Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:42 PM GMT

PDB ID	:	4YUB
Title	:	Crystal structure of human Nicotinic Acid Phosphoribosyltransferase
Authors	:	Garavaglia, S.; Rizzi, M.; Marletta, A.S.
Deposited on	:	2015-03-18
Resolution	:	2.90 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

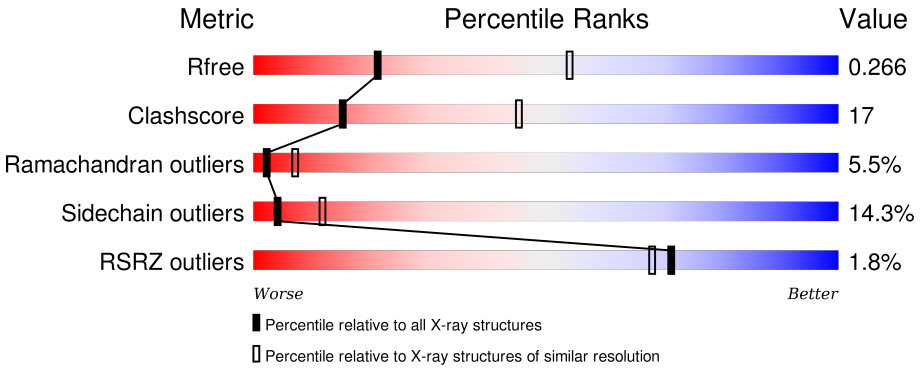
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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. 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	538	2% 54% 29% 8% • 7%
1	B	538	% 55% 28% 7% • 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7656 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 Nicotinate phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	500	Total	C	N	O	S	0	0	0
			3776	2409	668	684	15			
1	B	501	Total	C	N	O	S	0	0	0
			3782	2411	670	686	15			

- Molecule 2 is water.

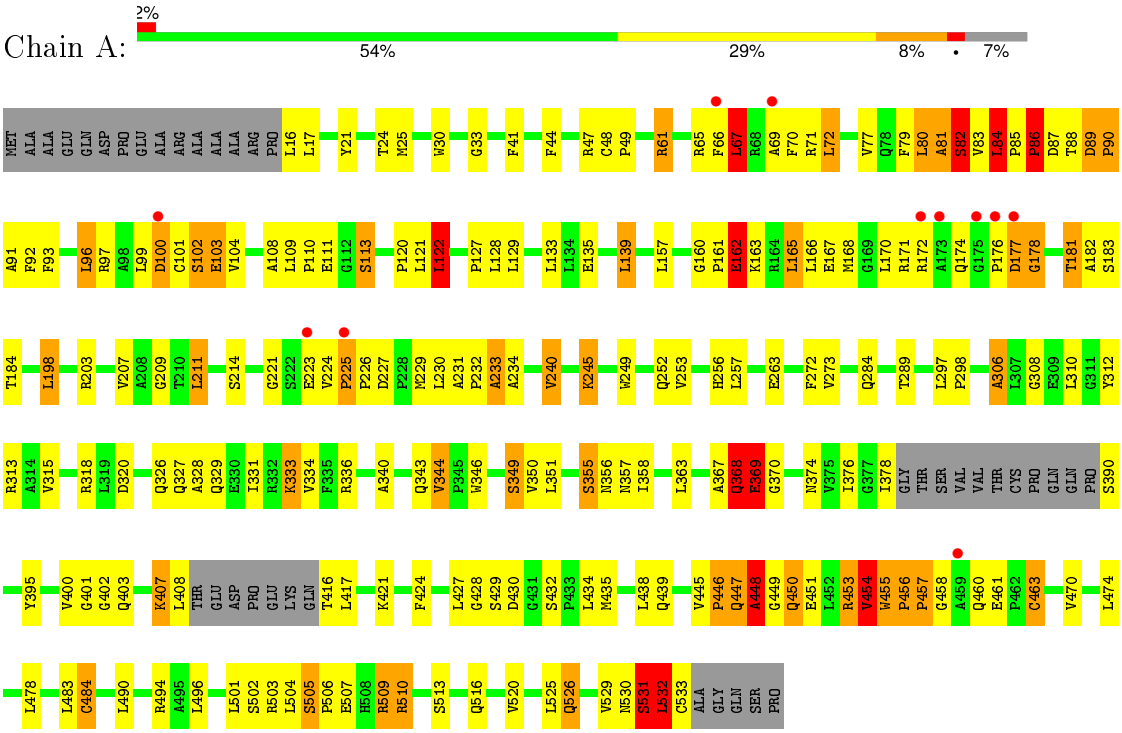
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	55	Total	O	0	0
			55	55		
2	B	43	Total	O	0	0
			43	43		

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 errors 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.

