Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 11:02 PM GMT

PDB ID	:	5F7C
Title	:	Crystal structure of Family 31 alpha-glucosidase (BT_0339) from Bacteroides thetaiotaomicron
Authors	:	Chaudet, M.M.; Rose, D.R.
Deposited on	:	2015-12-07
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
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:

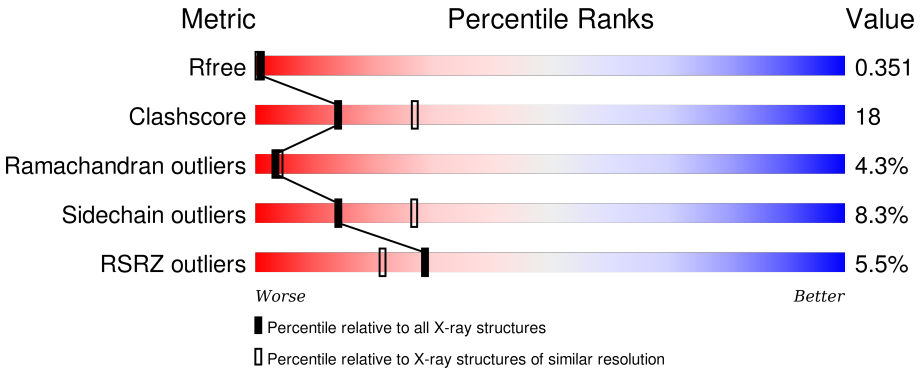
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 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	761	2% 50% 26% 6% • 18%
1	B	761	9% 53% 22% 5% 20%
1	C	761	3% 57% 23% • 17%
1	D	761	4% 51% 26% • 18%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 34019 atoms, of which 14026 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 Alpha-glucosidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	625	Total	C	H	N	O	S	0	0	0
			8422	3229	3426	837	901	29			
1	B	611	Total	C	H	N	O	S	0	0	0
			8403	3150	3512	832	881	28			
1	C	632	Total	C	H	N	O	S	0	0	0
			8637	3278	3548	865	917	29			
1	D	623	Total	C	H	N	O	S	0	0	0
			8490	3185	3540	840	895	30			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	LEU	PHE	conflict	UNP Q8AAX3
A	13	PHE	LEU	conflict	UNP Q8AAX3
A	750	HIS	-	expression tag	UNP Q8AAX3
A	751	HIS	-	expression tag	UNP Q8AAX3
A	752	HIS	-	expression tag	UNP Q8AAX3
A	753	HIS	-	expression tag	UNP Q8AAX3
A	754	HIS	-	expression tag	UNP Q8AAX3
A	755	HIS	-	expression tag	UNP Q8AAX3
A	756	LEU	-	expression tag	UNP Q8AAX3
A	757	ARG	-	expression tag	UNP Q8AAX3
A	758	VAL	-	expression tag	UNP Q8AAX3
A	759	PRO	-	expression tag	UNP Q8AAX3
A	760	ARG	-	expression tag	UNP Q8AAX3
A	761	GLY	-	expression tag	UNP Q8AAX3
A	762	SER	-	expression tag	UNP Q8AAX3
B	12	LEU	PHE	conflict	UNP Q8AAX3
B	13	PHE	LEU	conflict	UNP Q8AAX3
B	750	HIS	-	expression tag	UNP Q8AAX3
B	751	HIS	-	expression tag	UNP Q8AAX3
B	752	HIS	-	expression tag	UNP Q8AAX3
B	753	HIS	-	expression tag	UNP Q8AAX3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	754	HIS	-	expression tag	UNP Q8AAX3
B	755	HIS	-	expression tag	UNP Q8AAX3
B	756	LEU	-	expression tag	UNP Q8AAX3
B	757	ARG	-	expression tag	UNP Q8AAX3
B	758	VAL	-	expression tag	UNP Q8AAX3
B	759	PRO	-	expression tag	UNP Q8AAX3
B	760	ARG	-	expression tag	UNP Q8AAX3
B	761	GLY	-	expression tag	UNP Q8AAX3
B	762	SER	-	expression tag	UNP Q8AAX3
C	12	LEU	PHE	conflict	UNP Q8AAX3
C	13	PHE	LEU	conflict	UNP Q8AAX3
C	750	HIS	-	expression tag	UNP Q8AAX3
C	751	HIS	-	expression tag	UNP Q8AAX3
C	752	HIS	-	expression tag	UNP Q8AAX3
C	753	HIS	-	expression tag	UNP Q8AAX3
C	754	HIS	-	expression tag	UNP Q8AAX3
C	755	HIS	-	expression tag	UNP Q8AAX3
C	756	LEU	-	expression tag	UNP Q8AAX3
C	757	ARG	-	expression tag	UNP Q8AAX3
C	758	VAL	-	expression tag	UNP Q8AAX3
C	759	PRO	-	expression tag	UNP Q8AAX3
C	760	ARG	-	expression tag	UNP Q8AAX3
C	761	GLY	-	expression tag	UNP Q8AAX3
C	762	SER	-	expression tag	UNP Q8AAX3
D	12	LEU	PHE	conflict	UNP Q8AAX3
D	13	PHE	LEU	conflict	UNP Q8AAX3
D	750	HIS	-	expression tag	UNP Q8AAX3
D	751	HIS	-	expression tag	UNP Q8AAX3
D	752	HIS	-	expression tag	UNP Q8AAX3
D	753	HIS	-	expression tag	UNP Q8AAX3
D	754	HIS	-	expression tag	UNP Q8AAX3
D	755	HIS	-	expression tag	UNP Q8AAX3
D	756	LEU	-	expression tag	UNP Q8AAX3
D	757	ARG	-	expression tag	UNP Q8AAX3
D	758	VAL	-	expression tag	UNP Q8AAX3
D	759	PRO	-	expression tag	UNP Q8AAX3
D	760	ARG	-	expression tag	UNP Q8AAX3
D	761	GLY	-	expression tag	UNP Q8AAX3
D	762	SER	-	expression tag	UNP Q8AAX3

- Molecule 2 is water.

