Full wwPDB X-ray Structure Validation Report (i)

Oct 25, 2023 – 10:06 AM EDT

PDB ID	:	3HD8
Title	:	Crystal structure of the Triticum aestivum xylanase inhibitor-IIA in complex with bacillus subtilis xylanase
Authors	:	Sansen, S.; Pollet, A.; Raedschelders, G.; Gebruers, K.; Rabijns, A.; Courtin, C.M.
Deposited on	:	2009-05-07
Resolution	:	2.39 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 (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:

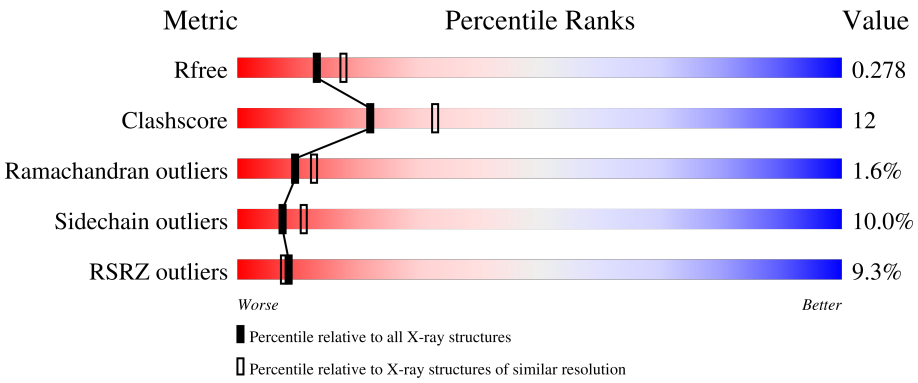
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	389	13% 67% 23% • • 5%
1	C	389	11% 74% 17% • • 5%
2	B	185	2% 75% 19% • • •
2	D	185	3% 72% 23% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8282 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 Xylanase inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	370	2682	1711	455	498	18	0	0	0
1	C	368	2672	1705	453	496	18	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	LYS	SEE REMARK 999	UNP Q53IQ4
A	163	PRO	ALA	SEE REMARK 999	UNP Q53IQ4
A	314	MET	LEU	SEE REMARK 999	UNP Q53IQ4
C	1	GLU	LYS	SEE REMARK 999	UNP Q53IQ4
C	163	PRO	ALA	SEE REMARK 999	UNP Q53IQ4
C	314	MET	LEU	SEE REMARK 999	UNP Q53IQ4

- Molecule 2 is a protein called Endo-1,4-beta-xylanase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	184	1443	909	248	284	2	0	0	0
2	D	184	1443	909	248	284	2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	147	THR	SER	SEE REMARK 999	UNP P18429
D	147	THR	SER	SEE REMARK 999	UNP P18429

- Molecule 3 is water.

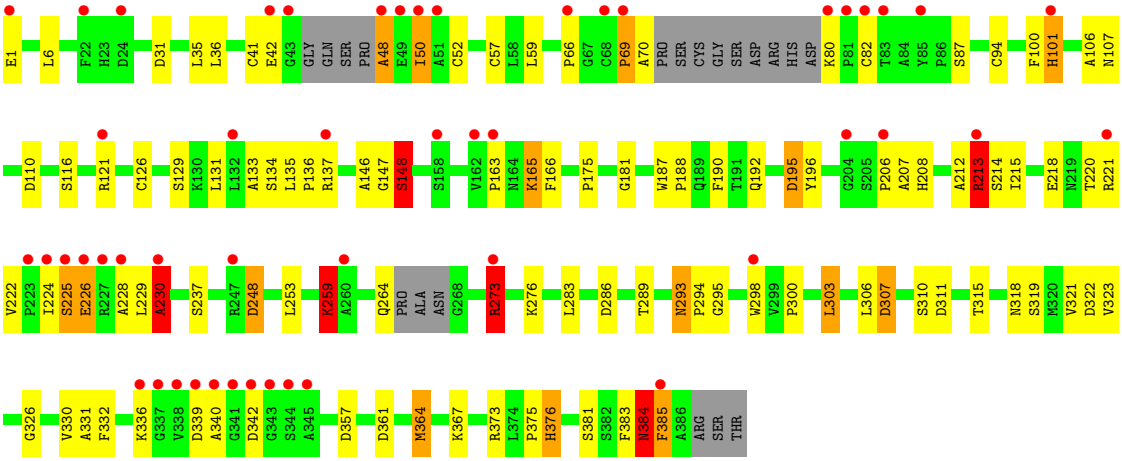
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	15	15	15	0	0
			Total	O		
3	B	7	7	7	0	0
			Total	O		
3	C	13	13	13	0	0
			Total	O		
3	D	7	7	7	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

