Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 06:18 PM JST

PDB ID	:	7WVH
Title	:	Structure of NAD+ glycohydrolase/Streptolysin O complex from Group A streptococcus
Authors	:	Tsai, W.-J.; Wang, S.-Y.
Deposited on	:	2022-02-10
Resolution	:	2.45 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:

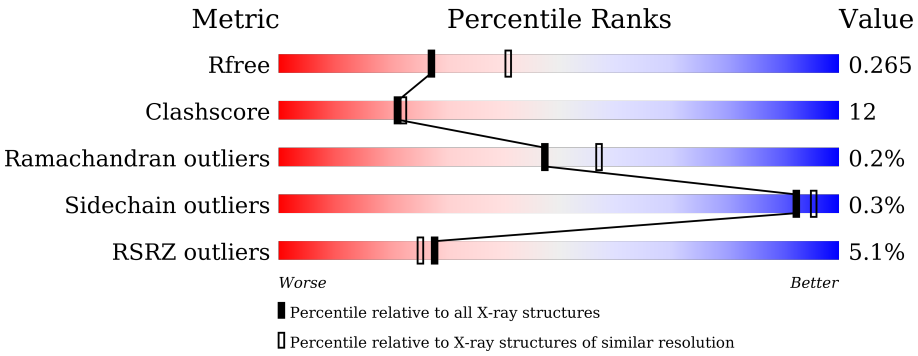
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	268	76% 17% 6%
1	B	268	12% 59% 25% • 14%
2	C	472	6% 66% 26% • 7%
2	D	472	% 78% 19% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11304 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 NAD+-glycohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	0	0
			2022	1279	339	397	7			
1	B	230	Total	C	N	O	S	0	0	0
			1861	1183	306	366	6			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	MET	-	initiating methionine	UNP D7S0C0
A	330	ASP	GLY	engineered mutation	UNP D7S0C0
A	368	ARG	GLY	engineered mutation	UNP D7S0C0
A	452	LEU	-	expression tag	UNP D7S0C0
A	453	GLU	-	expression tag	UNP D7S0C0
A	454	HIS	-	expression tag	UNP D7S0C0
A	455	HIS	-	expression tag	UNP D7S0C0
A	456	HIS	-	expression tag	UNP D7S0C0
A	457	HIS	-	expression tag	UNP D7S0C0
A	458	HIS	-	expression tag	UNP D7S0C0
A	459	HIS	-	expression tag	UNP D7S0C0
B	192	MET	-	initiating methionine	UNP D7S0C0
B	330	ASP	GLY	engineered mutation	UNP D7S0C0
B	368	ARG	GLY	engineered mutation	UNP D7S0C0
B	452	LEU	-	expression tag	UNP D7S0C0
B	453	GLU	-	expression tag	UNP D7S0C0
B	454	HIS	-	expression tag	UNP D7S0C0
B	455	HIS	-	expression tag	UNP D7S0C0
B	456	HIS	-	expression tag	UNP D7S0C0
B	457	HIS	-	expression tag	UNP D7S0C0
B	458	HIS	-	expression tag	UNP D7S0C0
B	459	HIS	-	expression tag	UNP D7S0C0

- Molecule 2 is a protein called Streptolysin O.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	455	Total	C	N	O	S	0	0	0
			3595	2273	609	708	5			
2	C	441	Total	C	N	O	S	0	0	0
			3500	2215	590	690	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	100	MET	-	initiating methionine	UNP P0C0I3
D	101	ALA	-	expression tag	UNP P0C0I3
D	102	SER	-	expression tag	UNP P0C0I3
D	450	SER	THR	conflict	UNP P0C0I3
C	100	MET	-	initiating methionine	UNP P0C0I3
C	101	ALA	-	expression tag	UNP P0C0I3
C	102	SER	-	expression tag	UNP P0C0I3
C	450	SER	THR	conflict	UNP P0C0I3

- Molecule 3 is water.

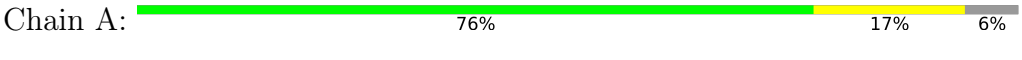
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	117	Total	O	0	0
			117	117		
3	D	145	Total	O	0	0
			145	145		
3	C	52	Total	O	0	0
			52	52		
3	B	12	Total	O	0	0
			12	12		

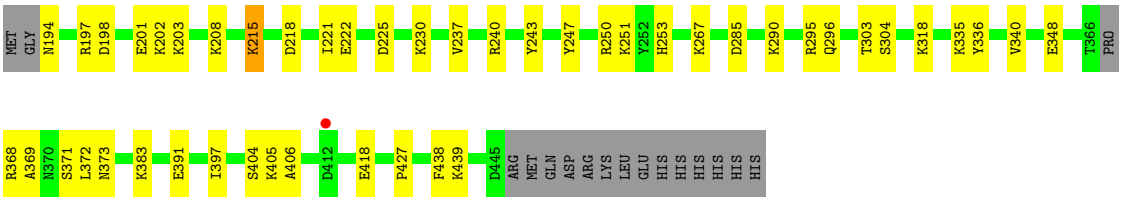
3 Residue-property plots (i)

