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	2768	0	2733	150	0
1	B	2768	0	2733	177	0
2	A	133	0	0	3	0
2	B	116	0	0	8	0
All	All	5785	0	5466	316	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 29.

All (316) 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:B:267:LEU:CD2	1:B:345:TYR:HB3	1.33	1.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LEU:CD2	1:A:345:TYR:HB3	1.34	1.53
1:A:266:TYR:CD2	1:A:278:VAL:HG12	1.72	1.24
1:B:266:TYR:CD2	1:B:278:VAL:HG12	1.73	1.23
1:B:317:MET:HB3	1:B:318:PRO:CD	1.74	1.17
1:B:255:GLN:OE1	1:B:295:GLY:HA2	1.46	1.15
1:B:67:ARG:HD2	1:B:181:ARG:CZ	1.77	1.14
1:B:267:LEU:CD2	1:B:345:TYR:CB	2.26	1.14
1:A:267:LEU:CD2	1:A:345:TYR:CB	2.28	1.11
1:B:267:LEU:HD23	1:B:345:TYR:HB3	1.30	1.11
1:A:267:LEU:HD23	1:A:345:TYR:HB3	1.33	1.10
1:B:317:MET:HB3	1:B:318:PRO:HD2	1.26	1.09
1:B:267:LEU:HD22	1:B:345:TYR:HB3	1.34	1.07
1:A:266:TYR:HD2	1:A:278:VAL:HG12	1.07	1.07
1:A:317:MET:HB3	1:A:318:PRO:HD2	1.33	1.07
1:A:260:LYS:HE3	1:A:266:TYR:CE1	1.89	1.06
1:A:255:GLN:OE1	1:A:295:GLY:HA2	1.56	1.04
1:A:317:MET:HB3	1:A:318:PRO:CD	1.86	1.04
1:B:345:TYR:HB2	1:B:373:ALA:HB3	1.39	1.04
1:A:267:LEU:HD22	1:A:345:TYR:HB3	1.34	1.04
1:B:266:TYR:HD2	1:B:278:VAL:HG12	1.08	1.03
1:A:266:TYR:CD2	1:A:278:VAL:CG1	2.42	1.02
1:A:258:ASN:HB3	1:A:260:LYS:NZ	1.74	1.02
1:A:251:GLU:HG3	1:A:299:ASN:OD1	1.61	1.01
1:B:266:TYR:CD2	1:B:278:VAL:CG1	2.42	1.01
1:B:27:PRO:HD3	1:B:65:TYR:CZ	1.96	1.00
1:A:345:TYR:HB2	1:A:373:ALA:HB3	1.37	1.00
1:B:313:THR:HG22	1:B:319:GLU:O	1.61	0.98
1:B:267:LEU:HD21	1:B:345:TYR:HB3	1.43	0.97
1:A:260:LYS:CE	1:A:266:TYR:CE1	2.46	0.97
1:A:267:LEU:HD21	1:A:345:TYR:HB3	1.45	0.97
1:A:23:ALA:HB1	2:A:458:HOH:O	1.65	0.95
1:A:266:TYR:HD2	1:A:278:VAL:CG1	1.78	0.93
1:A:259:SER:O	1:A:260:LYS:HG3	1.68	0.93
1:A:378:VAL:O	1:A:378:VAL:HG13	1.68	0.92
1:B:251:GLU:HG3	1:B:299:ASN:OD1	1.69	0.92
1:B:266:TYR:HD2	1:B:278:VAL:CG1	1.79	0.91
1:B:378:VAL:O	1:B:378:VAL:HG13	1.70	0.88
1:B:255:GLN:OE1	1:B:295:GLY:CA	2.20	0.88
1:B:27:PRO:CD	1:B:65:TYR:CZ	2.56	0.87
1:B:27:PRO:HD2	1:B:65:TYR:OH	1.74	0.86
1:B:67:ARG:HD2	1:B:181:ARG:NH1	1.89	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LYS:CE	1:A:266:TYR:HE1	1.89	0.85