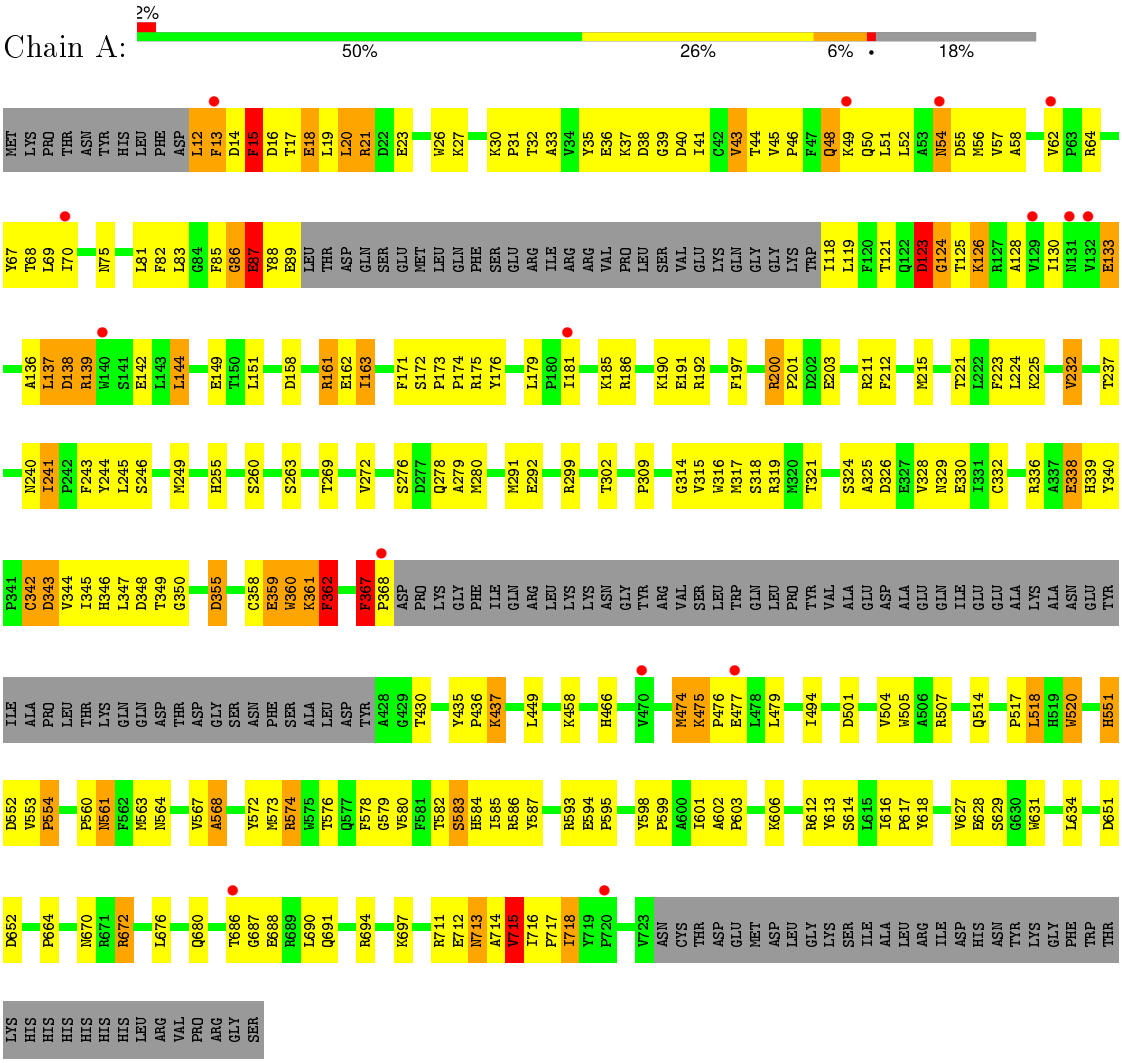
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	23	Total O 23 23	0	0
2	B	9	Total O 9 9	0	0
2	C	18	Total O 18 18	0	0
2	D	17	Total O 17 17	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