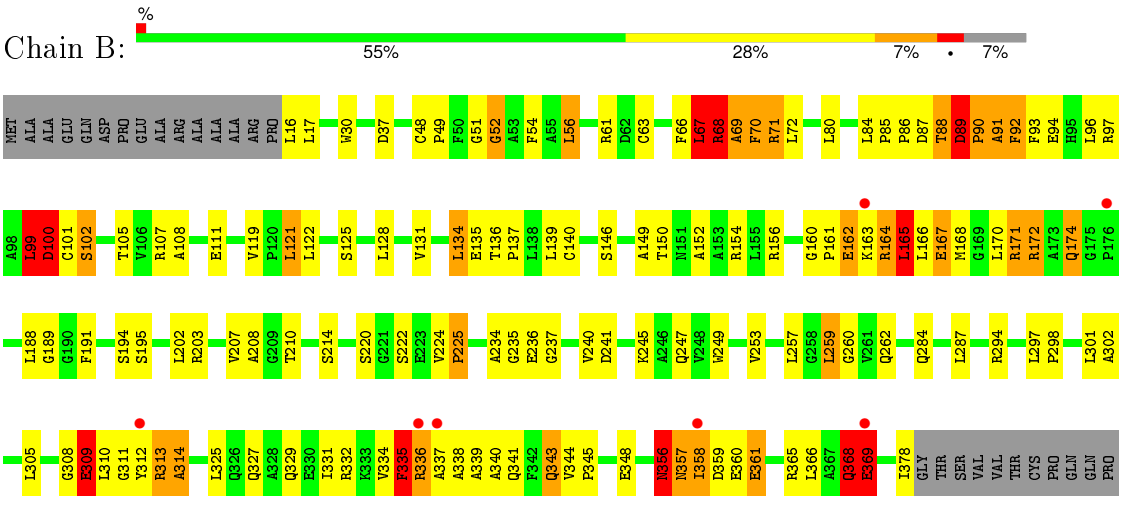
- Molecule 1: Nicotinate phosphoribosyltransferase

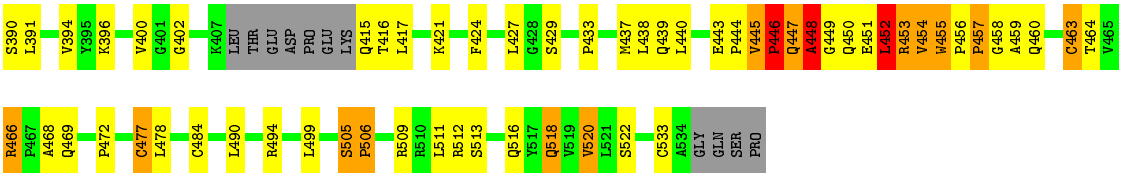
Chain A:



- Molecule 1: Nicotinate phosphoribosyltransferase

Chain B:




S390
L391
V394
Y395
K396
V400
G401
G402
K407
LEU
THR
GLU
ASP
PRO
GLU
LYS
Q415
T416
L417
K421
F424
L427
G428
S429
P433
M437
L438
Q439
L440
E443
P444
V445
P446
Q447
A448
G449
Q450
E451
L452
R453
V454
W455
P456
P457
G458
A459
Q460
C463
T464
V465
R466
P467
A468
Q469
P472
C477
L478
C484
L490
R494
L499
S505
P506
R509
R510
L511
R512
S513
Q516
Y517
Q518
V519
V520
L521
S522
C533
A534
GLY
GLN
SER
PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.02Å 101.09Å 125.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 58.64 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.90) 99.5 (58.64-2.90)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.28 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.197 , 0.243 0.205 , 0.266	Depositor DCC
R_{free} test set	124 reflections (0.49%)	DCC
Wilson B-factor (Å^2)	44.9	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 76.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 25261 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7656	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.75	0/3855	0.93	10/5246 (0.2%)
1	B	0.69	0/3861	0.88	5/5254 (0.1%)
All	All	0.72	0/7716	0.91	15/10500 (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
1	A	0	38
1	B	0	43
All	All	0	81

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	233	ALA	CB-CA-C	-9.60	95.70	110.10
1	A	446	PRO	CA-N-CD	-8.69	99.33	111.50
1	B	356	ASN	N-CA-C	-7.66	90.33	111.00
1	A	533	CYS	CA-CB-SG	-7.14	101.15	114.00
1	A	532	LEU	N-CA-C	-7.03	92.01	111.00
1	A	84	LEU	CB-CA-C	-6.89	97.11	110.20
1	A	90	PRO	CA-N-CD	-6.67	102.17	111.50
1	B	68	ARG	CB-CA-C	-6.34	97.72	110.40
1	B	356	ASN	C-N-CA	6.34	137.55	121.70
1	A	454	VAL	CB-CA-C	6.27	123.31	111.40
1	A	463	CYS	CA-CB-SG	5.81	124.46	114.00
1	B	484	CYS	CB-CA-C	5.37	121.15	110.40
1	A	100	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	67	LEU	CA-CB-CG	5.11	127.05	115.30
1	A	447	GLN	N-CA-C	5.08	124.71	111.00

There are no chirality outliers.