1:B:317:MET:CB	1:B:318:PRO:CD	2.53	0.85
1:A:255:GLN:OE1	1:A:295:GLY:CA	2.26	0.84
1:A:260:LYS:HE2	1:A:266:TYR:HE1	1.40	0.84
1:A:267:LEU:HD21	1:A:345:TYR:C	1.98	0.83
1:B:27:PRO:CD	1:B:65:TYR:OH	2.25	0.83
1:B:267:LEU:HD21	1:B:345:TYR:C	2.00	0.82
1:A:258:ASN:HB3	1:A:260:LYS:HZ1	1.46	0.79
1:A:269:LYS:HE3	1:A:271:ASN:HB2	1.64	0.78
1:B:333:LEU:N	1:B:333:LEU:HD12	1.99	0.78
1:B:67:ARG:HG3	1:B:181:ARG:HG3	1.64	0.78
1:A:330:ARG:HH12	1:A:332:GLN:HE21	1.31	0.77
1:A:339:ASN:N	1:A:340:PRO:CD	2.47	0.77
1:B:67:ARG:CD	1:B:181:ARG:NH1	2.47	0.77
1:B:269:LYS:HE3	1:B:271:ASN:HB2	1.65	0.76
1:B:339:ASN:N	1:B:340:PRO:CD	2.47	0.76
1:B:266:TYR:CE2	1:B:278:VAL:HG11	2.22	0.75
1:A:266:TYR:CE2	1:A:278:VAL:HG11	2.22	0.75
1:B:23:ALA:HB3	2:B:414:HOH:O	1.87	0.74
1:B:267:LEU:HD21	1:B:345:TYR:CB	2.07	0.73
1:B:23:ALA:HB1	2:B:490:HOH:O	1.89	0.73
1:B:223:PRO:HB3	1:B:229:TYR:CZ	2.24	0.73
1:A:378:VAL:O	1:A:378:VAL:CG1	2.38	0.72
1:A:259:SER:O	1:A:260:LYS:CG	2.38	0.71
1:B:333:LEU:HD12	1:B:333:LEU:H	1.55	0.71
1:A:266:TYR:CE2	1:A:278:VAL:CG1	2.73	0.71
1:B:317:MET:HB3	1:B:318:PRO:HD3	1.72	0.71
1:A:267:LEU:HD21	1:A:346:MET:N	2.06	0.71
1:B:266:TYR:CE2	1:B:278:VAL:CG1	2.74	0.70
1:A:257:ASP:C	1:A:258:ASN:HD22	1.94	0.70
1:A:267:LEU:HD21	1:A:345:TYR:CB	2.10	0.69
1:A:322:VAL:HG12	1:B:322:VAL:HG23	1.75	0.69
1:B:378:VAL:O	1:B:378:VAL:CG1	2.40	0.69
1:A:230:ILE:HG22	1:A:231:GLY:N	2.10	0.67
1:A:223:PRO:HB3	1:A:229:TYR:CZ	2.30	0.67
1:A:320:ILE:HD11	1:B:317:MET:CB	2.25	0.67
1:B:317:MET:CB	1:B:318:PRO:HD2	2.16	0.67
1:B:257:ASP:C	1:B:258:ASN:HD22	1.98	0.66
1:B:27:PRO:HG3	1:B:65:TYR:CE1	2.31	0.66
1:B:230:ILE:HG22	1:B:231:GLY:N	2.10	0.66
1:A:221:LEU:HD23	1:A:374:SER:H	1.61	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:LEU:HD21	1:B:346:MET:N	2.11	0.66
1:A:333:LEU:N	1:A:333:LEU:HD12	2.11	0.65
1:B:330:ARG:HH12	1:B:332:GLN:HE21	1.45	0.65
1:A:267:LEU:HG	1:A:346:MET:C	2.17	0.65
1:A:279:TYR:HB3	1:A:335:ALA:HB2	1.77	0.65
1:B:27:PRO:CG	1:B:65:TYR:CE1	2.80	0.65
1:A:258:ASN:CB	1:A:260:LYS:NZ	2.57	0.65
1:B:279:TYR:HB3	1:B:335:ALA:HB2	1.78	0.64