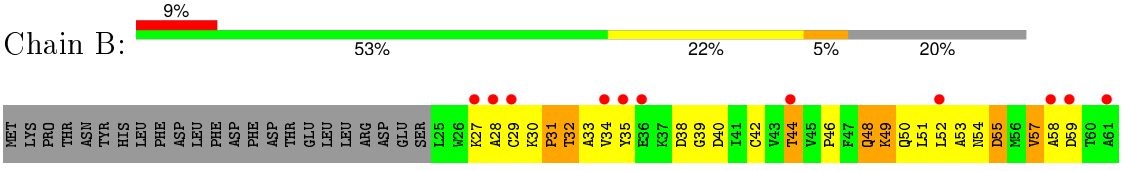
- Molecule 1: Alpha-glucosidase

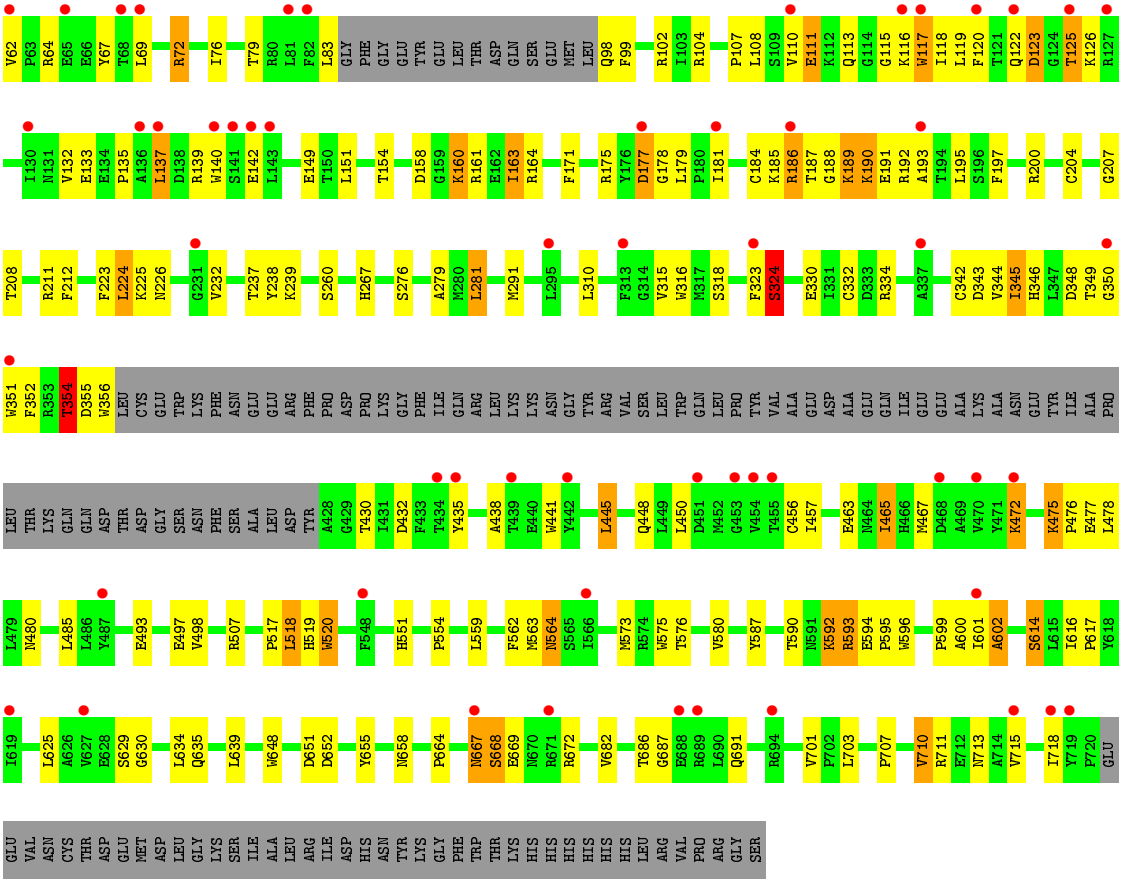
Chain A:



- Molecule 1: Alpha-glucosidase

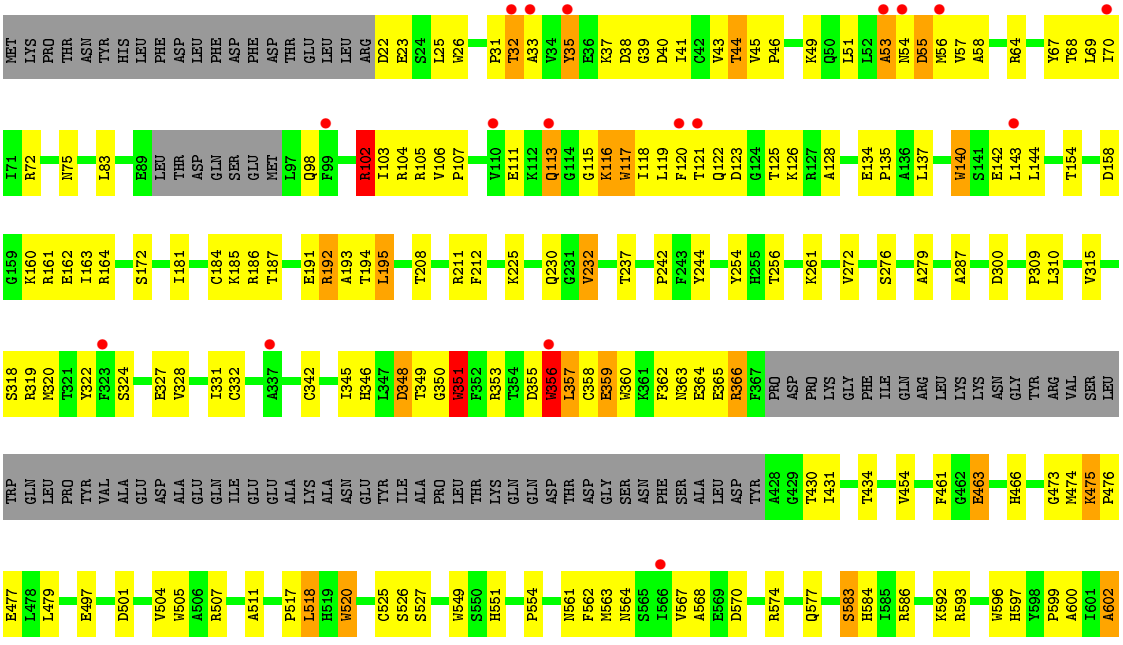
Chain B:

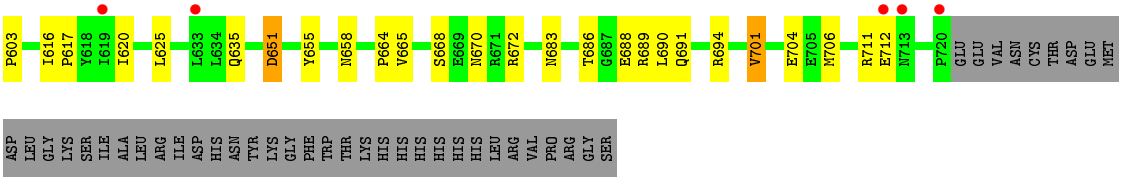




• Molecule 1: Alpha-glucosidase

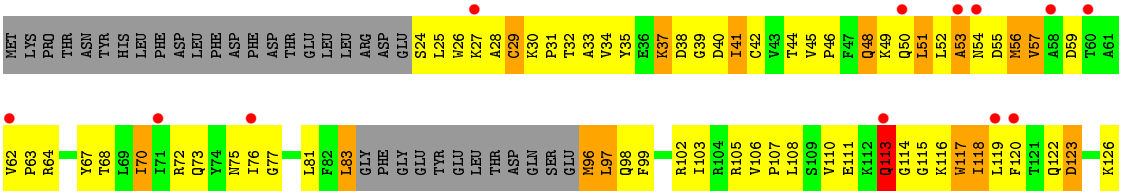
Chain C:

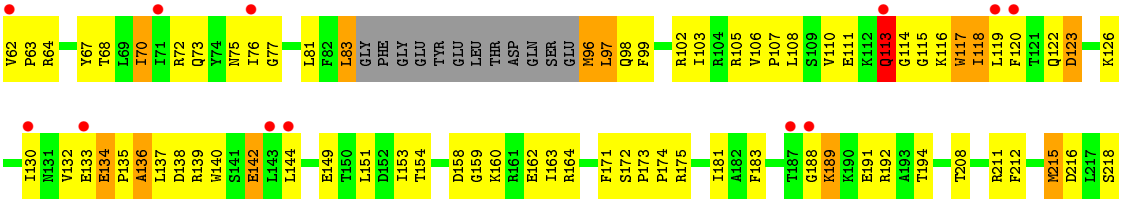


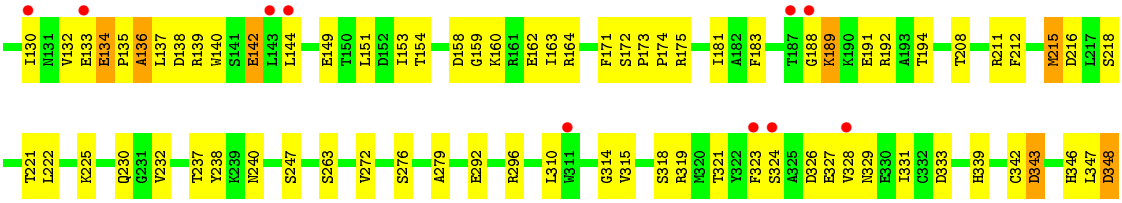


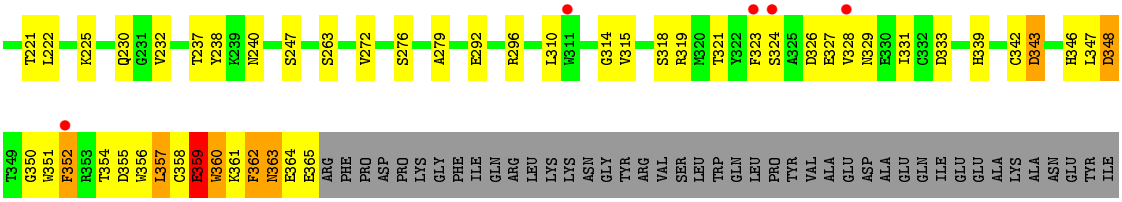
• Molecule 1: Alpha-glucosidase

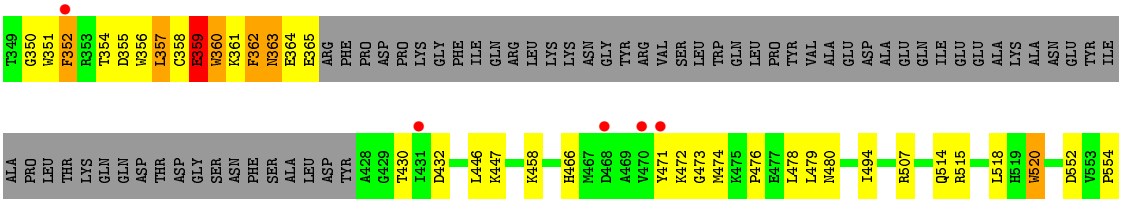
Chain D:

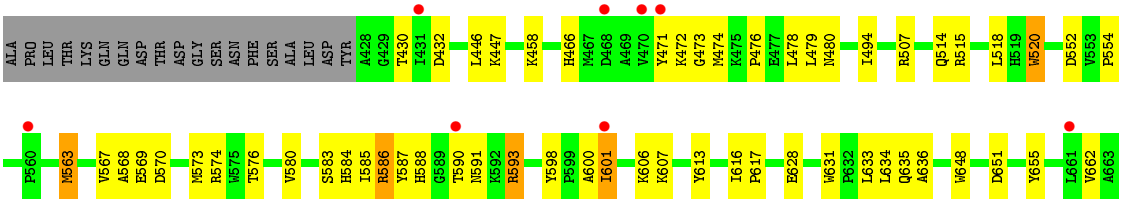


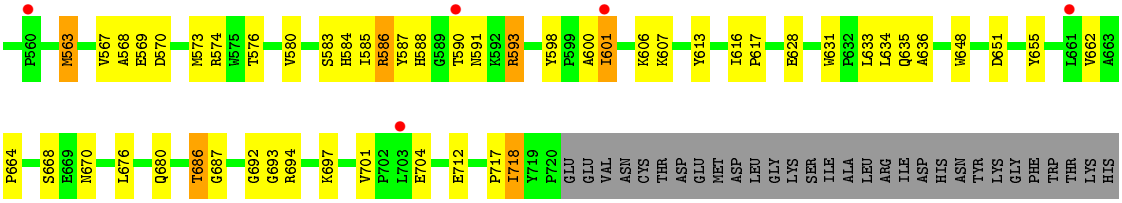












4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.34Å 75.00Å 232.86Å 90.00° 95.14° 90.00°	Depositor
Resolution (Å)	48.81 – 2.60 48.81 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.81-2.60) 100.0 (48.81-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.61Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.302 , 0.349 0.310 , 0.351	Depositor DCC
R_{free} test set	2000 reflections (2.34%)	DCC
Wilson B-factor (Å^2)	46.0	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 87516 reflections	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	34019	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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	0.66	1/5147 (0.0%)	0.58	1/7000 (0.0%)
1	B	0.71	2/5035 (0.0%)	0.48	1/6839 (0.0%)
1	C	0.74	2/5240 (0.0%)	0.55	1/7115 (0.0%)
1	D	0.74	2/5092 (0.0%)	0.54	1/6917 (0.0%)
All	All	0.71	7/20514 (0.0%)	0.54	4/27871 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	324	SER	CA-CB	-37.04	0.97	1.52
1	B	324	SER	CA-CB	-37.03	0.97	1.52
1	D	324	SER	CA-CB	-36.99	0.97	1.52
1	C	324	SER	CA-CB	-36.97	0.97	1.52
1	B	117	TRP	CA-CB	-25.68	0.97	1.53
1	C	117	TRP	CA-CB	-25.66	0.97	1.53
1	D	117	TRP	CA-CB	-25.66	0.97	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	476	PRO	N-CA-CB	5.63	110.06	103.30
1	D	476	PRO	N-CA-CB	5.57	109.99	103.30
1	A	476	PRO	N-CA-CB	5.31	109.67	103.30
1	C	476	PRO	N-CA-CB	5.24	109.58	103.30

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	4996	3426	4731	213	0
1	B	4891	3512	4668	166	0
1	C	5089	3548	4863	161	0
1	D	4950	3540	4704	182	0
2	A	23	0	0	0	0
2	B	9	0	0	0	0
2	C	18	0	0	0	0
2	D	17	0	0	2	0
All	All	19993	14026	18966	711	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 18.