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: NAD+-glycohydrolase

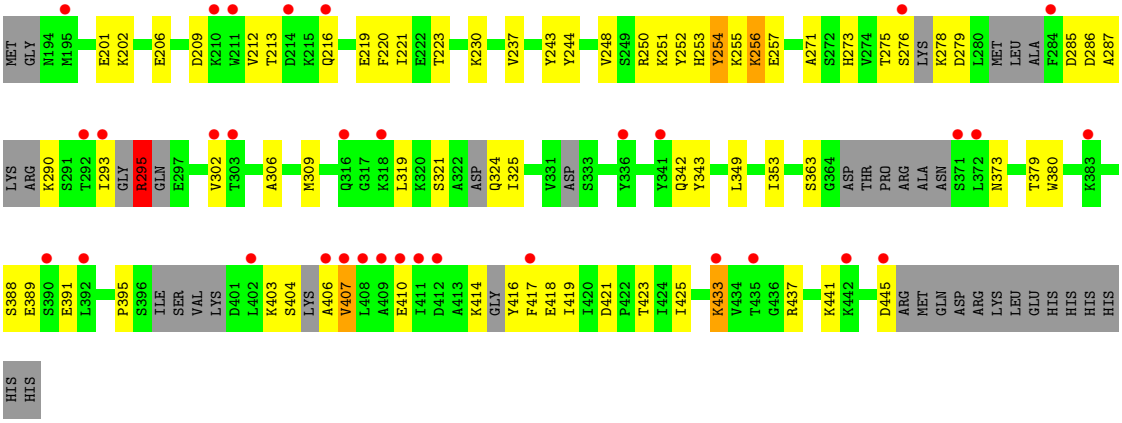
Chain A:





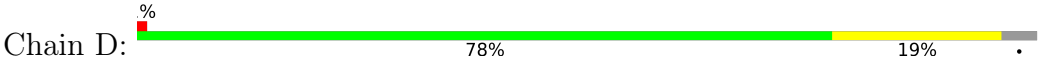
• Molecule 1: NAD+-glycohydrolase

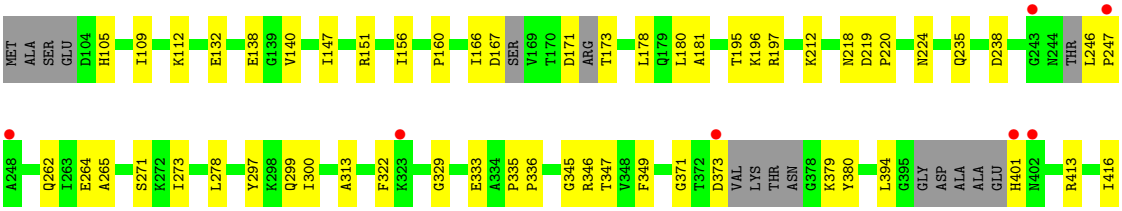
Chain B:

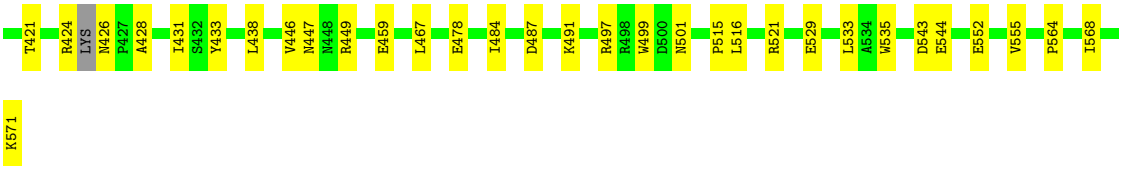


• Molecule 2: Streptolysin O

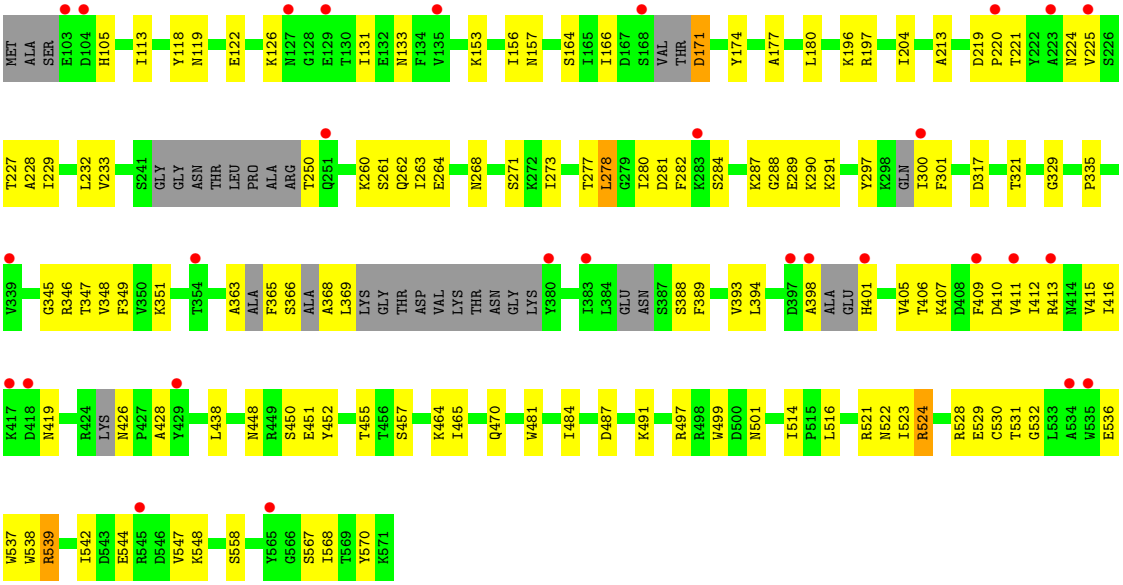
Chain D:







• Molecule 2: Streptolysin O



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	246.09Å 52.48Å 169.40Å 90.00° 132.04° 90.00°	Depositor
Resolution (Å)	26.12 – 2.45 26.12 – 2.45	Depositor EDS
% Data completeness (in resolution range)	92.2 (26.12-2.45) 92.1 (26.12-2.45)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.09 (at 2.44Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.213 , 0.265 0.213 , 0.265	Depositor DCC
R_{free} test set	2836 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å^2)	36.5	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 46.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.010 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11304	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 16.31% 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	0.58	0/2056	0.99	4/2752 (0.1%)
1	B	0.55	4/1885 (0.2%)	0.77	7/2510 (0.3%)
2	C	0.45	0/3561	0.70	6/4818 (0.1%)
2	D	0.50	0/3660	0.63	1/4957 (0.0%)
All	All	0.51	4/11162 (0.0%)	0.75	18/15037 (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
2	C	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	433	LYS	CD-CE	6.80	1.68	1.51
1	B	295	ARG	CG-CD	6.06	1.67	1.51
1	B	295	ARG	CZ-NH1	5.93	1.40	1.33
1	B	433	LYS	CB-CG	5.25	1.66	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	295	ARG	NE-CZ-NH1	26.30	133.45	120.30
1	A	295	ARG	NE-CZ-NH2	-22.18	109.21	120.30
2	C	171	ASP	CB-CG-OD2	-10.99	108.41	118.30
1	B	295	ARG	NE-CZ-NH1	9.61	125.10	120.30
2	C	171	ASP	CB-CG-OD1	8.84	126.26	118.30
1	A	295	ARG	CD-NE-CZ	8.61	135.65	123.60
1	B	256	LYS	CB-CG-CD	-7.90	91.06	111.60
1	B	407	VAL	CG1-CB-CG2	-7.67	98.62	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	433	LYS	CD-CE-NZ	-7.45	94.57	111.70
2	C	278	LEU	CB-CG-CD2	7.12	123.10	111.00
1	A	295	ARG	CG-CD-NE	6.37	125.18	111.80
1	B	295	ARG	NE-CZ-NH2	-6.23	117.18	120.30
2	C	539	ARG	NE-CZ-NH1	-6.15	117.23	120.30
2	C	539	ARG	CG-CD-NE	6.05	124.51	111.80
1	B	295	ARG	CA-CB-CG	6.05	126.71	113.40
1	B	295	ARG	CB-CA-C	5.24	120.88	110.40
2	C	291	LYS	CA-CB-CG	5.13	124.69	113.40
2	D	218	ASN	CB-CA-C	5.12	120.64	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	171	ASP	Sidechain

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	2022	0	2010	37	0
1	B	1861	0	1828	60	0
2	C	3500	0	3457	107	0
2	D	3595	0	3561	65	0
3	A	117	0	0	11	1
3	B	12	0	0	1	0
3	C	52	0	0	4	2
3	D	145	0	0	14	1
All	All	11304	0	10856	265	2

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 12.