1:B:227:GLY:HA3	1:B:338:LYS:NZ	2.12	0.64
1:A:312:ILE:HG22	1:A:313:THR:O	1.97	0.63
1:A:330:ARG:HH12	1:A:332:GLN:NE2	1.96	0.63
1:B:36:ILE:HD13	1:B:157:ILE:HD12	1.81	0.62
1:B:377:PRO:O	1:B:378:VAL:C	2.37	0.62
1:A:312:ILE:HG22	1:A:313:THR:N	2.14	0.62
1:A:377:PRO:O	1:A:378:VAL:C	2.38	0.62
1:B:277:LEU:HD12	1:B:277:LEU:O	1.99	0.62
1:B:267:LEU:HD22	1:B:345:TYR:CB	2.15	0.62
1:A:227:GLY:HA3	1:A:338:LYS:NZ	2.14	0.61
1:B:267:LEU:HG	1:B:346:MET:C	2.21	0.61
1:B:312:ILE:O	1:B:321:SER:HA	2.00	0.61
1:A:277:LEU:C	1:A:277:LEU:HD12	2.20	0.60
1:A:365:VAL:HG12	1:A:366:GLU:N	2.16	0.60
1:B:221:LEU:HD23	1:B:374:SER:H	1.67	0.60
1:A:258:ASN:HB3	1:A:260:LYS:HZ3	1.66	0.59
1:B:277:LEU:HD12	1:B:277:LEU:C	2.22	0.59
1:A:66:ASP:OD2	1:A:181:ARG:NH1	2.36	0.59
1:B:255:GLN:CD	1:B:295:GLY:HA2	2.22	0.58
1:B:348:ASN:OD1	1:B:369:ILE:O	2.22	0.58
1:A:277:LEU:HD12	1:A:277:LEU:O	2.04	0.58
1:A:348:ASN:OD1	1:A:369:ILE:O	2.22	0.57
1:B:273:ASP:O	1:B:275:LYS:HE3	2.04	0.57
1:B:339:ASN:N	1:B:340:PRO:HD2	2.19	0.57
1:A:255:GLN:CD	1:A:295:GLY:HA2	2.25	0.57
1:B:33:THR:HG23	2:B:477:HOH:O	2.04	0.57
1:A:62:HIS:CE1	1:A:64:LEU:HB2	2.39	0.57
1:A:267:LEU:HD22	1:A:345:TYR:CB	2.16	0.57
1:B:312:ILE:HG22	1:B:313:THR:O	2.05	0.57
1:A:266:TYR:HE2	1:A:278:VAL:HG11	1.68	0.57
1:A:357:SER:HB2	1:A:360:LEU:O	2.05	0.57
1:A:339:ASN:N	1:A:340:PRO:HD2	2.19	0.56
1:A:204:ILE:HG22	1:A:365:VAL:HG21	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:GLY:HA3	1:A:338:LYS:HZ2	1.70	0.56
1:B:27:PRO:HD3	1:B:65:TYR:OH	1.97	0.56
1:B:346:MET:HA	1:B:371:VAL:O	2.06	0.56
1:A:267:LEU:CD2	1:A:346:MET:N	2.69	0.56
1:B:211:PHE:CG	1:B:215:ALA:HB2	2.40	0.56
1:B:312:ILE:HG22	1:B:313:THR:N	2.19	0.56
1:B:204:ILE:HG22	1:B:365:VAL:HG21	1.88	0.55
1:B:267:LEU:HD23	1:B:345:TYR:CB	2.19	0.55
1:A:346:MET:HA	1:A:371:VAL:O	2.06	0.55
1:A:357:SER:CB	1:A:360:LEU:O	2.54	0.55
1:A:67:ARG:HB3	1:A:140:HIS:HB3	1.89	0.55
1:A:338:LYS:O	1:A:339:ASN:HB3	2.06	0.55
1:A:317:MET:CB	1:B:320:ILE:HD11	2.37	0.55
1:A:230:ILE:CG2	1:A:231:GLY:N	2.70	0.54
1:A:333:LEU:HD12	1:A:333:LEU:H	1.71	0.54
1:B:227:GLY:HA3	1:B:338:LYS:HZ2	1.72	0.54
1:A:322:VAL:HG12	1:B:322:VAL:CG2	2.37	0.54
1:A:70:PHE:HA	1:A:178:ASN:O	2.06	0.54