All (711) 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:D:49:LYS:HB2	1:D:64:ARG:HG2	1.26	1.12
1:A:14:ASP:HA	1:A:15:PHE:HB2	1.17	1.12
1:A:49:LYS:HB2	1:A:64:ARG:HD2	1.39	1.03
1:A:14:ASP:CA	1:A:15:PHE:HB2	1.94	0.98
1:A:37:LYS:HB2	1:A:39:GLY:H	1.26	0.96
1:A:136:ALA:HA	1:A:137:LEU:HG	1.49	0.92
1:A:36:GLU:CB	1:A:37:LYS:HG3	2.01	0.90
1:A:14:ASP:HA	1:A:15:PHE:CB	2.00	0.90
1:D:362:PHE:HB3	1:D:363:ASN:C	1.93	0.89
1:A:86:GLY:HA3	1:A:87:GLU:HG2	1.55	0.89
1:A:30:LYS:HE2	1:A:133:GLU:HG2	1.53	0.87
1:C:356:TRP:HA	1:C:357:LEU:HB2	1.55	0.87
1:A:37:LYS:HB2	1:A:39:GLY:N	1.90	0.87
1:A:652:ASP:OD2	1:A:672:ARG:NH2	2.09	0.86
1:A:315:VAL:HG22	1:A:342:CYS:HA	1.57	0.86
1:D:24:SER:N	2:D:801:HOH:O	2.09	0.85
1:A:21:ARG:HH12	1:A:186:ARG:HH11	1.26	0.83
1:D:49:LYS:CB	1:D:64:ARG:HG2	2.08	0.82
1:D:507:ARG:HB2	1:D:520:TRP:CZ3	2.13	0.82
1:B:49:LYS:HE3	1:B:58:ALA:HB1	1.60	0.82
1:A:119:LEU:HD12	1:A:128:ALA:HB3	1.61	0.82
1:A:430:THR:HG1	1:A:466:HIS:HD1	1.26	0.82
1:B:191:GLU:HG3	1:B:192:ARG:HG3	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:MET:HG3	1:A:479:LEU:HB2	1.61	0.81
1:D:49:LYS:HB2	1:D:64:ARG:CG	2.08	0.81
1:A:691:GLN:HB3	1:A:694:ARG:HE	1.45	0.81
1:A:136:ALA:HA	1:A:137:LEU:CG	2.10	0.80
1:C:507:ARG:HB2	1:C:520:TRP:CH2	2.16	0.80
1:B:350:GLY:HA2	1:B:352:PHE:H	1.46	0.80
1:B:57:VAL:HG12	1:B:58:ALA:H	1.45	0.80
1:B:238:TYR:CD2	1:B:507:ARG:HD3	2.16	0.80
1:A:664:PRO:O	1:A:672:ARG:NH1	2.15	0.80
1:D:362:PHE:HB3	1:D:363:ASN:CA	2.12	0.79
1:A:136:ALA:HA	1:A:137:LEU:CB	2.13	0.78
1:D:97:LEU:HD23	1:D:98:GLN:HG3	1.66	0.77
1:A:33:ALA:HB3	1:A:45:VAL:CG1	2.14	0.77
1:B:53:ALA:HA	1:B:54:ASN:HB3	1.64	0.77
1:C:574:ARG:NH2	1:C:670:ASN:OD1	2.18	0.77
1:A:49:LYS:HE2	1:A:58:ALA:HB1	1.66	0.76
1:A:136:ALA:HB1	1:A:137:LEU:HB2	1.65	0.76
1:C:191:GLU:HG3	1:C:192:ARG:HE	1.49	0.76
1:B:28:ALA:HA	1:B:48:GLN:HG3	1.66	0.76
1:B:29:CYS:SG	1:B:49:LYS:HG3	2.26	0.76
1:D:430:THR:OG1	1:D:466:HIS:ND1	2.19	0.76
1:D:113:GLN:HE21	1:D:119:LEU:HD21	1.51	0.75
1:A:12:LEU:HD12	1:A:13:PHE:N	2.02	0.75
1:C:664:PRO:O	1:C:672:ARG:NH1	2.20	0.75
1:D:318:SER:HB2	1:D:346:HIS:HB3	1.69	0.75
1:A:507:ARG:HB2	1:A:520:TRP:CH2	2.22	0.75
1:D:119:LEU:HD13	1:D:120:PHE:N	2.01	0.75
1:B:118:ILE:HG13	1:B:133:GLU:CG	2.17	0.74
1:B:564:ASN:HB3	1:D:139:ARG:HA	1.67	0.74
1:C:75:ASN:ND2	1:C:107:PRO:HD2	2.02	0.74
1:D:113:GLN:HG3	1:D:114:GLY:HA2	1.70	0.73
1:A:686:THR:O	1:A:688:GLU:N	2.22	0.73
1:A:46:PRO:HD2	1:A:67:TYR:O	1.88	0.73
1:D:99:PHE:O	1:D:515:ARG:NH2	2.21	0.73
1:A:136:ALA:CB	1:A:137:LEU:HB2	2.18	0.73
1:B:587:TYR:HB3	1:B:593:ARG:HG2	1.71	0.73
1:B:318:SER:HB2	1:B:346:HIS:HB3	1.71	0.72
1:C:318:SER:HB2	1:C:346:HIS:HB3	1.71	0.72
1:B:49:LYS:HB3	1:B:64:ARG:HG2	1.71	0.72
1:D:31:PRO:HA	1:D:46:PRO:HA	1.70	0.72
1:D:134:GLU:N	1:D:135:PRO:HD2	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:TYR:CD2	1:D:507:ARG:HD3	2.24	0.72
1:C:691:GLN:OE1	1:C:694:ARG:NH2	2.23	0.72
1:A:136:ALA:CA	1:A:137:LEU:HB2	2.19	0.72
1:D:97:LEU:HG	1:D:98:GLN:HA	1.70	0.71
1:C:362:PHE:O	1:C:364:GLU:N	2.22	0.71
1:A:348:ASP:OD2	1:A:349:THR:HG23	1.91	0.71
1:C:430:THR:HG1	1:C:466:HIS:HD1	0.72	0.71
1:A:712:GLU:O	1:A:713:ASN:HB2	1.90	0.71
1:C:689:ARG:NH2	1:C:712:GLU:OE2	2.23	0.70