All (265) 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)
2:C:389:PHE:HE1	2:C:409:PHE:CD1	1.81	0.97
2:C:389:PHE:CE1	2:C:409:PHE:HD1	1.81	0.97
2:C:300:ILE:HD11	2:C:346:ARG:H	1.33	0.93
2:C:389:PHE:HE1	2:C:409:PHE:HD1	0.94	0.91
1:B:250:ARG:HH22	1:B:373:ASN:HD21	1.10	0.90
1:B:319:LEU:HB3	1:B:445:ASP:HB3	1.58	0.86
2:D:171:ASP:O	2:D:173:THR:N	2.09	0.85
2:D:346:ARG:NH2	2:D:421:THR:O	2.10	0.85
1:A:368:ARG:N	1:A:391:GLU:OE1	2.11	0.81
2:C:250:THR:N	3:C:601:HOH:O	2.12	0.81
2:C:409:PHE:HD2	2:C:413:ARG:HD2	1.44	0.81
2:C:410:ASP:HA	2:C:413:ARG:HG2	1.64	0.79
2:D:497:ARG:NH1	3:D:605:HOH:O	2.17	0.77
2:D:166:ILE:HD12	2:D:273:ILE:HG13	1.68	0.75
2:C:409:PHE:CE2	2:C:413:ARG:HB3	2.22	0.75
1:A:208:LYS:NZ	3:A:504:HOH:O	2.21	0.74
2:D:195:THR:O	2:D:196:LYS:HE2	1.88	0.73
2:D:181:ALA:HB3	2:D:335:PRO:HD2	1.71	0.72
2:D:138:GLU:OE2	3:D:601:HOH:O	2.06	0.72
2:D:459:GLU:OE2	3:D:602:HOH:O	2.08	0.71
1:B:275:THR:OG1	1:B:279:ASP:OD1	2.08	0.71
1:A:194:ASN:ND2	3:A:505:HOH:O	2.23	0.70
1:B:250:ARG:NH2	1:B:373:ASN:HD21	1.88	0.69
2:C:156:ILE:HD11	2:C:450:SER:HB2	1.75	0.68
1:A:201:GLU:HG3	1:A:221:ILE:HD12	1.73	0.68
1:B:201:GLU:HG3	1:B:221:ILE:HD12	1.74	0.68
2:C:529:GLU:OE2	2:C:531:THR:HG22	1.94	0.68
1:A:427:PRO:O	3:A:501:HOH:O	2.12	0.68
2:C:455:THR:OG1	3:C:602:HOH:O	2.13	0.67
2:D:195:THR:C	2:D:196:LYS:HE2	2.15	0.67
2:C:131:ILE:HD13	2:C:153:LYS:HE2	1.77	0.66
2:D:371:GLY:HA2	2:D:413:ARG:HH21	1.59	0.66
1:B:286:ASP:OD2	1:B:287:ALA:N	2.29	0.66
1:A:405:LYS:NZ	3:A:503:HOH:O	2.20	0.66
2:C:363:ALA:O	2:C:365:PHE:N	2.28	0.66
2:D:167:ASP:O	3:D:603:HOH:O	2.14	0.65
2:C:228:ALA:O	2:C:232:LEU:HD23	1.97	0.64
2:D:552:GLU:OE1	2:D:571:LYS:HE3	1.97	0.64
1:B:251:LYS:HB3	1:B:253:HIS:NE2	2.13	0.63
1:B:319:LEU:CB	1:B:445:ASP:HB3	2.29	0.63
2:C:284:SER:CB	2:C:290:LYS:HZ1	2.12	0.62
2:C:174:TYR:CD1	2:C:225:VAL:HG21	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:LYS:O	1:B:416:TYR:N	2.33	0.62
2:D:156:ILE:HD11	2:D:262:GLN:HA	1.82	0.62
2:D:373:ASP:OD1	2:D:373:ASP:N	2.32	0.62
1:B:244:TYR:O	1:B:248:VAL:HG23	2.00	0.62
2:C:219:ASP:O	2:C:224:ASN:ND2	2.30	0.62
2:C:288:GLY:HA3	2:C:457:SER:HB2	1.81	0.62
1:B:290:LYS:HD2	1:B:290:LYS:N	2.15	0.61
1:B:209:ASP:O	1:B:212:VAL:HG22	2.00	0.61
2:C:531:THR:HG21	2:C:539:ARG:HD3	1.81	0.61
1:B:213:THR:HG23	1:B:216:GLN:H	1.64	0.61
1:A:368:ARG:HA	1:A:373:ASN:HB2	1.83	0.61
1:B:373:ASN:OD1	1:B:373:ASN:N	2.32	0.61
1:A:218:ASP:O	1:A:222:GLU:HG2	2.01	0.60
1:B:293:ILE:O	1:B:295:ARG:N	2.35	0.60
1:B:293:ILE:HD11	1:B:343:TYR:CZ	2.37	0.60
2:D:333:GLU:HG2	3:D:613:HOH:O	2.02	0.59
2:C:532:GLY:HA3	1:B:309:MET:CE	2.32	0.59
1:B:285:ASP:OD1	1:B:404:SER:N	2.33	0.59
1:B:202:LYS:O	1:B:206:GLU:HG2	2.03	0.58
1:A:335:LYS:NZ	3:A:506:HOH:O	2.25	0.58
2:C:409:PHE:CD2	2:C:413:ARG:HD2	2.34	0.58
2:C:197:ARG:HB2	2:C:220:PRO:HD2	1.84	0.58
2:D:173:THR:HG21	2:D:433:TYR:CD1	2.39	0.58
2:C:284:SER:OG	2:C:290:LYS:NZ	2.34	0.58
2:D:264:GLU:HG3	2:D:271:SER:HB3	1.85	0.57