1:B:67:ARG:CD	1:B:181:ARG:CZ	2.68	0.54
1:B:111:ILE:HG22	1:B:112:LYS:N	2.22	0.54
1:A:65:TYR:N	1:A:65:TYR:CD2	2.73	0.54
1:B:267:LEU:CD2	1:B:346:MET:N	2.71	0.54
1:A:267:LEU:HD23	1:A:345:TYR:CB	2.21	0.53
1:A:313:THR:HG22	1:A:319:GLU:O	2.09	0.53
1:B:357:SER:CB	1:B:360:LEU:O	2.56	0.53
1:B:266:TYR:HE2	1:B:278:VAL:HG11	1.69	0.53
1:B:67:ARG:CG	1:B:181:ARG:NH1	2.71	0.53
1:B:230:ILE:CG2	1:B:231:GLY:N	2.72	0.53
1:B:375:VAL:HG23	1:B:375:VAL:O	2.09	0.53
1:B:27:PRO:CD	1:B:65:TYR:CE1	2.91	0.53
1:A:312:ILE:CG2	1:A:313:THR:N	2.72	0.52
1:A:83:CYS:O	1:A:84:PRO:C	2.46	0.52
1:A:273:ASP:O	1:A:275:LYS:HE3	2.09	0.52
1:A:239:PHE:CE2	1:A:252:ILE:HD12	2.44	0.52
1:A:317:MET:HG3	1:B:320:ILE:HD11	1.91	0.52
1:B:267:LEU:CD1	1:B:371:VAL:HG12	2.39	0.52
1:A:330:ARG:NH1	1:A:332:GLN:HE21	2.03	0.52
1:A:221:LEU:HA	1:A:230:ILE:O	2.10	0.52
1:B:223:PRO:O	1:B:224:THR:CG2	2.58	0.51
1:A:30:GLU:HG3	1:A:190:TYR:HE1	1.74	0.51
1:A:339:ASN:N	1:A:340:PRO:HD3	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ILE:HD13	1:A:157:ILE:HD12	1.91	0.51
1:B:254:PHE:CE1	1:B:351:ILE:HG12	2.45	0.51
1:B:216:ARG:HA	1:B:370:THR:O	2.11	0.51
1:A:223:PRO:O	1:A:224:THR:CG2	2.59	0.51
1:B:99:ASN:ND2	1:B:118:LYS:HE2	2.26	0.50
1:B:218:ASP:OD2	1:B:220:ASN:N	2.39	0.50
1:B:211:PHE:CG	1:B:215:ALA:CB	2.95	0.50
1:B:357:SER:HB2	1:B:360:LEU:O	2.11	0.50
1:B:239:PHE:CE2	1:B:252:ILE:HD12	2.47	0.50
1:A:254:PHE:CE1	1:A:351:ILE:HG12	2.47	0.49
1:B:338:LYS:O	1:B:339:ASN:HB3	2.11	0.49
1:B:83:CYS:O	1:B:84:PRO:C	2.50	0.49
1:B:228:THR:CG2	1:B:229:TYR:N	2.73	0.49
1:A:99:ASN:OD1	1:A:116:GLN:NE2	2.42	0.49
1:A:272:ASP:OD2	1:A:275:LYS:HB2	2.13	0.49
1:A:317:MET:CB	1:A:318:PRO:CD	2.64	0.49
1:B:66:ASP:OD2	1:B:67:ARG:HG2	2.13	0.49
1:B:223:PRO:HB3	1:B:229:TYR:CE2	2.47	0.49
1:B:339:ASN:N	1:B:340:PRO:HD3	2.26	0.49
1:B:365:VAL:HG12	1:B:366:GLU:N	2.27	0.49
1:B:259:SER:O	1:B:260:LYS:HD3	2.13	0.48
1:B:238:CYS:HB3	1:B:326:CYS:SG	2.53	0.48
1:B:80:ASN:HB2	2:B:456:HOH:O	2.12	0.48
1:A:159:ALA:O	2:A:496:HOH:O	2.20	0.48
1:B:330:ARG:HH12	1:B:332:GLN:NE2	2.10	0.48
1:A:232:ARG:HA	1:A:333:LEU:O	2.13	0.48
1:B:272:ASP:OD2	1:B:275:LYS:HB2	2.12	0.48