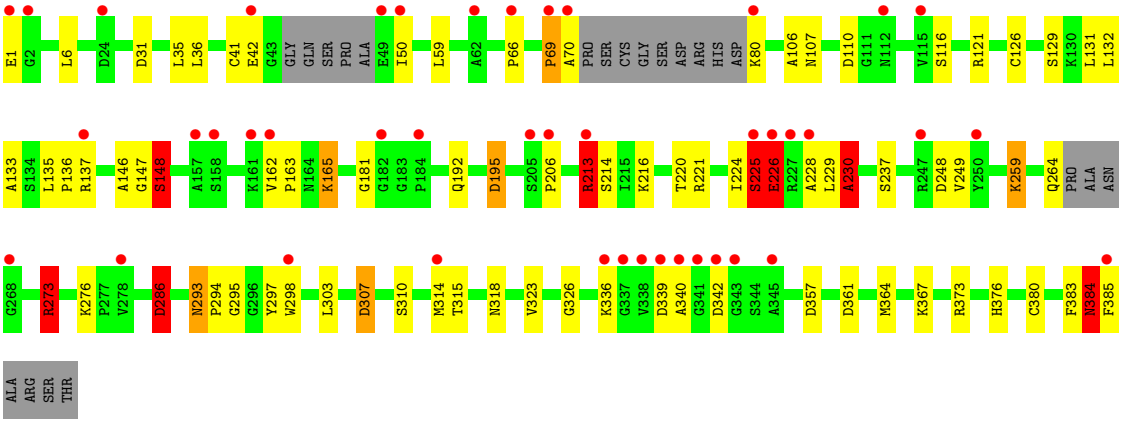
• Molecule 1: Xylanase inhibitor

Chain A:



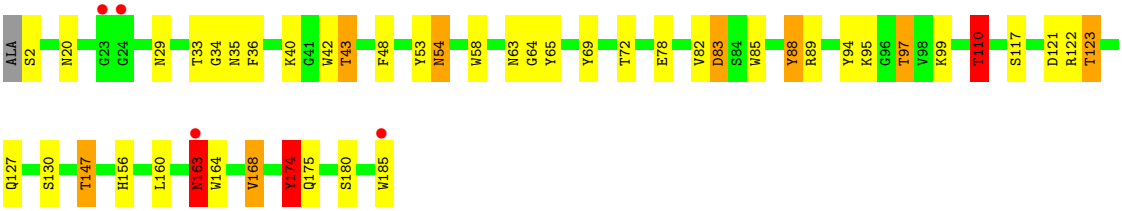
• Molecule 1: Xylanase inhibitor

Chain C:



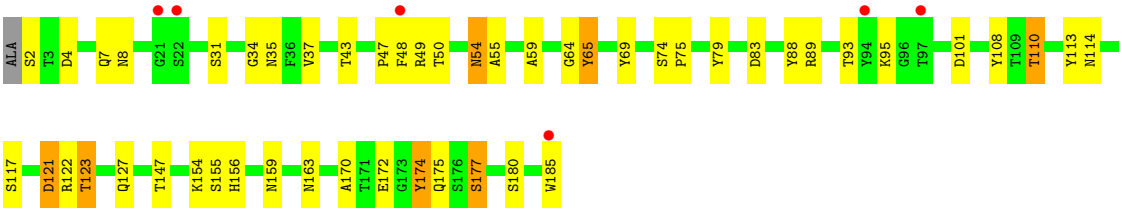
• Molecule 2: Endo-1,4-beta-xylanase A

Chain B:



• Molecule 2: Endo-1,4-beta-xylanase A

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.35Å 60.30Å 134.19Å 90.00° 101.49° 90.00°	Depositor
Resolution (Å)	38.52 – 2.39 38.52 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.8 (38.52-2.39) 98.7 (38.52-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	5.13 (at 2.39Å)	Xtriage
Refinement program	CNS, REFMAC 5.1.19	Depositor
R, R_{free}	0.223 , 0.275 0.236 , 0.278	Depositor DCC
R_{free} test set	2427 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	32.1	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 37.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8282	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% 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 (i)

5.1 Standard geometry (i)

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	1.23	10/2746 (0.4%)	1.17	16/3747 (0.4%)
1	C	1.28	9/2736 (0.3%)	1.16	15/3733 (0.4%)
2	B	1.39	11/1491 (0.7%)	1.12	6/2043 (0.3%)
2	D	1.30	8/1491 (0.5%)	1.17	9/2043 (0.4%)
All	All	1.29	38/8464 (0.4%)	1.16	46/11566 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	C	0	5
2	B	0	1
All	All	0	11