All (81) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	ALA	Peptide
1	A	122	LEU	Peptide
1	A	160	GLY	Peptide
1	A	162	GLU	Peptide
1	A	163	LYS	Peptide
1	A	166	LEU	Peptide
1	A	168	MET	Peptide
1	A	177	ASP	Peptide
1	A	178	GLY	Peptide
1	A	209	GLY	Peptide
1	A	221	GLY	Peptide
1	A	230	LEU	Peptide
1	A	306	ALA	Peptide
1	A	308	GLY	Peptide
1	A	315	VAL	Peptide
1	A	349	SER	Peptide
1	A	356	ASN	Peptide
1	A	357	ASN	Peptide
1	A	367	ALA	Peptide
1	A	368	GLN	Peptide
1	A	369	GLU	Peptide
1	A	370	GLY	Peptide
1	A	416	THR	Peptide
1	A	427	LEU	Peptide
1	A	428	GLY	Peptide
1	A	429	SER	Peptide
1	A	438	LEU	Peptide
1	A	448	ALA	Peptide
1	A	449	GLY	Peptide
1	A	450	GLN	Peptide
1	A	457	PRO	Peptide
1	A	67	LEU	Peptide
1	A	70	PHE	Peptide
1	A	72	LEU	Peptide
1	A	79	PHE	Peptide
1	A	81	ALA	Peptide
1	A	82	SER	Peptide
1	A	86	PRO	Peptide
1	B	100	ASP	Peptide
1	B	101	CYS	Peptide

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Mol	Chain	Res	Type	Group
1	B	16	LEU	Peptide
1	B	160	GLY	Peptide
1	B	163	LYS	Peptide
1	B	165	LEU	Peptide
1	B	168	MET	Peptide
1	B	171	ARG	Peptide
1	B	172	ARG	Peptide
1	B	174	GLN	Peptide
1	B	220	SER	Peptide
1	B	235	GLY	Peptide
1	B	259	LEU	Peptide
1	B	287	LEU	Peptide
1	B	308	GLY	Peptide
1	B	311	GLY	Peptide
1	B	314	ALA	Peptide
1	B	335	PHE	Peptide
1	B	356	ASN	Peptide
1	B	358	ILE	Peptide
1	B	359	ASP	Peptide
1	B	361	GLU	Peptide
1	B	368	GLN	Peptide
1	B	369	GLU	Peptide
1	B	390	SER	Peptide
1	B	444	PRO	Peptide
1	B	446	PRO	Peptide
1	B	448	ALA	Peptide
1	B	449	GLY	Peptide
1	B	452	LEU	Peptide
1	B	456	PRO	Peptide
1	B	463	CYS	Peptide
1	B	51	GLY	Peptide
1	B	518	GLN	Peptide
1	B	54	PHE	Peptide
1	B	69	ALA	Peptide
1	B	86	PRO	Peptide
1	B	88	THR	Peptide
1	B	89	ASP	Peptide
1	B	90	PRO	Peptide
1	B	91	ALA	Peptide
1	B	92	PHE	Peptide
1	B	99	LEU	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	3776	0	3827	137	0
1	B	3782	0	3831	133	0
2	A	55	0	0	6	0
2	B	43	0	0	8	0
All	All	7656	0	7658	265	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 17.