1:A:405:LYS:HD3	1:A:406:ALA:N	2.20	0.57
2:D:543:ASP:OD2	3:D:604:HOH:O	2.17	0.57
1:B:254:TYR:N	1:B:254:TYR:CD1	2.71	0.57
2:C:281:ASP:HB3	2:C:290:LYS:HE3	1.85	0.57
1:B:319:LEU:HD11	1:B:325:ILE:HD11	1.86	0.57
1:B:403:LYS:O	1:B:406:ALA:HB3	2.05	0.56
2:D:167:ASP:O	3:D:606:HOH:O	2.17	0.56
2:C:412:ILE:O	2:C:416:ILE:HD12	2.06	0.56
1:A:198:ASP:HB3	1:A:202:LYS:NZ	2.21	0.55
1:A:230:LYS:HE3	3:A:544:HOH:O	2.05	0.55
2:C:300:ILE:HD11	2:C:346:ARG:N	2.14	0.55
1:A:318:LYS:NZ	3:A:509:HOH:O	2.32	0.55
2:D:197:ARG:HB2	2:D:220:PRO:HD2	1.89	0.55
2:D:180:LEU:HD11	2:D:329:GLY:HA3	1.88	0.55
2:D:297:TYR:CZ	2:D:416:ILE:HD13	2.42	0.54
1:B:257:GLU:H	1:B:257:GLU:CD	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:VAL:HG21	1:A:243:TYR:HB2	1.90	0.54
1:A:368:ARG:HG2	1:A:373:ASN:CB	2.38	0.54
2:D:219:ASP:HB3	2:D:224:ASN:HD22	1.73	0.54
2:C:410:ASP:HA	2:C:413:ARG:CG	2.35	0.54
2:C:118:TYR:CE1	2:C:335:PRO:HB3	2.43	0.54
2:C:389:PHE:HD1	2:C:412:ILE:HD12	1.72	0.54
2:C:532:GLY:HA3	1:B:309:MET:HE1	1.90	0.54
1:B:417:PHE:HE1	1:B:419:ILE:CG1	2.22	0.53
1:A:368:ARG:HA	1:A:373:ASN:CB	2.37	0.53
2:D:426:ASN:OD1	2:D:426:ASN:N	2.41	0.53
1:B:255:LYS:HD2	1:B:255:LYS:N	2.23	0.53
2:C:522:ASN:O	2:C:524:ARG:NE	2.39	0.53
1:B:254:TYR:N	1:B:254:TYR:HD1	2.07	0.53
1:A:383:LYS:NZ	3:A:512:HOH:O	2.38	0.53
2:C:389:PHE:CE1	2:C:409:PHE:CD1	2.71	0.53
2:C:131:ILE:HG21	2:C:153:LYS:HE2	1.89	0.53
1:B:220:PHE:HA	1:B:380:TRP:CZ2	2.43	0.53
2:D:219:ASP:HB3	2:D:224:ASN:ND2	2.23	0.53
2:C:126:LYS:HD3	2:C:448:ASN:ND2	2.24	0.53
2:D:499:TRP:CZ2	2:D:501:ASN:HB2	2.43	0.52
2:C:180:LEU:HD11	2:C:329:GLY:HA3	1.91	0.52
2:C:287:LYS:HB2	2:C:289:GLU:HG3	1.90	0.52
1:B:306:ALA:O	1:B:309:MET:HG2	2.10	0.52
1:B:418:GLU:OE2	1:B:437:ARG:NE	2.37	0.52
2:C:297:TYR:HB2	2:C:348:VAL:HB	1.91	0.52
2:C:278:LEU:HD22	2:C:351:LYS:HB2	1.92	0.52
2:D:487:ASP:OD2	2:D:491:LYS:HB3	2.10	0.52
1:B:237:VAL:HG21	1:B:243:TYR:HB2	1.91	0.52
1:B:306:ALA:HA	1:B:309:MET:SD	2.50	0.52
1:A:251:LYS:HE2	1:A:253:HIS:CD2	2.46	0.51
2:D:196:LYS:HE2	2:D:196:LYS:HA	1.91	0.51
2:C:464:LYS:NZ	3:C:606:HOH:O	2.44	0.51
2:C:411:VAL:O	2:C:415:VAL:HG23	2.11	0.50
2:C:119:ASN:HB3	2:C:122:GLU:HB2	1.93	0.50
2:C:531:THR:OG1	2:C:536:GLU:O	2.26	0.50
1:B:423:THR:HG23	1:B:433:LYS:HD2	1.92	0.50
1:A:397:ILE:HG13	1:A:438:PHE:CE1	2.47	0.50
1:A:405:LYS:HD3	1:A:405:LYS:C	2.32	0.50
2:D:173:THR:N	3:D:607:HOH:O	2.45	0.50
2:D:300:ILE:HD13	2:D:431:ILE:HD11	1.94	0.50
2:D:112:LYS:HB3	2:D:322:PHE:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:VAL:O	1:B:410:GLU:N	2.45	0.50
1:B:403:LYS:O	1:B:407:VAL:HG12	2.12	0.49
2:D:347:THR:HB	2:D:394:LEU:HD13	1.94	0.49
2:C:300:ILE:HG13	2:C:345:GLY:HA3	1.94	0.49
2:C:481:TRP:O	2:C:497:ARG:HB3	2.12	0.49
2:C:349:PHE:CD1	2:C:394:LEU:HD21	2.46	0.49
2:C:365:PHE:O	2:C:369:LEU:HD23	2.11	0.49
2:C:487:ASP:OD1	2:C:491:LYS:N	2.45	0.49
1:B:342:GLN:OE1	1:B:441:LYS:HE3	2.12	0.49
2:C:301:PHE:HD2	2:C:428:ALA:HB2	1.77	0.49