1:C:191:GLU:HA	1:C:279:ALA:HB2	1.73	0.70
1:D:46:PRO:HD2	1:D:67:TYR:O	1.91	0.70
1:C:116:LYS:HD2	1:C:120:PHE:CE2	2.26	0.70
1:D:119:LEU:HD12	1:D:130:ILE:HD13	1.72	0.70
1:A:86:GLY:HA3	1:A:87:GLU:CG	2.21	0.70
1:A:49:LYS:HB2	1:A:64:ARG:CD	2.19	0.69
1:A:17:THR:N	1:A:19:LEU:H	1.90	0.69
1:B:350:GLY:HA2	1:B:351:TRP:CB	2.22	0.69
1:D:29:CYS:HB3	1:D:149:GLU:HB2	1.75	0.69
1:A:574:ARG:NH2	1:A:670:ASN:OD1	2.26	0.69
1:C:35:TYR:CG	1:C:119:LEU:HG	2.27	0.69
1:D:72:ARG:HD3	1:D:108:LEU:HD22	1.75	0.69
1:C:353:ARG:HA	1:C:362:PHE:CD2	2.28	0.68
1:C:430:THR:OG1	1:C:466:HIS:ND1	2.10	0.68
1:B:42:CYS:SG	1:B:111:GLU:HG2	2.33	0.68
1:D:328:VAL:CG2	1:D:347:LEU:HD11	2.24	0.68
1:B:118:ILE:HG13	1:B:133:GLU:HG3	1.75	0.68
1:A:37:LYS:HB2	1:A:38:ASP:CA	2.24	0.68
1:A:507:ARG:HB2	1:A:520:TRP:CZ3	2.29	0.68
1:C:106:VAL:N	1:C:107:PRO:HD3	2.08	0.68
1:A:336:ARG:NH1	1:A:340:TYR:O	2.27	0.67
1:D:111:GLU:OE2	1:D:111:GLU:N	2.26	0.67
1:C:44:THR:O	1:C:46:PRO:HD3	1.94	0.67
1:D:507:ARG:HB2	1:D:520:TRP:CH2	2.28	0.67
1:B:475:LYS:HE3	1:B:478:LEU:HG	1.74	0.67
1:A:338:GLU:O	1:A:606:LYS:NZ	2.23	0.67
1:A:124:GLY:HA2	1:A:125:THR:O	1.95	0.67
1:A:43:VAL:HB	1:A:70:ILE:HG22	1.76	0.67
1:B:315:VAL:HG13	1:B:342:CYS:HA	1.75	0.67
1:C:704:GLU:OE1	1:C:704:GLU:N	2.27	0.67
1:D:32:THR:N	1:D:45:VAL:O	2.27	0.67
1:B:29:CYS:HB3	1:B:149:GLU:HG3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:GLU:OE2	1:B:507:ARG:HD2	1.95	0.66
1:A:27:LYS:HB2	1:A:51:LEU:HD21	1.76	0.66
1:D:154:THR:HG23	1:D:164:ARG:HB3	1.76	0.66
1:A:30:LYS:HG3	1:A:149:GLU:HB3	1.78	0.66
1:C:51:LEU:HG	1:C:56:MET:SD	2.36	0.66
1:D:686:THR:OG1	1:D:687:GLY:N	2.27	0.66
1:B:46:PRO:HD2	1:B:67:TYR:O	1.95	0.66
1:C:43:VAL:HG13	1:C:68:THR:HG23	1.79	0.65
1:A:191:GLU:HA	1:A:279:ALA:HB2	1.77	0.65
1:D:41:ILE:HG13	1:D:70:ILE:HD12	1.78	0.65
1:C:31:PRO:HA	1:C:46:PRO:HA	1.78	0.65
1:C:35:TYR:CD1	1:C:119:LEU:HG	2.31	0.65
1:D:35:TYR:HB3	1:D:119:LEU:HG	1.77	0.65
1:B:49:LYS:CB	1:B:64:ARG:HG2	2.26	0.65
1:B:191:GLU:HA	1:B:279:ALA:HB2	1.79	0.65
1:A:86:GLY:N	1:A:87:GLU:HB2	2.12	0.65
1:C:51:LEU:HD12	1:C:56:MET:HG2	1.79	0.65
1:A:54:ASN:HA	1:A:55:ASP:HB3	1.79	0.65
1:A:318:SER:HB2	1:A:346:HIS:HB3	1.79	0.65
1:C:103:ILE:HG22	1:C:104:ARG:H	1.59	0.65
1:B:192:ARG:HA	1:B:276:SER:O	1.97	0.65
1:C:22:ASP:O	1:C:187:THR:N	2.30	0.65
1:A:18:GLU:OE2	1:A:20:LEU:HB2	1.96	0.65
1:D:32:THR:HB	1:D:45:VAL:HG13	1.78	0.64
1:D:447:LYS:HB2	1:D:494:ILE:HD11	1.79	0.64
1:D:144:LEU:HD12	1:D:173:PRO:HD2	1.79	0.64
1:C:38:ASP:O	1:C:40:ASP:N	2.30	0.64
1:A:37:LYS:HD3	1:A:40:ASP:H	1.62	0.64
1:A:51:LEU:HG	1:A:56:MET:SD	2.37	0.64
1:D:97:LEU:CB	1:D:98:GLN:HA	2.28	0.64
1:C:51:LEU:HD13	1:C:58:ALA:HA	1.78	0.64
1:A:37:LYS:HB2	1:A:38:ASP:HA	1.79	0.64
1:C:22:ASP:HB3	1:C:187:THR:HA	1.80	0.64
1:D:25:LEU:HD23	1:D:56:MET:CE	2.28	0.64
1:A:435:TYR:O	1:A:437:LYS:N	2.31	0.63
1:B:576:THR:O	1:B:580:VAL:HG23	1.99	0.63
1:B:49:LYS:HD3	1:B:50:GLN:N	2.12	0.63
1:C:75:ASN:CG	1:C:107:PRO:HD2	2.18	0.63
1:A:121:THR:O	1:A:123:ASP:HB3	1.99	0.63
1:C:507:ARG:HB2	1:C:520:TRP:CZ3	2.33	0.63
1:C:331:ILE:HG23	1:C:596:TRP:CH2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:682:VAL:HG13	1:B:710:VAL:HG23	1.79	0.63
1:D:49:LYS:HD3	1:D:64:ARG:HE	1.63	0.63
1:D:328:VAL:HG21	1:D:347:LEU:HD11	1.80	0.63