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)
1:A:435:MET:SD	1:A:453:ARG:NH1	1.94	1.40
1:B:455:TRP:CZ2	1:B:463:CYS:SG	2.38	1.16
1:B:356:ASN:O	1:B:358:ILE:HG23	1.45	1.16
1:A:435:MET:SD	1:A:453:ARG:CZ	2.33	1.16
1:B:455:TRP:NE1	1:B:463:CYS:SG	2.24	1.10
1:B:455:TRP:CE2	1:B:463:CYS:SG	2.48	1.05
1:B:453:ARG:NH2	1:B:520:VAL:HG13	1.70	1.04
1:B:162:GLU:OE1	1:B:165:LEU:HG	1.60	1.01
1:A:67:LEU:HD23	1:A:101:CYS:CB	1.92	1.00
1:A:435:MET:SD	1:A:453:ARG:NH2	2.38	0.97
1:A:446:PRO:HG2	1:A:470:VAL:HG11	1.50	0.94
1:B:455:TRP:HZ2	1:B:463:CYS:SG	1.89	0.93
1:A:532:LEU:CD1	2:A:650:HOH:O	2.17	0.93
1:A:67:LEU:HD23	1:A:101:CYS:HB2	1.56	0.87
1:A:67:LEU:CD2	1:A:101:CYS:CB	2.53	0.86
1:B:453:ARG:HH21	1:B:520:VAL:HG13	1.39	0.85
1:A:532:LEU:HD12	2:A:650:HOH:O	1.75	0.85
1:A:80:LEU:O	1:A:81:ALA:HB3	1.74	0.85
1:B:100:ASP:OD2	1:B:102:SER:OG	1.93	0.85
1:A:368:GLN:O	1:A:369:GLU:HG3	1.76	0.84
1:A:458:GLY:N	1:A:460:GLN:OE1	2.09	0.84
1:B:437:MET:HA	1:B:453:ARG:HH22	1.43	0.83
1:B:85:PRO:O	1:B:88:THR:HG23	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:CD2	1:A:101:CYS:HB3	2.09	0.82
1:A:453:ARG:NH1	1:A:520:VAL:HG21	1.94	0.82
1:A:89:ASP:O	1:A:91:ALA:N	2.11	0.82
1:B:309:GLU:HB2	1:B:310:LEU:HD12	1.61	0.82
1:B:368:GLN:HB3	1:B:369:GLU:HG2	1.60	0.81
1:B:357:ASN:HB3	2:B:637:HOH:O	1.82	0.80
1:B:455:TRP:HE1	1:B:463:CYS:CB	1.95	0.79
1:B:89:ASP:O	1:B:91:ALA:N	2.16	0.79
1:B:100:ASP:N	1:B:100:ASP:OD1	2.15	0.78
1:A:162:GLU:HB2	1:A:165:LEU:CD1	2.13	0.78
1:B:445:VAL:HB	1:B:446:PRO:HD3	1.67	0.77
1:A:99:LEU:O	1:A:100:ASP:OD1	2.03	0.77
1:B:294:ARG:CZ	2:B:602:HOH:O	2.34	0.76
1:A:446:PRO:C	1:A:447:GLN:HG2	2.07	0.75
1:A:478:LEU:HD13	1:A:483:LEU:HD23	1.69	0.74
1:B:61:ARG:NH1	1:B:111:GLU:OE1	2.19	0.74
1:B:131:VAL:HA	1:B:134:LEU:HD22	1.68	0.74
1:A:526:GLN:HE21	1:A:526:GLN:CA	2.01	0.73
1:A:80:LEU:O	1:A:81:ALA:CB	2.36	0.73
1:B:80:LEU:O	1:B:84:LEU:HD12	1.89	0.72
1:B:445:VAL:O	2:B:601:HOH:O	2.06	0.72
1:B:294:ARG:NH2	2:B:602:HOH:O	2.21	0.72
1:B:457:PRO:O	1:B:459:ALA:N	2.23	0.72
1:B:437:MET:HA	1:B:453:ARG:NH2	2.04	0.71
1:A:83:VAL:HG13	1:A:85:PRO:HD2	1.73	0.70
1:A:455:TRP:HB3	1:A:456:PRO:CD	2.23	0.68
1:B:162:GLU:CD	1:B:165:LEU:HG	2.13	0.68
1:B:96:LEU:O	1:B:99:LEU:HD23	1.93	0.68
1:A:455:TRP:HB3	1:A:456:PRO:HD2	1.74	0.68
1:A:532:LEU:HD13	2:A:650:HOH:O	1.85	0.67
1:A:445:VAL:HG12	1:A:446:PRO:CD	2.23	0.67
1:A:344:VAL:O	1:A:344:VAL:HG12	1.92	0.67
1:A:447:GLN:O	1:A:448:ALA:HB2	1.95	0.67
1:A:453:ARG:NH2	1:A:520:VAL:HG11	2.10	0.66
1:A:21:TYR:HA	1:A:24:THR:HB	1.78	0.66
1:B:334:VAL:O	1:B:338:ALA:N	2.29	0.66
1:B:56:LEU:HD12	1:B:56:LEU:C	2.16	0.65
1:B:453:ARG:NH1	1:B:520:VAL:C	2.50	0.65
1:B:56:LEU:HD11	1:B:149:ALA:HB1	1.76	0.65
1:B:164:ARG:CZ	1:B:164:ARG:HB3	2.26	0.64
1:B:191:PHE:O	1:B:494:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:GLU:HB2	1:A:165:LEU:HD13	1.80	0.64
1:A:530:ASN:O	1:A:531:SER:OG	2.13	0.63
1:B:240:VAL:HG21	1:B:245:LYS:HD3	1.81	0.63
1:A:445:VAL:HG12	1:A:446:PRO:HD2	1.80	0.62
1:B:453:ARG:NH1	1:B:520:VAL:O	2.30	0.62
1:A:83:VAL:O	1:A:84:LEU:HB2	1.99	0.62
1:B:170:LEU:HD13	2:B:607:HOH:O	2.00	0.62
1:A:47:ARG:O	1:A:49:PRO:HD3	2.00	0.62
1:B:49:PRO:HB3	1:B:391:LEU:HD23	1.83	0.61
1:B:437:MET:HG3	1:B:453:ARG:NH1	2.16	0.61
1:B:452:LEU:HA	1:B:463:CYS:O	2.01	0.61
1:A:344:VAL:CG1	1:A:344:VAL:O	2.47	0.61
1:A:224:VAL:C	1:A:226:PRO:HD3	2.20	0.61
1:B:253:VAL:HG12	1:B:257:LEU:HD12	1.81	0.61
1:A:453:ARG:CZ	1:A:520:VAL:HG11	2.31	0.60
1:A:82:SER:O	1:A:84:LEU:CD1	2.50	0.60
1:A:344:VAL:HG22	1:A:346:TRP:CH2	2.36	0.60
1:A:102:SER:O	1:A:103:GLU:CB	2.43	0.60
1:B:195:SER:HA	1:B:208:ALA:O	2.01	0.60
1:A:484:CYS:O	1:B:468:ALA:HB1	2.02	0.60
1:A:82:SER:O	1:A:84:LEU:HD13	2.01	0.59
1:A:453:ARG:CZ	1:A:520:VAL:HG21	2.31	0.59
1:B:162:GLU:HG3	1:B:165:LEU:HD21	1.84	0.59
1:B:63:CYS:O	1:B:67:LEU:HD12	2.03	0.59
1:B:162:GLU:CD	1:B:165:LEU:CD2	2.71	0.58