1:A:178:ASN:OD1	1:A:189:THR:OG1	2.32	0.48
1:B:36:ILE:CD1	1:B:157:ILE:HD12	2.42	0.48
1:A:218:ASP:OD2	1:A:220:ASN:N	2.44	0.48
1:A:319:GLU:O	1:A:320:ILE:C	2.51	0.48
1:A:338:LYS:O	1:A:339:ASN:CB	2.61	0.48
1:A:312:ILE:O	1:A:321:SER:HA	2.13	0.48
1:A:211:PHE:CD1	1:A:215:ALA:HA	2.48	0.47
1:A:257:ASP:O	1:A:258:ASN:ND2	2.39	0.47
1:B:375:VAL:O	1:B:375:VAL:CG2	2.61	0.47
1:A:227:GLY:CA	1:A:338:LYS:HZ2	2.27	0.47
1:B:256:ASP:O	1:B:258:ASN:N	2.43	0.47
1:A:31:ASN:OD1	1:A:191:THR:HB	2.15	0.47
1:B:312:ILE:CG2	1:B:313:THR:N	2.77	0.47
1:B:289:ASN:O	1:B:290:LEU:HD23	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ASP:OD2	1:A:180:LYS:NZ	2.47	0.46
1:A:267:LEU:CD1	1:A:371:VAL:HG12	2.45	0.46
1:B:30:GLU:OE2	2:B:480:HOH:O	2.20	0.46
1:B:223:PRO:O	1:B:224:THR:HG22	2.15	0.46
1:B:313:THR:CG2	1:B:319:GLU:O	2.48	0.46
1:A:342:ALA:HA	1:A:375:VAL:HG11	1.98	0.46
1:B:99:ASN:OD1	1:B:116:GLN:NE2	2.48	0.46
1:B:267:LEU:HD21	1:B:345:TYR:CA	2.45	0.46
1:A:338:LYS:C	1:A:340:PRO:HD3	2.35	0.46
1:A:67:ARG:C	2:A:443:HOH:O	2.54	0.46
1:A:267:LEU:HD21	1:A:345:TYR:CA	2.45	0.46
1:B:270:ILE:HG12	1:B:344:GLN:O	2.15	0.46
1:B:343:GLY:H	1:B:375:VAL:HG21	1.79	0.46
1:A:36:ILE:HG23	1:A:48:TYR:CD2	2.50	0.46
1:A:258:ASN:CB	1:A:260:LYS:HZ3	2.25	0.46
1:A:228:THR:CG2	1:A:229:TYR:N	2.77	0.46
1:A:275:LYS:HA	1:A:275:LYS:HD3	1.71	0.46
1:B:227:GLY:CA	1:B:338:LYS:HZ2	2.28	0.46
1:B:308:ASN:ND2	1:B:328:PRO:HG3	2.31	0.46
1:A:312:ILE:O	1:A:321:SER:HB2	2.17	0.45
1:B:221:LEU:HA	1:B:230:ILE:O	2.17	0.45
1:B:245:THR:HB	1:B:327:TRP:CZ2	2.52	0.45
1:A:317:MET:HB3	1:B:320:ILE:HD11	1.98	0.45
1:B:205:GLN:HA	1:B:365:VAL:HG11	1.99	0.45
1:A:226:GLY:C	1:A:228:THR:H	2.20	0.45
1:B:67:ARG:HG2	1:B:181:ARG:NH1	2.31	0.45
1:B:338:LYS:C	1:B:340:PRO:HD3	2.36	0.45
1:A:67:ARG:CB	1:A:140:HIS:HB3	2.47	0.45
1:A:312:ILE:HG21	1:A:312:ILE:HD13	1.68	0.45
1:A:317:MET:HB3	1:A:318:PRO:HD3	1.90	0.45
1:A:259:SER:C	1:A:260:LYS:HG3	2.35	0.45
1:B:166:PRO:HD2	1:B:171:TRP:CH2	2.52	0.45
1:B:57:ALA:HB1	1:B:65:TYR:CG	2.52	0.45
1:B:216:ARG:HB3	1:B:370:THR:HB	1.98	0.44
1:A:99:ASN:ND2	1:A:118:LYS:HE2	2.31	0.44
1:A:365:VAL:CG1	1:A:366:GLU:N	2.80	0.44
1:B:338:LYS:O	1:B:339:ASN:CB	2.65	0.44