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	164	TRP	CB-CG	-8.75	1.34	1.50
1	C	195	ASP	CB-CG	8.64	1.69	1.51
1	A	385	PHE	CD1-CE1	7.37	1.53	1.39
2	B	163	ASN	CB-CG	-7.36	1.34	1.51
1	C	148	SER	CA-CB	7.33	1.64	1.52
2	B	130	SER	CB-OG	-6.79	1.33	1.42
1	A	165	LYS	CE-NZ	6.74	1.66	1.49
1	A	384	ASN	CB-CG	-6.49	1.36	1.51
2	D	174	TYR	CE1-CZ	-6.46	1.30	1.38
1	A	195	ASP	CB-CG	6.45	1.65	1.51
2	B	82	VAL	CB-CG2	-6.43	1.39	1.52
1	A	384	ASN	CA-C	6.42	1.69	1.52
1	A	148	SER	CA-CB	6.39	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	213	ARG	CZ-NH2	6.37	1.41	1.33
1	C	385	PHE	CD1-CE1	6.35	1.51	1.39
2	D	48	PHE	CD1-CE1	6.18	1.51	1.39
1	C	384	ASN	CA-C	5.84	1.68	1.52
1	C	165	LYS	CE-NZ	5.77	1.63	1.49
1	C	230	ALA	CA-CB	5.76	1.64	1.52
2	D	170	ALA	CA-CB	-5.75	1.40	1.52
2	B	174	TYR	CB-CG	-5.70	1.43	1.51
2	B	58	TRP	CB-CG	-5.64	1.40	1.50
1	A	196	TYR	CD1-CE1	5.57	1.47	1.39
2	B	88	TYR	CB-CG	5.53	1.59	1.51
1	C	216	LYS	CD-CE	5.53	1.65	1.51
1	A	319	SER	CB-OG	5.53	1.49	1.42
2	D	172	GLU	CD-OE2	5.50	1.31	1.25
1	A	230	ALA	CA-CB	5.49	1.64	1.52
2	D	79	TYR	CD2-CE2	5.46	1.47	1.39
2	B	174	TYR	CD2-CE2	-5.42	1.31	1.39
2	D	65	TYR	CE1-CZ	-5.27	1.31	1.38
2	B	42	TRP	CB-CG	-5.20	1.40	1.50
2	D	59	ALA	CA-CB	-5.20	1.41	1.52
2	B	174	TYR	CD1-CE1	-5.17	1.31	1.39
1	C	385	PHE	CD2-CE2	5.14	1.49	1.39
2	D	177	SER	CB-OG	5.05	1.48	1.42
1	A	259	LYS	CD-CE	5.03	1.63	1.51
2	B	99	LYS	CE-NZ	5.00	1.61	1.49

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	213	ARG	CA-CB-CG	14.79	145.94	113.40
1	A	213	ARG	CA-CB-CG	11.86	139.49	113.40
1	C	307	ASP	CB-CG-OD2	10.07	127.36	118.30
1	A	384	ASN	N-CA-C	8.71	134.53	111.00
2	B	163	ASN	CB-CA-C	8.60	127.60	110.40
1	C	384	ASN	N-CA-C	8.50	133.96	111.00
2	D	4	ASP	CB-CG-OD2	8.12	125.61	118.30
1	A	357	ASP	CB-CG-OD2	8.10	125.59	118.30
1	C	342	ASP	CB-CG-OD2	7.86	125.37	118.30
1	A	273	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	C	165	LYS	CD-CE-NZ	7.58	129.13	111.70
1	C	273	ARG	NE-CZ-NH1	7.52	124.06	120.30
2	D	101	ASP	CB-CG-OD2	7.28	124.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	185	TRP	CA-C-O	7.10	135.01	120.10
1	A	110	ASP	CB-CG-OD2	6.85	124.47	118.30
1	A	307	ASP	CB-CG-OD2	6.84	124.45	118.30
1	C	286	ASP	CB-CG-OD1	6.75	124.37	118.30
1	C	361	ASP	CB-CG-OD2	6.74	124.36	118.30
1	A	248	ASP	CB-CG-OD2	6.73	124.36	118.30
1	C	195	ASP	CB-CG-OD1	6.67	124.31	118.30
1	A	361	ASP	CB-CG-OD2	6.56	124.20	118.30
2	D	121	ASP	CB-CG-OD2	6.47	124.12	118.30
2	D	174	TYR	CE1-CZ-OH	-6.21	103.33	120.10
2	B	185	TRP	CA-C-O	6.16	133.04	120.10
1	A	307	ASP	CB-CG-OD1	-5.99	112.91	118.30
1	C	213	ARG	CB-CG-CD	-5.97	96.08	111.60
1	A	213	ARG	CB-CA-C	-5.89	98.61	110.40
2	D	89	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	C	273	ARG	NE-CZ-NH2	-5.82	117.39	120.30
2	D	49	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	A	342	ASP	CB-CG-OD2	5.75	123.47	118.30
2	D	174	TYR	OH-CZ-CE2	5.72	135.56	120.10
1	A	273	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	31	ASP	CB-CG-OD2	5.44	123.19	118.30
1	C	31	ASP	CB-CG-OD2	5.41	123.16	118.30
2	B	168	VAL	CB-CA-C	-5.33	101.28	111.40
2	B	121	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	36	LEU	CB-CA-C	-5.25	100.23	110.20
1	A	385	PHE	CB-CG-CD1	5.16	124.41	120.80
1	C	195	ASP	OD1-CG-OD2	-5.12	113.58	123.30
1	A	322	ASP	CB-CG-OD2	5.06	122.85	118.30
1	C	110	ASP	CB-CG-OD2	5.06	122.85	118.30
2	D	50	THR	OG1-CB-CG2	-5.05	98.39	110.00
2	B	110	THR	N-CA-CB	-5.02	100.76	110.30
2	B	147	THR	OG1-CB-CG2	-5.02	98.46	110.00
1	C	286	ASP	CB-CA-C	5.01	120.42	110.40