1:A:184:THR:HG23	1:A:490:LEU:HD11	1.85	0.58
1:B:156:ARG:HH12	1:B:165:LEU:HD13	1.67	0.58
1:A:526:GLN:HA	1:A:526:GLN:HE21	1.68	0.58
1:B:335:PHE:HD1	1:B:335:PHE:N	2.02	0.58
1:B:427:LEU:HD12	1:B:469:GLN:HB2	1.86	0.58
1:A:447:GLN:O	1:A:448:ALA:CB	2.52	0.57
1:A:368:GLN:O	1:A:369:GLU:CG	2.52	0.57
1:B:453:ARG:CZ	1:B:520:VAL:HG13	2.33	0.57
1:A:67:LEU:HD21	1:A:101:CYS:HB3	1.86	0.57
1:A:110:PRO:O	1:A:113:SER:OG	2.22	0.57
1:B:100:ASP:HB2	1:B:102:SER:HA	1.87	0.57
1:A:460:GLN:HG2	1:A:461:GLU:HG2	1.86	0.57
1:B:335:PHE:CD1	1:B:335:PHE:N	2.71	0.57
1:A:67:LEU:HD23	1:A:101:CYS:SG	2.45	0.57
1:A:525:LEU:O	1:A:529:VAL:HG23	2.05	0.56
1:B:194:SER:O	1:B:207:VAL:HA	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LEU:C	1:A:17:LEU:HD23	2.26	0.55
1:B:122:LEU:N	1:B:122:LEU:HD12	2.21	0.55
1:B:447:GLN:O	1:B:448:ALA:HB2	2.07	0.55
1:B:453:ARG:CZ	1:B:520:VAL:HG22	2.37	0.55
1:B:440:LEU:HB2	1:B:443:GLU:HG3	1.89	0.54
1:B:154:ARG:NH2	1:B:511:LEU:O	2.39	0.54
1:A:122:LEU:HD12	1:A:122:LEU:N	2.22	0.54
1:B:455:TRP:NE1	1:B:463:CYS:CB	2.65	0.54
1:B:511:LEU:C	1:B:512:ARG:HD3	2.28	0.54
1:A:504:LEU:HD23	1:A:509:ARG:HG3	1.89	0.54
1:A:445:VAL:CG1	1:A:446:PRO:CD	2.85	0.54
1:A:496:LEU:HD12	1:A:496:LEU:O	2.08	0.53
1:A:306:ALA:O	1:A:310:LEU:HD12	2.09	0.53
1:A:30:TRP:CZ2	1:A:92:PHE:CD2	2.96	0.53
1:A:167:GLU:HB3	1:A:376:ILE:O	2.07	0.53
1:B:107:ARG:HG3	1:B:107:ARG:HH11	1.74	0.53
1:A:67:LEU:CD2	1:A:101:CYS:HB2	2.31	0.53
1:A:162:GLU:CB	1:A:165:LEU:HD13	2.38	0.53
1:A:446:PRO:O	1:A:446:PRO:HD2	2.08	0.53
1:B:89:ASP:C	1:B:91:ALA:N	2.62	0.53
1:B:446:PRO:HB2	1:B:447:GLN:HA	1.91	0.53
1:A:249:TRP:O	1:A:253:VAL:HG23	2.09	0.53
1:B:162:GLU:CD	1:B:165:LEU:CG	2.76	0.53
1:B:297:LEU:HB3	1:B:298:PRO:CD	2.38	0.52
1:A:505:SER:HB2	1:A:506:PRO:HD2	1.92	0.52
1:A:526:GLN:NE2	1:A:526:GLN:CA	2.73	0.52
1:B:136:THR:N	1:B:137:PRO:HD2	2.25	0.51
1:B:451:GLU:O	1:B:464:THR:HA	2.10	0.51
1:B:337:ALA:HA	1:B:340:ALA:HB3	1.92	0.51
1:B:162:GLU:CG	1:B:165:LEU:HD21	2.41	0.50
1:A:454:VAL:HB	1:A:526:GLN:HG3	1.92	0.50
1:A:177:ASP:O	1:A:181:THR:HG23	2.11	0.50
1:B:325:LEU:HD22	1:B:365:ARG:HE	1.77	0.50
1:A:129:LEU:HD12	1:A:129:LEU:O	2.11	0.50
1:B:105:THR:HA	1:B:478:LEU:O	2.12	0.50
1:A:526:GLN:HE21	1:A:526:GLN:C	2.15	0.49
1:B:249:TRP:O	1:B:253:VAL:HG23	2.13	0.49
1:B:453:ARG:NH2	1:B:520:VAL:CG1	2.61	0.49
1:B:165:LEU:HD12	1:B:165:LEU:N	2.28	0.49
1:B:427:LEU:HD23	1:B:433:PRO:HA	1.94	0.49
1:B:210:THR:OG1	1:B:284:GLN:OE1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:VAL:HG21	1:A:245:LYS:CE	2.43	0.49
1:A:83:VAL:O	1:A:84:LEU:CB	2.61	0.49
1:B:170:LEU:HD22	2:B:607:HOH:O	2.12	0.49
1:B:477:CYS:SG	2:B:624:HOH:O	2.44	0.48
1:B:260:GLY:HA3	1:B:262:GLN:NE2	2.28	0.48
1:B:69:ALA:O	1:B:71:ARG:N	2.46	0.48
1:B:156:ARG:CZ	1:B:166:LEU:HD22	2.42	0.48
1:B:167:GLU:O	1:B:378:ILE:N	2.46	0.48
1:A:234:ALA:CB	1:B:343:GLN:HG2	2.44	0.48
1:B:437:MET:CA	1:B:453:ARG:NH2	2.76	0.48
1:A:445:VAL:CG1	1:A:446:PRO:HD3	2.44	0.48
1:B:361:GLU:HG2	1:B:361:GLU:O	2.12	0.48
1:A:526:GLN:HA	1:A:526:GLN:NE2	2.29	0.48
1:A:102:SER:C	1:A:104:VAL:H	2.17	0.48
1:B:455:TRP:NE1	1:B:463:CYS:HB2	2.29	0.47
1:A:109:LEU:HD12	1:A:121:LEU:HD22	1.96	0.47
1:B:309:GLU:H	1:B:309:GLU:HG2	1.38	0.47
1:A:135:GLU:O	1:A:139:LEU:HB2	2.15	0.47
1:B:162:GLU:CD	1:B:165:LEU:HD21	2.34	0.47
1:B:17:LEU:C	1:B:17:LEU:HD23	2.35	0.47
1:A:432:SER:CB	1:A:503:ARG:O	2.63	0.47
1:B:224:VAL:HA	1:B:225:PRO:HD3	1.83	0.47
1:A:109:LEU:HD12	1:A:121:LEU:CD2	2.45	0.47
1:B:301:LEU:O	1:B:302:ALA:C	2.51	0.47
1:A:417:LEU:O	1:A:421:LYS:NZ	2.44	0.47
1:A:333:LYS:O	1:A:336:ARG:HB3	2.15	0.47
1:A:272:PHE:O	1:A:273:VAL:C	2.48	0.47
1:A:390:SER:HB3	2:A:634:HOH:O	2.13	0.46
1:A:71:ARG:O	1:A:72:LEU:HD22	2.16	0.46
1:A:320:ASP:HA	1:A:355:SER:O	2.15	0.46
1:B:249:TRP:CE3	1:B:305:LEU:HD13	2.51	0.46
1:A:167:GLU:O	1:A:378:ILE:N	2.49	0.46
1:A:510:ARG:NH2	1:A:513:SER:O	2.31	0.46