1:A:70:PHE:O	1:A:71:LEU:HD23	2.17	0.44
1:B:181:ARG:HB2	1:B:187:TYR:OH	2.18	0.44
1:A:320:ILE:HD11	1:B:317:MET:HG3	2.00	0.44
1:A:365:VAL:HG12	1:A:366:GLU:H	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:PRO:C	1:B:224:THR:HG23	2.38	0.44
1:A:223:PRO:C	1:A:224:THR:HG23	2.38	0.44
1:B:99:ASN:HD21	1:B:118:LYS:HE2	1.82	0.44
1:B:281:LEU:HB3	1:B:331:LEU:HD11	2.00	0.44
1:A:320:ILE:HD11	1:B:317:MET:HB3	2.00	0.44
1:B:181:ARG:HG2	1:B:184:ASP:CB	2.48	0.44
1:B:259:SER:O	1:B:260:LYS:HG2	2.18	0.44
1:A:211:PHE:CG	1:A:215:ALA:HB2	2.53	0.44
1:A:168:ASP:O	1:A:244:SER:OG	2.25	0.43
1:A:181:ARG:HB3	1:A:184:ASP:HB3	1.99	0.43
1:A:269:LYS:HG2	1:A:271:ASN:H	1.84	0.43
1:A:260:LYS:HE3	1:A:266:TYR:CD1	2.45	0.43
1:B:324:VAL:HG12	2:B:475:HOH:O	2.19	0.43
1:A:301:ASN:OD1	1:A:302:THR:N	2.51	0.43
1:B:43:GLY:N	2:B:482:HOH:O	2.46	0.43
1:A:272:ASP:OD2	1:A:275:LYS:CG	2.66	0.43
1:B:253:ARG:CG	1:B:254:PHE:N	2.81	0.42
1:B:285:LEU:CD2	1:B:300:ILE:HD13	2.49	0.42
1:B:62:HIS:CE1	1:B:64:LEU:HB2	2.53	0.42
1:B:272:ASP:OD2	1:B:275:LYS:CG	2.67	0.42
1:A:223:PRO:O	1:A:224:THR:HG22	2.19	0.42
1:A:253:ARG:CG	1:A:254:PHE:N	2.82	0.42
1:B:211:PHE:CD2	1:B:215:ALA:CB	3.02	0.42
1:B:343:GLY:N	1:B:375:VAL:HG21	2.35	0.42
1:A:317:MET:CG	1:B:320:ILE:HD11	2.48	0.42
1:B:330:ARG:NH1	1:B:332:GLN:HE21	2.14	0.42
1:B:51:LEU:HD23	1:B:51:LEU:HA	1.86	0.42
1:B:262:ASP:HB3	1:B:264:LYS:HG2	2.02	0.42
1:A:312:ILE:HD12	1:A:324:VAL:HG21	2.02	0.42
1:B:263:GLY:O	1:B:294:ASN:N	2.41	0.42
1:B:301:ASN:OD1	1:B:302:THR:N	2.53	0.42
1:A:279:TYR:CB	1:A:335:ALA:HB2	2.45	0.42
1:B:269:LYS:HG2	1:B:270:ILE:N	2.35	0.42
1:B:46:PRO:HG2	1:B:48:TYR:CZ	2.54	0.42
1:B:26:ASN:HA	1:B:27:PRO:HD3	1.85	0.41
1:B:31:ASN:OD1	1:B:191:THR:HB	2.20	0.41
1:B:338:LYS:HD3	1:B:339:ASN:H	1.84	0.41
1:A:118:LYS:O	1:A:155:LEU:HA	2.20	0.41
1:B:315:VAL:HG12	1:B:316:THR:HG23	2.02	0.41
1:A:320:ILE:HD11	1:B:317:MET:HB2	2.02	0.41
1:B:70:PHE:CE2	1:B:179:VAL:HG13	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:LYS:HD3	1:B:275:LYS:HA	1.68	0.41
1:A:238:CYS:HB3	1:A:326:CYS:SG	2.60	0.41
1:B:31:ASN:HB3	2:B:433:HOH:O	2.20	0.41
1:B:73:LEU:HD23	1:B:73:LEU:HA	1.77	0.41