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	GLU	Peptide
1	A	146	ALA	Peptide
1	A	225	SER	Peptide
1	A	384	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	A	48	ALA	Peptide
2	B	33	THR	Peptide
1	C	1	GLU	Peptide
1	C	146	ALA	Peptide
1	C	225	SER	Peptide
1	C	36	LEU	Peptide
1	C	384	ASN	Peptide

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	2682	0	2679	71	0
1	C	2672	0	2669	69	0
2	B	1443	0	1314	33	0
2	D	1443	0	1314	31	0
3	A	15	0	0	2	0
3	B	7	0	0	2	0
3	C	13	0	0	3	0
3	D	7	0	0	0	0
All	All	8282	0	7976	191	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 12.

All (191) 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:D:117:SER:OG	2:D:123:THR:HG21	1.53	1.09
1:C:35:LEU:HD21	1:C:206:PRO:CB	1.81	1.09
1:A:385:PHE:HB3	3:A:404:HOH:O	1.54	1.07
1:A:35:LEU:HD21	1:A:206:PRO:CB	1.85	1.05
1:A:318:ASN:HD21	1:A:373:ARG:HH12	1.06	1.01
2:B:43:THR:HG22	3:B:188:HOH:O	1.59	1.01
1:C:35:LEU:HD21	1:C:206:PRO:CG	1.94	0.96
1:A:35:LEU:HD21	1:A:206:PRO:CG	1.96	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:ARG:HB3	1:C:213:ARG:CZ	1.98	0.93
1:C:318:ASN:HD21	1:C:373:ARG:HH12	0.97	0.91
2:D:154:LYS:HG3	2:D:159:ASN:ND2	1.87	0.90
1:A:383:PHE:O	1:A:384:ASN:HB2	1.73	0.89
1:C:213:ARG:NH2	1:C:307:ASP:OD1	2.05	0.89
1:C:383:PHE:O	1:C:384:ASN:HB2	1.71	0.88
1:A:315:THR:H	1:A:318:ASN:HD22	1.21	0.88
2:B:117:SER:OG	2:B:123:THR:HG21	1.74	0.87
1:C:318:ASN:ND2	1:C:373:ARG:HH12	1.73	0.86
1:A:35:LEU:HD21	1:A:206:PRO:HB3	1.58	0.86
1:C:35:LEU:HD11	1:C:206:PRO:HG2	1.58	0.85
1:A:107:ASN:ND2	3:A:396:HOH:O	2.11	0.84
1:C:315:THR:H	1:C:318:ASN:HD22	1.22	0.83
1:C:35:LEU:HD21	1:C:206:PRO:HB3	1.62	0.82
1:A:48:ALA:HB3	1:A:100:PHE:HA	1.63	0.80
1:A:318:ASN:ND2	1:A:373:ARG:HH12	1.80	0.80
1:C:107:ASN:ND2	3:C:395:HOH:O	2.15	0.79
1:C:264:GLN:OE1	1:C:298:TRP:CD1	2.37	0.76
2:B:110:THR:HG22	2:B:127:GLN:OE1	1.85	0.75
2:D:64:GLY:O	2:D:65:TYR:HD1	1.70	0.75
2:B:110:THR:CG2	2:B:127:GLN:OE1	2.35	0.74
1:A:190:PHE:HB3	2:B:174:TYR:OH	1.87	0.74
1:A:35:LEU:HD11	1:A:206:PRO:HG2	1.69	0.73
2:B:95:LYS:O	2:B:156:HIS:CD2	2.41	0.73
2:D:110:THR:HG22	2:D:127:GLN:OE1	1.88	0.73
1:C:35:LEU:CD2	1:C:206:PRO:HB3	2.18	0.73
1:C:35:LEU:HD21	1:C:206:PRO:HG2	1.70	0.72
1:A:147:GLY:O	1:A:148:SER:HB3	1.89	0.72
2:D:110:THR:CG2	2:D:127:GLN:OE1	2.37	0.72
1:C:264:GLN:OE1	1:C:298:TRP:HD1	1.72	0.72
2:B:95:LYS:O	2:B:156:HIS:HD2	1.71	0.72
1:A:213:ARG:NH2	1:A:307:ASP:OD1	2.24	0.71
1:A:35:LEU:CD2	1:A:206:PRO:HB3	2.22	0.70
2:D:95:LYS:O	2:D:156:HIS:HD2	1.75	0.69
1:C:318:ASN:HD21	1:C:373:ARG:NH1	1.82	0.68
1:A:35:LEU:HD21	1:A:206:PRO:HG2	1.76	0.68
1:C:147:GLY:O	1:C:148:SER:HB3	1.93	0.68
1:C:286:ASP:HA	1:C:326:GLY:O	1.94	0.68
1:C:273:ARG:HH11	1:C:273:ARG:HG2	1.59	0.67
2:D:154:LYS:HG3	2:D:159:ASN:HD21	1.59	0.67
1:C:35:LEU:CD2	1:C:206:PRO:CG	2.71	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:64:GLY:O	2:D:65:TYR:CD1	2.49	0.66
1:A:273:ARG:HG2	1:A:273:ARG:HH11	1.61	0.65
2:D:95:LYS:O	2:D:156:HIS:CD2	2.50	0.65
2:D:54:ASN:HD22	2:D:54:ASN:C	2.00	0.64
1:C:35:LEU:CD2	1:C:206:PRO:CB	2.65	0.63