1:B:139:LEU:O	1:B:140:CYS:C	2.53	0.46
1:B:52:GLY:HA3	2:B:614:HOH:O	2.15	0.46
1:A:446:PRO:O	1:A:447:GLN:HG2	2.15	0.46
1:B:70:PHE:HB3	1:B:99:LEU:HD13	1.98	0.46
1:B:331:ILE:O	1:B:335:PHE:CZ	2.69	0.46
1:A:313:ARG:HH22	1:B:313:ARG:HG3	1.81	0.46
1:A:174:GLN:CB	1:A:178:GLY:HA3	2.45	0.46
1:A:424:PHE:CE1	1:A:445:VAL:HG13	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:TRP:NE1	1:B:89:ASP:OD2	2.48	0.46
1:B:447:GLN:O	1:B:448:ALA:CB	2.63	0.46
1:A:225:PRO:O	1:A:226:PRO:C	2.49	0.45
1:A:89:ASP:O	1:A:92:PHE:N	2.43	0.45
1:B:394:VAL:HG12	1:B:396:LYS:HG2	1.98	0.45
1:A:233:ALA:HB2	1:A:312:TYR:CZ	2.51	0.45
1:B:332:ARG:NH1	1:B:348:GLU:O	2.49	0.45
1:A:162:GLU:HB2	1:A:165:LEU:HD11	1.97	0.45
1:B:108:ALA:HA	1:B:121:LEU:O	2.16	0.45
1:A:446:PRO:HB3	1:A:451:GLU:OE2	2.16	0.45
1:A:504:LEU:HD12	2:A:614:HOH:O	2.16	0.45
1:B:368:GLN:HG2	1:B:369:GLU:HA	1.99	0.45
1:B:439:GLN:HB2	1:B:443:GLU:OE2	2.17	0.45
1:B:361:GLU:CG	1:B:361:GLU:O	2.64	0.45
1:A:401:GLY:O	1:A:403:GLN:N	2.50	0.45
1:B:66:PHE:O	1:B:69:ALA:N	2.45	0.45
1:A:256:HIS:CD2	1:A:257:LEU:HD12	2.52	0.44
1:B:437:MET:HB2	1:B:453:ARG:CZ	2.48	0.44
1:A:44:PHE:HB3	1:A:120:PRO:HA	1.99	0.44
1:A:458:GLY:HA2	1:A:460:GLN:HE22	1.83	0.44
1:A:232:PRO:O	1:A:233:ALA:HB3	2.18	0.44
1:A:181:THR:O	1:A:182:ALA:C	2.55	0.44
1:B:94:GLU:OE1	1:B:97:ARG:NH1	2.51	0.44
1:B:344:VAL:HA	1:B:345:PRO:HD2	1.81	0.44
1:B:454:VAL:C	1:B:520:VAL:HG23	2.38	0.44
1:A:232:PRO:O	1:A:310:LEU:O	2.37	0.43
1:B:72:LEU:HA	1:B:72:LEU:HD12	1.87	0.43
1:B:37:ASP:O	1:B:128:LEU:N	2.50	0.43
1:B:49:PRO:HB3	1:B:391:LEU:CD2	2.48	0.43
1:A:133:LEU:HA	1:A:133:LEU:HD23	1.88	0.43
1:B:152:ALA:HB3	1:B:189:GLY:HA3	2.00	0.43
1:B:337:ALA:O	1:B:341:GLN:HB2	2.18	0.43
1:A:297:LEU:HB3	1:A:298:PRO:CD	2.48	0.43
1:A:234:ALA:HB2	1:B:343:GLN:OE1	2.19	0.43
1:A:93:PHE:O	1:A:96:LEU:HB2	2.19	0.43
1:A:490:LEU:O	1:A:494:ARG:HB2	2.18	0.43
1:A:66:PHE:O	1:A:69:ALA:N	2.52	0.43
1:A:77:VAL:HG21	1:A:97:ARG:HG2	2.01	0.43
1:A:326:GLN:O	1:A:327:GLN:C	2.55	0.42
1:A:127:PRO:O	1:A:128:LEU:C	2.56	0.42
1:A:41:PHE:CD2	1:A:395:TYR:CE2	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:ARG:NE	1:B:520:VAL:HG22	2.34	0.42
1:A:102:SER:O	1:A:103:GLU:HB3	2.16	0.42
1:A:93:PHE:CD2	1:A:93:PHE:N	2.86	0.42
1:A:227:ASP:OD1	1:A:229:MET:HB2	2.19	0.42
1:B:450:GLN:HB3	1:B:466:ARG:CD	2.48	0.42
1:B:325:LEU:HD13	1:B:366:LEU:HD23	2.00	0.42
1:A:24:THR:HG22	1:A:25:MET:N	2.35	0.42
1:B:505:SER:HA	1:B:506:PRO:HD2	1.86	0.42
1:A:211:LEU:HD21	1:A:284:GLN:HB2	2.01	0.42
1:A:81:ALA:N	1:A:83:VAL:H	2.18	0.42
1:A:435:MET:CG	1:A:453:ARG:NH1	2.79	0.42
1:A:458:GLY:CA	1:A:460:GLN:OE1	2.68	0.42
1:B:446:PRO:HG2	1:B:447:GLN:CG	2.50	0.42
1:A:65:ARG:HG2	1:A:66:PHE:N	2.35	0.42
1:B:325:LEU:O	1:B:329:GLN:HG3	2.20	0.41
1:B:424:PHE:CE2	1:B:472:PRO:HB3	2.55	0.41
1:A:456:PRO:HD2	1:A:457:PRO:HD2	2.02	0.41
1:B:339:ALA:O	1:B:343:GLN:HA	2.19	0.41
1:B:119:VAL:HG13	1:B:438:LEU:HD21	2.01	0.41
1:A:89:ASP:C	1:A:91:ALA:N	2.72	0.41
1:B:331:ILE:O	1:B:335:PHE:CE1	2.74	0.41
1:A:33:GLY:HA2	2:A:621:HOH:O	2.19	0.41
1:B:339:ALA:O	1:B:343:GLN:N	2.52	0.41
1:A:340:ALA:HA	1:B:234:ALA:HB1	2.02	0.41
1:A:162:GLU:C	1:A:165:LEU:HD13	2.41	0.41
1:B:146:SER:O	1:B:150:THR:OG1	2.34	0.41
1:A:446:PRO:O	1:A:446:PRO:CD	2.69	0.41
1:A:198:LEU:H	1:A:198:LEU:HG	1.59	0.41
1:A:351:LEU:HA	1:A:374:ASN:OD1	2.20	0.41
1:A:407:LYS:N	1:A:407:LYS:HD3	2.36	0.40
1:A:61:ARG:CG	1:A:111:GLU:OE2	2.69	0.40
1:B:455:TRP:HA	1:B:520:VAL:HB	2.04	0.40
1:B:96:LEU:O	1:B:99:LEU:CD2	2.64	0.40
1:A:21:TYR:CD1	1:A:21:TYR:C	2.94	0.40
1:B:134:LEU:O	1:B:135:GLU:C	2.59	0.40
1:A:328:ALA:HA	1:A:331:ILE:HD12	2.03	0.40
1:B:417:LEU:HB2	1:B:421:LYS:HE2	2.03	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	494/538 (92%)	407 (82%)	66 (13%)	21 (4%)	3 13
1	B	495/538 (92%)	411 (83%)	51 (10%)	33 (7%)	1 4
All	All	989/1076 (92%)	818 (83%)	117 (12%)	54 (6%)	2 7