1:A:66:ASP:OD2	1:A:67:ARG:N	2.54	0.41
1:A:257:ASP:C	1:A:258:ASN:ND2	2.69	0.41
1:A:322:VAL:HG12	1:B:322:VAL:CB	2.50	0.41
1:B:227:GLY:HA3	1:B:338:LYS:HZ1	1.81	0.41
1:B:269:LYS:HG2	1:B:271:ASN:H	1.85	0.41
1:A:269:LYS:HA	1:A:344:GLN:O	2.21	0.41
1:B:211:PHE:CB	1:B:215:ALA:HB2	2.51	0.41
1:B:342:ALA:HA	1:B:375:VAL:HG21	2.02	0.41
1:A:274:SER:O	1:A:275:LYS:CE	2.69	0.40
1:B:211:PHE:CD2	1:B:215:ALA:HB1	2.56	0.40
1:B:221:LEU:HD13	1:B:230:ILE:O	2.21	0.40
1:B:230:ILE:HG22	1:B:231:GLY:H	1.85	0.40
1:B:259:SER:O	1:B:260:LYS:CD	2.70	0.40
1:A:118:LYS:HD3	1:A:118:LYS:HA	1.91	0.40
1:A:136:LEU:HA	1:A:136:LEU:HD23	1.83	0.40
1:B:70:PHE:O	1:B:71:LEU:HD23	2.22	0.40
1:B:223:PRO:C	1:B:224:THR:CG2	2.90	0.40
1:B:230:ILE:CG2	1:B:231:GLY:H	2.34	0.40
1:B:312:ILE:HD13	1:B:312:ILE:HG21	1.70	0.40
1:B:339:ASN:H	1:B:340:PRO:HD2	1.87	0.40
1:A:211:PHE:CD2	1:A:215:ALA:CB	3.05	0.40
1:A:230:ILE:CG2	1:A:231:GLY:H	2.35	0.40
1:B:226:GLY:C	1:B:228:THR:H	2.24	0.40
1:B:333:LEU:N	1:B:333:LEU:CD1	2.71	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	354/356 (99%)	339 (96%)	15 (4%)	0	100	100
1	B	354/356 (99%)	339 (96%)	15 (4%)	0	100	100
All	All	708/712 (99%)	678 (96%)	30 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	312/312 (100%)	306 (98%)	6 (2%)	52	75
1	B	312/312 (100%)	307 (98%)	5 (2%)	58	79
All	All	624/624 (100%)	613 (98%)	11 (2%)	54	77

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	ASP
1	A	184	ASP
1	A	243	TYR
1	A	251	GLU
1	A	338	LYS
1	A	360	LEU
1	B	61	SER
1	B	184	ASP
1	B	243	TYR
1	B	338	LYS
1	B	363	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	99	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	116	GLN
1	A	163	ASN
1	A	205	GLN
1	A	258	ASN
1	A	310	ASN
1	A	332	GLN
1	A	362	ASN
1	B	99	ASN
1	B	116	GLN
1	B	210	GLN
1	B	258	ASN
1	B	332	GLN
1	B	362	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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, 95th 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	356/356 (100%)	0.26	58 (16%) 5 4	15, 38, 162, 212	0
1	B	356/356 (100%)	0.27	58 (16%) 5 4	15, 39, 139, 176	0