2:B:34:GLY:HA2	2:B:175:GLN:NE2	2.14	0.62
2:D:117:SER:HG	2:D:123:THR:HG21	1.59	0.62
1:A:229:LEU:O	1:A:230:ALA:O	2.18	0.62
1:C:35:LEU:HD11	1:C:206:PRO:CG	2.30	0.62
1:A:69:PRO:O	1:A:70:ALA:HB2	2.01	0.61
1:C:376:HIS:H	2:D:35:ASN:ND2	1.98	0.61
1:A:163:PRO:HD2	1:A:181:GLY:O	2.01	0.61
1:C:213:ARG:CZ	1:C:307:ASP:OD1	2.48	0.61
1:C:376:HIS:H	2:D:35:ASN:HD21	1.49	0.61
1:C:163:PRO:HD2	1:C:181:GLY:O	2.00	0.60
1:A:192:GLN:NE2	2:B:88:TYR:OH	2.34	0.60
1:C:35:LEU:CD1	1:C:206:PRO:HG2	2.29	0.60
1:C:293:ASN:HB2	1:C:294:PRO:CD	2.32	0.59
1:A:35:LEU:CD2	1:A:206:PRO:CG	2.77	0.59
2:D:117:SER:CB	2:D:123:THR:HG21	2.31	0.58
1:C:315:THR:H	1:C:318:ASN:ND2	1.97	0.58
1:A:293:ASN:HB2	1:A:294:PRO:CD	2.34	0.58
1:C:315:THR:N	1:C:318:ASN:HD22	1.99	0.58
1:A:48:ALA:HB1	1:A:101:HIS:CE1	2.39	0.57
1:A:225:SER:OG	1:A:228:ALA:HB2	2.03	0.57
1:A:293:ASN:C	1:A:293:ASN:HD22	2.08	0.57
1:C:383:PHE:O	1:C:384:ASN:CB	2.48	0.57
2:B:29:ASN:ND2	1:C:213:ARG:HD3	2.20	0.57
1:A:293:ASN:HB2	1:A:294:PRO:HD2	1.87	0.57
2:D:34:GLY:HA2	2:D:175:GLN:HE21	1.70	0.56
1:A:293:ASN:ND2	1:A:295:GLY:H	2.04	0.56
1:A:213:ARG:CZ	1:A:307:ASP:OD1	2.54	0.56
1:A:286:ASP:HA	1:A:326:GLY:O	2.06	0.56
1:A:383:PHE:O	1:A:384:ASN:CB	2.52	0.56
1:C:248:ASP:HB3	1:C:340:ALA:HB1	1.89	0.55
1:A:293:ASN:HD22	1:A:295:GLY:H	1.53	0.55
1:A:273:ARG:HB2	1:A:289:THR:HG21	1.88	0.54
1:A:213:ARG:NH1	1:A:307:ASP:OD1	2.41	0.54
1:A:6:LEU:O	1:A:106:ALA:HB1	2.07	0.53
2:B:34:GLY:HA2	2:B:175:GLN:HE21	1.74	0.53
1:A:190:PHE:HB3	2:B:174:TYR:HH	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:HIS:HE2	2:D:37:VAL:HG21	1.74	0.53
1:A:248:ASP:HB3	1:A:340:ALA:HB1	1.90	0.53
1:A:35:LEU:HD11	1:A:206:PRO:CG	2.38	0.53
1:C:273:ARG:HH11	1:C:273:ARG:CG	2.21	0.53
2:D:93:THR:O	2:D:108:TYR:HA	2.09	0.53
1:C:192:GLN:NE2	2:D:88:TYR:OH	2.42	0.52
1:C:225:SER:HB2	1:C:226:GLU:O	2.10	0.52
1:C:225:SER:OG	1:C:228:ALA:HB2	2.09	0.52
2:B:94:TYR:OH	2:B:97:THR:HG22	2.10	0.51
1:C:35:LEU:CD2	1:C:206:PRO:HG2	2.38	0.51
1:C:293:ASN:HB2	1:C:294:PRO:HD2	1.92	0.51
1:A:315:THR:H	1:A:318:ASN:ND2	2.00	0.51
2:B:117:SER:CB	2:B:123:THR:HG21	2.40	0.51
1:C:264:GLN:CD	1:C:298:TRP:HE1	2.15	0.50
2:B:54:ASN:C	2:B:54:ASN:HD22	2.15	0.50
2:D:47:PRO:O	2:D:147:THR:HG22	2.12	0.50
2:D:110:THR:HG21	2:D:127:GLN:OE1	2.10	0.50
2:D:34:GLY:HA2	2:D:175:GLN:NE2	2.27	0.49
1:A:187:TRP:N	1:A:188:PRO:CD	2.75	0.49
1:C:293:ASN:HD22	1:C:295:GLY:H	1.59	0.49
1:A:293:ASN:HD22	1:A:295:GLY:N	2.10	0.49
1:A:69:PRO:O	1:A:70:ALA:CB	2.61	0.49
1:A:87:SER:HB3	1:A:94:CYS:HB3	1.95	0.48
1:A:376:HIS:ND1	1:A:376:HIS:C	2.67	0.48
1:C:163:PRO:O	1:C:181:GLY:HA2	2.13	0.48
1:C:229:LEU:C	3:C:402:HOH:O	2.51	0.48
1:A:376:HIS:H	2:B:35:ASN:HD21	1.61	0.48
1:A:133:ALA:O	1:A:134:SER:HB3	2.13	0.48
1:C:69:PRO:O	1:C:70:ALA:HB2	2.13	0.48
1:C:264:GLN:CD	1:C:298:TRP:NE1	2.67	0.48
1:A:52:CYS:HA	1:A:57:CYS:SG	2.53	0.48
1:A:376:HIS:H	2:B:35:ASN:ND2	2.12	0.48
1:C:229:LEU:O	1:C:230:ALA:O	2.32	0.48
1:C:264:GLN:C	3:C:393:HOH:O	2.52	0.48
1:C:147:GLY:CA	1:C:364:MET:HE3	2.44	0.47
2:B:85:TRP:CE2	2:B:89:ARG:HB2	2.49	0.47
1:C:213:ARG:NH1	1:C:307:ASP:OD1	2.48	0.47