1:A:348:GLU:OE2	3:A:502:HOH:O	2.20	0.48
2:D:171:ASP:O	3:D:607:HOH:O	2.20	0.48
2:C:260:LYS:HG3	2:C:261:SER:N	2.28	0.48
2:C:388:SER:HB2	2:C:407:LYS:HE3	1.94	0.48
1:A:203:LYS:HE2	1:A:250:ARG:HD3	1.94	0.48
1:A:285:ASP:OD2	1:A:404:SER:OG	2.29	0.48
2:D:156:ILE:HD12	2:D:265:ALA:HB3	1.96	0.48
2:C:389:PHE:HB3	2:C:412:ILE:CD1	2.44	0.48
2:D:238:ASP:OD1	2:D:424:ARG:NH1	2.47	0.48
2:D:533:LEU:HD13	2:D:535:TRP:CZ2	2.48	0.48
2:C:409:PHE:HE2	2:C:413:ARG:HB3	1.71	0.48
1:B:251:LYS:HE2	1:B:251:LYS:HA	1.95	0.48
2:C:465:ILE:HD11	2:C:516:LEU:HD11	1.96	0.48
1:B:407:VAL:CG2	1:B:417:PHE:CD2	2.97	0.48
1:A:225:ASP:HB3	1:A:240:ARG:HH21	1.80	0.47
1:A:369:ALA:HB3	1:A:372:LEU:HB2	1.95	0.47
2:D:156:ILE:CD1	2:D:262:GLN:HA	2.43	0.47
2:C:470:GLN:HB2	2:C:558:SER:HB3	1.94	0.47
1:B:276:SER:O	1:B:278:LYS:N	2.47	0.47
2:C:221:THR:HG23	2:C:224:ASN:H	1.78	0.47
2:C:224:ASN:O	2:C:227:THR:OG1	2.28	0.47
1:A:290:LYS:HD3	1:A:296:GLN:HG2	1.97	0.47
2:D:345:GLY:N	2:D:428:ALA:HB1	2.30	0.47
2:D:401:HIS:N	3:D:637:HOH:O	2.48	0.47
2:C:406:THR:HG21	2:C:411:VAL:HG11	1.97	0.47
1:B:321:SER:O	1:B:324:GLN:N	2.48	0.47
1:B:407:VAL:HG23	1:B:417:PHE:CD2	2.49	0.47
2:D:167:ASP:HB2	3:D:603:HOH:O	2.14	0.47
2:D:109:ILE:HB	2:D:313:ALA:HB2	1.95	0.47
1:B:423:THR:HG23	1:B:433:LYS:CD	2.44	0.47
2:C:366:SER:O	2:C:368:ALA:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:544:GLU:HG3	2:C:568:ILE:HD13	1.96	0.46
2:D:544:GLU:HG3	2:D:568:ILE:HD12	1.97	0.46
2:C:465:ILE:HB	2:C:514:ILE:HB	1.96	0.46
2:D:246:LEU:N	3:D:635:HOH:O	2.48	0.46
1:B:273:HIS:O	1:B:342:GLN:HA	2.15	0.46
2:C:389:PHE:O	2:C:405:VAL:HG13	2.16	0.46
2:D:166:ILE:HD12	2:D:273:ILE:CG1	2.42	0.46
2:C:412:ILE:O	2:C:415:VAL:HB	2.15	0.46
2:D:160:PRO:HD2	2:D:446:VAL:O	2.14	0.46
2:D:467:LEU:HD23	2:D:555:VAL:HB	1.97	0.46
2:C:499:TRP:CZ2	2:C:501:ASN:HB2	2.50	0.46
1:B:410:GLU:HG3	1:B:416:TYR:O	2.15	0.46
2:C:499:TRP:CE2	2:C:501:ASN:HB2	2.51	0.46
2:C:542:ILE:HD11	2:C:567:SER:N	2.31	0.46
1:B:271:ALA:HB1	1:B:302:VAL:HG21	1.98	0.46
2:C:264:GLU:HG3	2:C:271:SER:HB3	1.97	0.46
1:B:417:PHE:HE1	1:B:419:ILE:HG13	1.81	0.46
1:B:319:LEU:H	1:B:445:ASP:HB3	1.80	0.45
2:C:389:PHE:HB3	2:C:412:ILE:HD11	1.99	0.45
2:C:300:ILE:CG1	2:C:345:GLY:HA3	2.46	0.45
2:C:416:ILE:HD12	2:C:416:ILE:H	1.81	0.45
2:D:447:ASN:ND2	2:D:449:ARG:HD3	2.32	0.45
2:D:478:GLU:OE1	3:D:608:HOH:O	2.21	0.45
2:D:212:LYS:HD3	2:D:235:GLN:HE22	1.82	0.45
2:C:229:ILE:O	2:C:233:VAL:HG23	2.16	0.45
1:A:267:LYS:NZ	3:A:510:HOH:O	2.34	0.45
2:C:529:GLU:O	2:C:538:TRP:HA	2.16	0.45
1:A:247:TYR:O	1:A:250:ARG:HD2	2.17	0.45
2:C:393:VAL:HG21	2:C:419:ASN:CG	2.37	0.45
1:B:379:THR:HG23	1:B:389:GLU:O	2.16	0.44
1:A:215:LYS:HE3	1:A:215:LYS:HB3	1.73	0.44
1:A:368:ARG:HG2	1:A:373:ASN:HB3	1.99	0.44
2:C:528:ARG:HD2	2:C:538:TRP:HB3	1.98	0.44
2:C:196:LYS:HE3	2:C:317:ASP:HB3	2.00	0.44
2:C:532:GLY:HA3	1:B:309:MET:HE2	1.98	0.44
2:D:278:LEU:HD11	2:D:349:PHE:HB3	1.98	0.44
2:C:225:VAL:O	2:C:229:ILE:HG13	2.18	0.44