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	CYS
1	A	84	LEU
1	A	87	ASP
1	A	89	ASP
1	A	90	PRO
1	A	176	PRO
1	A	231	ALA
1	A	358	ILE
1	A	369	GLU
1	A	402	GLY
1	A	448	ALA
1	A	531	SER
1	B	52	GLY
1	B	68	ARG
1	B	70	PHE
1	B	89	ASP
1	B	99	LEU
1	B	236	GLU
1	B	314	ALA
1	B	336	ARG
1	B	445	VAL
1	B	448	ALA
1	B	457	PRO
1	B	533	CYS
1	A	80	LEU

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Mol	Chain	Res	Type
1	A	161	PRO
1	A	368	GLN
1	A	455	TRP
1	A	510	ARG
1	B	67	LEU
1	B	93	PHE
1	B	241	ASP
1	B	312	TYR
1	B	446	PRO
1	B	447	GLN
1	B	453	ARG
1	B	87	ASP
1	B	90	PRO
1	B	490	LEU
1	A	456	PRO
1	B	225	PRO
1	B	356	ASN
1	B	357	ASN
1	A	225	PRO
1	B	161	PRO
1	B	309	GLU
1	B	368	GLN
1	A	86	PRO
1	B	237	GLY
1	A	350	VAL
1	B	48	CYS
1	B	506	PRO
1	B	402	GLY
1	B	458	GLY