All	All	712/712 (100%)	0.26	116 (16%) 5 4	15, 39, 146, 212	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	317	MET	6.7
1	B	318	PRO	6.6
1	A	317	MET	6.1
1	A	318	PRO	5.7
1	B	320	ILE	5.1
1	A	185	THR	5.1
1	B	319	GLU	5.0
1	B	340	PRO	4.8
1	A	261	SER	4.6
1	B	185	THR	4.6
1	A	378	VAL	4.4
1	B	263	GLY	4.3
1	B	359	THR	4.3
1	B	378	VAL	4.3
1	B	337	VAL	4.2
1	B	261	SER	4.0
1	B	360	LEU	4.0
1	B	227	GLY	3.9
1	A	360	LEU	3.9
1	A	359	THR	3.7
1	A	316	THR	3.7
1	A	217	VAL	3.6
1	A	66	ASP	3.6
1	A	320	ILE	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	262	ASP	3.4
1	B	375	VAL	3.4
1	A	225	GLY	3.4
1	A	340	PRO	3.4
1	A	377	PRO	3.4
1	A	259	SER	3.2
1	B	342	ALA	3.2
1	A	337	VAL	3.2
1	A	347	GLY	3.2
1	A	274	SER	3.1
1	A	263	GLY	3.1
1	A	272	ASP	3.1
1	A	319	GLU	3.1
1	A	230	ILE	3.1
1	A	278	VAL	3.1
1	B	255	GLN	3.1
1	B	260	LYS	3.0
1	B	377	PRO	3.0
1	A	322	VAL	3.0
1	B	213	SER	3.0
1	A	364	GLN	3.0
1	A	42	GLY	3.0
1	A	342	ALA	2.9
1	B	265	PHE	2.9
1	A	270	ILE	2.9
1	B	374	SER	2.9
1	B	65	TYR	2.9
1	B	316	THR	2.9
1	B	262	ASP	2.9
1	B	212	LYS	2.9
1	A	362	ASN	2.8
1	A	336	LYS	2.8
1	A	224	THR	2.8
1	B	224	THR	2.8
1	B	362	ASN	2.8
1	A	371	VAL	2.8
1	B	264	LYS	2.8
1	B	373	ALA	2.8
1	A	265	PHE	2.7
1	B	348	ASN	2.7
1	B	215	ALA	2.7
1	B	335	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	374	SER	2.7
1	A	227	GLY	2.7
1	B	266	TYR	2.6
1	A	23	ALA	2.6
1	A	212	LYS	2.6
1	B	272	ASP	2.6
1	B	338	LYS	2.5
1	A	279	TYR	2.5
1	A	264	LYS	2.5
1	B	278	VAL	2.5
1	B	42	GLY	2.5
1	B	267	LEU	2.4
1	B	357	SER	2.4
1	A	255	GLN	2.4
1	A	363	LYS	2.4
1	B	344	GLN	2.4
1	B	238	CYS	2.4
1	A	228	THR	2.4
1	B	372	THR	2.4
1	B	336	LYS	2.4
1	A	375	VAL	2.4
1	A	219	LEU	2.4
1	A	346	MET	2.3
1	B	321	SER	2.3
1	A	223	PRO	2.3
1	A	216	ARG	2.3
1	B	259	SER	2.2
1	B	363	LYS	2.2
1	A	214	ASN	2.2
1	B	230	ILE	2.2
1	A	277	LEU	2.2
1	B	223	PRO	2.1
1	A	213	SER	2.1
1	A	266	TYR	2.1
1	A	273	ASP	2.1
1	A	358	GLN	2.1
1	A	280	THR	2.1
1	A	338	LYS	2.1
1	B	222	ARG	2.1
1	B	314	ALA	2.1
1	B	219	LEU	2.1
1	A	335	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	226	GLY	2.1
1	B	274	SER	2.1
1	A	267	LEU	2.1
1	B	23	ALA	2.1
1	B	270	ILE	2.0
1	B	277	LEU	2.0
1	B	346	MET	2.0
1	B	220	ASN	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.