2:D:154:LYS:HG3	2:D:159:ASN:HD22	1.75	0.47
1:A:35:LEU:CD1	1:A:206:PRO:HG2	2.42	0.47
1:C:132:LEU:O	1:C:133:ALA:C	2.52	0.47
1:A:375:PRO:HG3	2:B:174:TYR:CZ	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:GLN:CD	1:C:298:TRP:CD1	2.89	0.46
2:D:113:TYR:O	2:D:114:ASN:C	2.53	0.46
1:A:273:ARG:HH11	1:A:273:ARG:CG	2.26	0.46
1:C:135:LEU:HB3	1:C:136:PRO:CD	2.46	0.46
1:C:297:TYR:CE2	2:D:121:ASP:HB2	2.51	0.46
1:C:224:ILE:HD13	1:C:249:VAL:HG13	1.96	0.46
2:B:64:GLY:O	2:B:65:TYR:HD1	1.98	0.46
1:A:376:HIS:C	1:A:376:HIS:HD1	2.19	0.45
2:D:54:ASN:C	2:D:54:ASN:ND2	2.69	0.45
2:D:47:PRO:O	2:D:147:THR:CG2	2.65	0.45
1:A:225:SER:OG	1:A:228:ALA:CB	2.65	0.45
1:C:147:GLY:HA2	1:C:364:MET:HE3	1.98	0.45
1:A:190:PHE:CB	2:B:174:TYR:HH	2.29	0.45
1:C:293:ASN:HD22	1:C:293:ASN:C	2.20	0.45
2:B:48:PHE:HA	2:B:147:THR:HG23	1.99	0.45
1:C:293:ASN:ND2	1:C:295:GLY:H	2.14	0.45
1:C:293:ASN:HD22	1:C:295:GLY:N	2.15	0.45
1:C:357:ASP:HA	1:C:380:CYS:SG	2.57	0.45
1:A:321:VAL:HG23	1:A:331:ALA:HB2	1.98	0.44
2:B:110:THR:HG21	2:B:127:GLN:OE1	2.16	0.44
1:A:259:LYS:HD3	1:A:259:LYS:HA	1.85	0.44
1:A:215:ILE:HG21	1:A:253:LEU:HD13	1.98	0.44
1:A:208:HIS:HE2	1:A:364:MET:CE	2.31	0.44
1:A:147:GLY:HA2	1:A:364:MET:HE3	2.00	0.44
2:B:20:ASN:OD1	2:B:40:LYS:CE	2.66	0.44
1:C:6:LEU:O	1:C:106:ALA:HB1	2.18	0.44
1:A:218:GLU:HG2	1:A:300:PRO:HB3	1.99	0.43
2:B:94:TYR:OH	2:B:97:THR:CG2	2.66	0.43
1:A:166:PHE:HE2	1:A:364:MET:HE2	1.83	0.43
1:C:147:GLY:O	1:C:148:SER:CB	2.64	0.43
1:A:50:ILE:HG22	1:A:82:CYS:HB2	2.01	0.43
2:B:163:ASN:HD22	2:B:163:ASN:C	2.22	0.43
1:A:306:LEU:O	1:A:307:ASP:C	2.57	0.43
1:C:314:MET:HA	1:C:318:ASN:HD22	1.84	0.42
2:D:54:ASN:HD22	2:D:55:ALA:N	2.16	0.42
2:D:74:SER:N	2:D:75:PRO:CA	2.82	0.42
1:A:264:GLN:OE1	1:A:298:TRP:CD1	2.72	0.42
1:C:147:GLY:CA	1:C:364:MET:CE	2.98	0.42
2:B:36:PHE:CD1	2:B:36:PHE:C	2.93	0.42
1:C:259:LYS:HD3	1:C:259:LYS:HA	1.89	0.42
2:B:48:PHE:HA	2:B:147:THR:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:GLU:O	2:B:127:GLN:HA	2.19	0.42
2:D:31:SER:HA	2:D:177:SER:OG	2.18	0.42
1:C:293:ASN:OD1	1:C:298:TRP:CE3	2.73	0.42
1:C:162:VAL:HG21	1:C:181:GLY:HA3	2.02	0.42
2:B:65:TYR:CZ	3:B:192:HOH:O	2.57	0.42
1:A:175:PRO:O	1:A:381:SER:HA	2.20	0.41
1:C:35:LEU:CD1	1:C:206:PRO:CG	2.95	0.41
1:C:273:ARG:CG	1:C:273:ARG:NH1	2.83	0.41
2:D:64:GLY:C	2:D:65:TYR:CD1	2.93	0.41
1:A:330:VAL:HG12	1:A:332:PHE:CD2	2.55	0.41
1:A:303:LEU:HD23	1:A:311:ASP:HB3	2.03	0.41
2:B:72:THR:HG21	2:B:160:LEU:HB3	2.03	0.41
1:A:50:ILE:HG22	1:A:50:ILE:O	2.21	0.41
1:A:135:LEU:HB3	1:A:136:PRO:CD	2.51	0.41
1:A:222:VAL:HG12	1:A:224:ILE:HG13	2.03	0.40
1:A:212:ALA:O	1:A:229:LEU:HB3	2.21	0.40
2:B:53:TYR:OH	2:B:83:ASP:OD2	2.24	0.40
2:B:63:ASN:HB2	2:B:174:TYR:O	2.21	0.40
2:D:154:LYS:HZ2	2:D:154:LYS:HB3	1.86	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	362/389 (93%)	334 (92%)	19 (5%)	9 (2%)	5 6
1	C	360/389 (92%)	335 (93%)	17 (5%)	8 (2%)	6 7
2	B	182/185 (98%)	177 (97%)	5 (3%)	0	100 100
2	D	182/185 (98%)	177 (97%)	5 (3%)	0	100 100
All	All	1086/1148 (95%)	1023 (94%)	46 (4%)	17 (2%)	9 13