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	392/422 (93%)	330 (84%)	62 (16%)	3 9
1	B	392/422 (93%)	342 (87%)	50 (13%)	5 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	784/844 (93%)	672 (86%)	112 (14%)	4 12

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	61	ARG
1	A	67	LEU
1	A	82	SER
1	A	84	LEU
1	A	86	PRO
1	A	88	THR
1	A	96	LEU
1	A	102	SER
1	A	103	GLU
1	A	113	SER
1	A	122	LEU
1	A	139	LEU
1	A	157	LEU
1	A	162	GLU
1	A	165	LEU
1	A	170	LEU
1	A	171	ARG
1	A	172	ARG
1	A	181	THR
1	A	183	SER
1	A	198	LEU
1	A	203	ARG
1	A	207	VAL
1	A	211	LEU
1	A	214	SER
1	A	223	GLU
1	A	240	VAL
1	A	245	LYS
1	A	252	GLN
1	A	263	GLU
1	A	289	THR
1	A	318	ARG
1	A	329	GLN
1	A	333	LYS
1	A	334	VAL
1	A	343	GLN

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Mol	Chain	Res	Type
1	A	344	VAL
1	A	349	SER
1	A	355	SER
1	A	363	LEU
1	A	400	VAL
1	A	407	LYS
1	A	408	LEU
1	A	430	ASP
1	A	434	LEU
1	A	439	GLN
1	A	450	GLN
1	A	453	ARG
1	A	454	VAL
1	A	463	CYS
1	A	474	LEU
1	A	484	CYS
1	A	501	LEU
1	A	502	SER
1	A	505	SER
1	A	507	GLU
1	A	509	ARG
1	A	516	GLN
1	A	526	GLN
1	A	531	SER
1	A	532	LEU
1	B	56	LEU
1	B	68	ARG
1	B	71	ARG
1	B	89	ASP
1	B	92	PHE
1	B	100	ASP
1	B	102	SER
1	B	121	LEU
1	B	125	SER
1	B	134	LEU
1	B	162	GLU
1	B	164	ARG
1	B	165	LEU
1	B	167	GLU
1	B	171	ARG
1	B	172	ARG
1	B	174	GLN

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Mol	Chain	Res	Type
1	B	188	LEU
1	B	202	LEU
1	B	203	ARG
1	B	214	SER
1	B	222	SER
1	B	247	GLN
1	B	259	LEU
1	B	309	GLU
1	B	313	ARG
1	B	327	GLN
1	B	335	PHE
1	B	336	ARG
1	B	343	GLN
1	B	360	GLU
1	B	369	GLU
1	B	400	VAL
1	B	415	GLN
1	B	416	THR
1	B	429	SER
1	B	452	LEU
1	B	454	VAL
1	B	455	TRP
1	B	460	GLN
1	B	466	ARG
1	B	477	CYS
1	B	499	LEU
1	B	505	SER
1	B	509	ARG
1	B	513	SER
1	B	516	GLN
1	B	518	GLN
1	B	520	VAL
1	B	522	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	HIS
1	A	327	GLN
1	A	329	GLN
1	A	480	GLN
1	A	526	GLN

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Mol	Chain	Res	Type
1	A	530	ASN
1	B	357	ASN
1	B	480	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	500/538 (92%)	-0.27	11 (2%) 65 60	16, 34, 86, 161	0
1	B	501/538 (93%)	-0.16	7 (1%) 78 76	14, 36, 79, 164	0
All	All	1001/1076 (93%)	-0.22	18 (1%) 71 68	14, 35, 83, 164	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	337	ALA	7.9
1	B	336	ARG	6.9
1	A	175	GLY	5.2
1	A	173	ALA	3.8
1	A	459	ALA	3.7
1	B	369	GLU	3.5
1	B	312	TYR	3.1
1	A	100	ASP	3.1
1	A	176	PRO	2.8
1	B	358	ILE	2.7
1	A	223	GLU	2.5
1	A	177	ASP	2.4
1	A	225	PRO	2.4
1	A	69	ALA	2.3
1	B	176	PRO	2.2
1	B	163	LYS	2.1
1	A	172	ARG	2.1
1	A	66	PHE	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.