2:C:250:THR:HA	2:C:300:ILE:HG22	1.98	0.44
1:B:256:LYS:HE2	1:B:256:LYS:HB2	1.95	0.44
2:C:156:ILE:HG23	2:C:452:TYR:HE1	1.82	0.44
1:B:252:TYR:HB2	1:B:363:SER:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:132:GLU:OE1	2:D:132:GLU:N	2.41	0.43
2:C:410:ASP:HA	2:C:413:ARG:CD	2.47	0.43
1:B:219:GLU:O	1:B:223:THR:HG23	2.18	0.43
1:B:349:LEU:O	1:B:353:ILE:HG13	2.17	0.43
2:D:246:LEU:HD12	2:D:247:PRO:HD2	1.99	0.43
1:B:391:GLU:HG3	3:B:505:HOH:O	2.19	0.43
2:C:263:ILE:HD12	2:C:263:ILE:HA	1.86	0.43
2:C:346:ARG:NH2	2:C:426:ASN:HB3	2.33	0.43
2:D:379:LYS:HG3	2:D:380:TYR:CD1	2.54	0.43
2:C:347:THR:HB	2:C:394:LEU:HD23	2.01	0.43
2:C:523:ILE:HB	2:C:547:VAL:HB	2.00	0.43
1:B:257:GLU:OE1	1:B:257:GLU:N	2.25	0.43
2:D:151:ARG:NH1	3:D:620:HOH:O	2.37	0.43
2:D:178:LEU:HD23	2:D:197:ARG:NH1	2.33	0.43
2:C:531:THR:HG21	2:C:539:ARG:CD	2.48	0.43
1:B:250:ARG:O	1:B:251:LYS:HE2	2.19	0.43
1:A:369:ALA:O	1:A:371:SER:N	2.52	0.43
2:C:113:ILE:HD13	2:C:438:LEU:HD23	2.01	0.42
2:C:548:LYS:HB3	2:C:570:TYR:CE2	2.54	0.42
2:C:105:HIS:CE1	2:C:321:THR:HG22	2.54	0.42
2:C:164:SER:OG	2:C:268:ASN:O	2.37	0.42
1:B:279:ASP:OD2	1:B:279:ASP:N	2.52	0.42
2:D:529:GLU:OE2	2:D:564:PRO:HG3	2.19	0.42
2:C:156:ILE:HD13	2:C:262:GLN:HA	2.00	0.42
2:D:421:THR:HG23	2:D:426:ASN:HD22	1.85	0.42
2:C:153:LYS:NZ	2:C:451:GLU:OE1	2.53	0.42
1:A:369:ALA:CB	1:A:372:LEU:HB2	2.50	0.42
2:C:349:PHE:CE1	2:C:394:LEU:HD21	2.54	0.42
2:C:537:TRP:HZ2	1:B:309:MET:O	2.03	0.41
2:C:411:VAL:HG13	2:C:412:ILE:N	2.35	0.41
2:D:299:GLN:O	2:D:345:GLY:HA3	2.21	0.41
1:A:303:THR:HG23	1:A:304:SER:O	2.20	0.41
2:D:515:PRO:O	2:D:516:LEU:HD23	2.21	0.41
1:B:230:LYS:HE3	1:B:388:SER:HB3	2.03	0.41
2:C:484:ILE:HG13	2:C:521:ARG:NE	2.35	0.41
1:A:418:GLU:HG3	1:A:439:LYS:HG2	2.03	0.41
2:D:105:HIS:O	2:D:109:ILE:HG12	2.21	0.41
2:D:336:PRO:HG2	2:D:438:LEU:HB3	2.03	0.41
2:C:280:ILE:HG21	2:C:282:PHE:CZ	2.56	0.41
2:C:410:ASP:OD1	2:C:413:ARG:HD3	2.21	0.41
2:C:411:VAL:HG13	2:C:412:ILE:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:530:CYS:HB2	2:C:538:TRP:CZ3	2.56	0.41
1:A:336:TYR:HB3	1:A:340:VAL:HG22	2.02	0.41
2:C:156:ILE:HG23	2:C:452:TYR:CE1	2.56	0.41
2:D:140:VAL:HG13	2:D:147:ILE:HB	2.03	0.40
2:C:398:ALA:HB2	2:C:401:HIS:HE2	1.85	0.40
2:C:122:GLU:OE1	3:C:603:HOH:O	2.21	0.40
2:C:157:ASN:HA	2:C:448:ASN:O	2.20	0.40
2:C:174:TYR:CD2	2:C:177:ALA:HB2	2.56	0.40
2:C:277:THR:OG1	2:C:278:LEU:HD12	2.21	0.40
2:D:499:TRP:CE2	2:D:501:ASN:HB2	2.56	0.40
2:C:166:ILE:HD12	2:C:273:ILE:HG13	2.02	0.40
1:A:197:ARG:NH1	1:A:225:ASP:OD2	2.55	0.40
2:C:290:LYS:HB2	2:C:290:LYS:HE2	1.83	0.40
1:B:395:PRO:HB3	1:B:425:ILE:O	2.21	0.40
1:A:369:ALA:HB1	3:A:590:HOH:O	2.20	0.40
2:D:196:LYS:HE2	2:D:196:LYS:CA	2.52	0.40
2:D:484:ILE:HG13	2:D:521:ARG:HD3	2.02	0.40
2:C:204:ILE:O	2:C:213:ALA:HB1	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:720:HOH:O	3:C:648:HOH:O[3_445]	1.88	0.32
3:A:592:HOH:O	3:C:651:HOH:O[3_455]	2.13	0.07