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	PRO
1	A	230	ALA
1	A	283	LEU
1	A	384	ASN
1	C	69	PRO
1	C	230	ALA
1	C	384	ASN
1	A	50	ILE
1	A	148	SER
1	A	226	GLU
1	C	50	ILE
1	C	148	SER
1	A	66	PRO
1	C	226	GLU
1	A	207	ALA
1	C	66	PRO
1	C	225	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	283/301 (94%)	252 (89%)	31 (11%)	6 8
1	C	283/301 (94%)	254 (90%)	29 (10%)	7 10
2	B	151/151 (100%)	138 (91%)	13 (9%)	10 16
2	D	151/151 (100%)	137 (91%)	14 (9%)	9 13
All	All	868/904 (96%)	781 (90%)	87 (10%)	7 11

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	CYS
1	A	42	GLU
1	A	59	LEU

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Mol	Chain	Res	Type
1	A	80	LYS
1	A	101	HIS
1	A	116	SER
1	A	121	ARG
1	A	126	CYS
1	A	129	SER
1	A	131	LEU
1	A	137	ARG
1	A	165	LYS
1	A	195	ASP
1	A	213	ARG
1	A	214	SER
1	A	220	THR
1	A	221	ARG
1	A	226	GLU
1	A	237	SER
1	A	259	LYS
1	A	273	ARG
1	A	276	LYS
1	A	293	ASN
1	A	303	LEU
1	A	310	SER
1	A	323	VAL
1	A	336	LYS
1	A	339	ASP
1	A	364	MET
1	A	367	LYS
1	A	376	HIS
2	B	2	SER
2	B	43	THR
2	B	54	ASN
2	B	69	TYR
2	B	83	ASP
2	B	97	THR
2	B	110	THR
2	B	122	ARG
2	B	123	THR
2	B	163	ASN
2	B	168	VAL
2	B	174	TYR
2	B	180	SER
1	C	41	CYS

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Mol	Chain	Res	Type
1	C	42	GLU
1	C	59	LEU
1	C	80	LYS
1	C	116	SER
1	C	121	ARG
1	C	126	CYS
1	C	129	SER
1	C	131	LEU
1	C	137	ARG
1	C	165	LYS
1	C	195	ASP
1	C	213	ARG
1	C	214	SER
1	C	220	THR
1	C	221	ARG
1	C	226	GLU
1	C	237	SER
1	C	259	LYS
1	C	273	ARG
1	C	276	LYS
1	C	286	ASP
1	C	293	ASN
1	C	303	LEU
1	C	310	SER
1	C	323	VAL
1	C	336	LYS
1	C	339	ASP
1	C	367	LYS
2	D	2	SER
2	D	7	GLN
2	D	8	ASN
2	D	43	THR
2	D	54	ASN
2	D	69	TYR
2	D	83	ASP
2	D	110	THR
2	D	122	ARG
2	D	123	THR
2	D	155	SER
2	D	163	ASN
2	D	174	TYR
2	D	180	SER