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	247/268 (92%)	238 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	207/268 (77%)	200 (97%)	6 (3%)	1 (0%)	29 34
2	C	421/472 (89%)	402 (96%)	18 (4%)	1 (0%)	47 57
2	D	441/472 (93%)	429 (97%)	12 (3%)	0	100 100
All	All	1316/1480 (89%)	1269 (96%)	45 (3%)	2 (0%)	47 57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	133	ASN
1	B	421	ASP

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	219/235 (93%)	218 (100%)	1 (0%)	88 93
1	B	202/235 (86%)	200 (99%)	2 (1%)	76 84
2	C	392/414 (95%)	391 (100%)	1 (0%)	92 95
2	D	401/414 (97%)	401 (100%)	0	100 100
All	All	1214/1298 (94%)	1210 (100%)	4 (0%)	92 95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	LYS
2	C	524	ARG
1	B	254	TYR
1	B	295	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	127	ASN
2	D	235	GLN
2	D	402	ASN
2	D	426	ASN
2	C	448	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	251/268 (93%)	-0.11	1 (0%) 92 93	17, 36, 58, 82	0
1	B	230/268 (85%)	0.91	33 (14%) 2 1	48, 83, 109, 141	0
2	C	441/472 (93%)	0.40	29 (6%) 18 14	31, 61, 97, 122	0
2	D	455/472 (96%)	-0.01	7 (1%) 73 71	17, 47, 80, 109	0
All	All	1377/1480 (93%)	0.25	70 (5%) 28 25	17, 54, 97, 141	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	398	ALA	4.8
1	B	402	LEU	4.6
1	B	409	ALA	4.5
1	B	210	LYS	4.3
1	B	318	LYS	4.2
2	C	103	GLU	4.0
1	B	316	GLN	4.0
1	B	211	TRP	3.9
1	B	408	LEU	3.9
2	C	409	PHE	3.6
2	C	104	ASP	3.5
2	D	373	ASP	3.5
1	B	292	THR	3.4
1	B	284	PHE	3.3
1	B	411	ILE	3.3
2	D	401	HIS	3.1
1	B	276	SER	3.1
2	C	127	ASN	3.0
2	C	168	SER	3.0
2	C	411	VAL	3.0
2	D	247	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	372	LEU	2.9
1	B	406	ALA	2.9
2	C	283	LYS	2.9
1	B	390	SER	2.9
2	C	417	LYS	2.9
1	B	195	MET	2.8
2	C	565	TYR	2.8
2	C	380	TYR	2.8
2	C	418	ASP	2.8
1	B	302	VAL	2.8
1	B	341	TYR	2.8
1	B	433	LYS	2.8
2	C	135	VAL	2.7
2	C	397	ASP	2.7
1	B	435	THR	2.7
1	B	417	PHE	2.7
1	B	303	THR	2.6
2	C	545	ARG	2.6
2	C	223	ALA	2.6
1	B	214	ASP	2.6
1	B	371	SER	2.5
2	C	383	ILE	2.5
2	C	413	ARG	2.4
2	C	429	TYR	2.4
2	C	534	ALA	2.4
1	B	392	LEU	2.4
2	D	248	ALA	2.4
2	C	129	GLU	2.4
2	D	323	LYS	2.3
1	B	336	TYR	2.3
1	B	442	LYS	2.3
2	C	354	THR	2.3
2	C	535	TRP	2.3
2	C	300	ILE	2.3
2	C	251	GLN	2.3
1	B	410	GLU	2.3
1	B	216	GLN	2.2
2	C	220	PRO	2.2
2	D	402	ASN	2.1
1	B	293	ILE	2.1
1	A	412	ASP	2.1
1	B	445	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	243	GLY	2.1
2	C	225	VAL	2.1
2	C	339	VAL	2.1
2	C	401	HIS	2.1
1	B	412	ASP	2.0
1	B	383	LYS	2.0
1	B	407	VAL	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.