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

Mol	Chain	Res	Type
1	A	61	ASN
1	A	107	ASN
1	A	192	GLN
1	A	293	ASN
1	A	318	ASN
2	B	8	ASN
2	B	35	ASN
2	B	54	ASN
2	B	133	GLN
2	B	148	ASN
2	B	159	ASN
2	B	163	ASN
2	B	175	GLN
1	C	61	ASN
1	C	107	ASN
1	C	192	GLN
1	C	293	ASN
1	C	318	ASN
2	D	8	ASN
2	D	35	ASN
2	D	54	ASN
2	D	133	GLN
2	D	148	ASN
2	D	159	ASN
2	D	163	ASN
2	D	175	GLN

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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	370/389 (95%)	0.79	50 (13%)	3	2	24, 43, 69, 85	0
1	C	368/389 (94%)	0.89	43 (11%)	4	4	24, 43, 68, 84	0
2	B	184/185 (99%)	0.20	4 (2%)	62	60	23, 32, 40, 52	0
2	D	184/185 (99%)	0.28	6 (3%)	46	45	24, 32, 40, 52	0
All	All	1106/1148 (96%)	0.64	103 (9%)	8	8	23, 37, 63, 85	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	339	ASP	10.7
1	A	340	ALA	9.6
1	C	338	VAL	8.2
1	C	342	ASP	7.3
1	C	227	ARG	7.1
1	C	340	ALA	7.0
1	A	342	ASP	7.0
1	A	338	VAL	6.7
1	C	1	GLU	6.5
1	A	341	GLY	6.3
1	C	343	GLY	6.1
1	C	337	GLY	5.5
1	A	49	GLU	5.4
1	C	70	ALA	5.4
1	C	226	GLU	5.3
1	A	343	GLY	5.2
1	A	226	GLU	5.2
1	C	206	PRO	4.9
1	A	385	PHE	4.8
1	C	385	PHE	4.8
1	A	339	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	247	ARG	4.8
1	C	341	GLY	4.7
1	A	50	ILE	4.6
1	C	345	ALA	4.6
1	A	1	GLU	4.5
1	C	247	ARG	4.3
1	C	158	SER	4.2
1	A	227	ARG	4.2
1	A	228	ALA	4.2
2	D	185	TRP	3.8
1	C	298	TRP	3.7
1	A	43	GLY	3.7
1	A	42	GLU	3.6
1	A	221	ARG	3.6
1	C	137	ARG	3.6
1	C	49	GLU	3.5
1	A	51	ALA	3.5
1	C	24	ASP	3.4
1	A	337	GLY	3.4
1	A	206	PRO	3.4
1	A	48	ALA	3.2
2	D	94	TYR	3.2
1	A	345	ALA	3.2
1	A	24	ASP	3.1
2	D	48	PHE	3.1
1	A	83	THR	3.1
1	A	22	PHE	3.1
1	C	228	ALA	3.0
1	C	80	LYS	3.0
2	D	22	SER	3.0
1	A	81	PRO	3.0
1	A	163	PRO	3.0
2	B	185	TRP	2.9
1	C	115	VAL	2.9
1	A	80	LYS	2.9
1	A	298	TRP	2.9
1	C	336	LYS	2.8
1	C	2	GLY	2.8
1	C	184	PRO	2.7
1	A	204	GLY	2.7
1	C	66	PRO	2.7
1	C	162	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	42	GLU	2.6
2	B	23	GLY	2.6
1	C	161	LYS	2.5
1	A	230	ALA	2.5
1	C	62	ALA	2.5
1	A	66	PRO	2.5
1	A	121	ARG	2.5
1	C	112	ASN	2.5
1	A	336	LYS	2.5
1	C	182	GLY	2.5
1	A	344	SER	2.5
1	C	278	VAL	2.4
1	A	213	ARG	2.4
2	B	163	ASN	2.4
2	B	24	GLY	2.4
1	C	69	PRO	2.4
1	C	225	SER	2.4
1	C	213	ARG	2.3
1	A	224	ILE	2.3
1	A	85	TYR	2.3
1	A	260	ALA	2.3
2	D	97	THR	2.3
1	A	69	PRO	2.3
1	C	314	MET	2.2
1	A	273	ARG	2.2
2	D	21	GLY	2.2
1	A	68	CYS	2.2
1	C	205	SER	2.2
1	A	82	CYS	2.1
1	C	268	GLY	2.1
1	A	101	HIS	2.1
1	A	137	ARG	2.1
1	A	223	PRO	2.1
1	A	132	LEU	2.1
1	A	162	VAL	2.1
1	C	157	ALA	2.0
1	A	225	SER	2.0
1	C	50	ILE	2.0
1	C	250	TYR	2.0
1	A	158	SER	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.