1:A:325:ALA:O	1:A:329:ASN:ND2	2.23	0.63
1:A:136:ALA:CA	1:A:137:LEU:CB	2.77	0.63
1:A:86:GLY:HA3	1:A:87:GLU:CB	2.29	0.62
1:B:30:LYS:HG3	1:B:132:VAL:HG12	1.80	0.62
1:B:507:ARG:HB2	1:B:520:TRP:CZ3	2.34	0.62
1:D:97:LEU:CG	1:D:98:GLN:HA	2.29	0.62
1:A:86:GLY:CA	1:A:87:GLU:HB2	2.29	0.62
1:D:352:PHE:HA	1:D:361:LYS:HA	1.81	0.62
1:C:23:GLU:HA	1:C:185:LYS:O	1.99	0.62
1:B:49:LYS:HZ2	1:B:50:GLN:H	1.48	0.62
1:D:34:VAL:CB	1:D:45:VAL:HG12	2.30	0.62
1:B:35:TYR:CZ	1:B:119:LEU:HD13	2.35	0.62
1:C:322:TYR:O	1:C:350:GLY:HA3	2.00	0.61
1:A:37:LYS:CB	1:A:38:ASP:HA	2.29	0.61
1:C:310:LEU:HD13	1:C:620:ILE:HD11	1.83	0.61
1:D:52:LEU:HD22	1:D:57:VAL:CG1	2.29	0.61
1:A:203:GLU:OE1	1:A:246:SER:OG	2.19	0.61
1:A:37:LYS:HG2	1:A:40:ASP:CA	2.30	0.61
1:D:552:ASP:OD1	1:D:586:ARG:NH1	2.33	0.61
1:A:136:ALA:HA	1:A:137:LEU:HB2	1.80	0.61
1:A:50:GLN:HB3	1:A:62:VAL:HG11	1.82	0.61
1:C:116:LYS:HD2	1:C:120:PHE:HE2	1.65	0.61
1:A:124:GLY:HA2	1:A:125:THR:C	2.20	0.61
1:C:103:ILE:HG22	1:C:104:ARG:N	2.16	0.61
1:D:362:PHE:HB2	1:D:364:GLU:HG3	1.82	0.60
1:B:64:ARG:NH1	1:B:149:GLU:OE1	2.33	0.60
1:B:350:GLY:HA2	1:B:352:PHE:N	2.15	0.60
1:C:53:ALA:N	1:C:54:ASN:HB2	2.15	0.60
1:B:44:THR:HG23	1:B:69:LEU:HB3	1.83	0.60
1:B:53:ALA:HB1	1:B:54:ASN:C	2.21	0.60
1:B:35:TYR:CD1	1:B:119:LEU:HD22	2.36	0.60
1:B:186:ARG:HD2	1:B:187:THR:HG23	1.82	0.60
1:B:122:GLN:HB3	1:B:125:THR:CG2	2.31	0.60
1:B:601:ILE:HD12	1:B:601:ILE:O	2.01	0.60
1:A:192:ARG:HA	1:A:276:SER:O	2.01	0.60
1:C:364:GLU:C	1:C:365:GLU:HG2	2.19	0.60
1:A:30:LYS:HD3	1:A:133:GLU:OE1	2.02	0.60
1:A:475:LYS:NZ	1:A:475:LYS:HB3	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:LEU:HD12	1:B:108:LEU:O	2.02	0.60
1:B:49:LYS:HG2	1:B:64:ARG:NE	2.17	0.60
1:A:30:LYS:CE	1:A:133:GLU:HG2	2.31	0.59
1:D:27:LYS:HG2	1:D:50:GLN:HG2	1.84	0.59
1:B:49:LYS:HE3	1:B:58:ALA:CB	2.30	0.59
1:D:49:LYS:HE2	1:D:64:ARG:HH21	1.67	0.59
1:D:569:GLU:HB3	1:D:601:ILE:HG13	1.83	0.59
1:C:103:ILE:HG13	1:C:300:ASP:HA	1.84	0.59
1:C:683:ASN:OD1	1:C:686:THR:N	2.35	0.59
1:B:151:LEU:HD23	1:B:181:ILE:HD12	1.85	0.59
1:B:49:LYS:HB3	1:B:64:ARG:CG	2.31	0.59
1:A:360:TRP:O	1:A:362:PHE:N	2.36	0.59
1:A:86:GLY:CA	1:A:87:GLU:CB	2.81	0.58
1:D:35:TYR:CD2	1:D:119:LEU:HB2	2.38	0.58
1:D:563:MET:HG3	1:D:590:THR:HB	1.85	0.58
1:B:151:LEU:CD2	1:B:181:ILE:HD12	2.33	0.58
1:D:171:PHE:HB3	1:D:175:ARG:HB3	1.86	0.58
1:A:17:THR:H	1:A:19:LEU:H	1.50	0.58
1:D:35:TYR:CG	1:D:119:LEU:HG	2.38	0.58
1:B:69:LEU:HB2	1:B:83:LEU:HD12	1.85	0.58
1:D:598:TYR:O	1:D:601:ILE:HB	2.02	0.58
1:A:211:ARG:NH2	1:A:240:ASN:OD1	2.36	0.58
1:C:118:ILE:HD11	1:C:120:PHE:CZ	2.39	0.58
1:C:315:VAL:HG13	1:C:342:CYS:HA	1.85	0.58
1:B:450:LEU:HB3	1:B:498:VAL:HG21	1.86	0.58
1:A:139:ARG:HA	1:C:564:ASN:OD1	2.04	0.58
1:C:315:VAL:CG1	1:C:342:CYS:HA	2.33	0.58
1:D:587:TYR:HB3	1:D:593:ARG:HG2	1.86	0.58
1:B:154:THR:HG23	1:B:164:ARG:HB3	1.85	0.58
1:A:245:LEU:HB3	1:A:291:MET:HE1	1.85	0.58
1:A:315:VAL:CG2	1:A:342:CYS:HA	2.30	0.58
1:B:475:LYS:H	1:B:475:LYS:HD3	1.69	0.58
1:B:40:ASP:CB	1:B:110:VAL:HG12	2.34	0.58
1:D:113:GLN:NE2	1:D:119:LEU:HD21	2.19	0.57
1:A:713:ASN:OD1	1:B:658:ASN:ND2	2.37	0.57
1:C:35:TYR:CD2	1:C:119:LEU:HG	2.39	0.57
1:A:359:GLU:O	1:A:361:LYS:N	2.36	0.57
1:B:50:GLN:CB	1:B:58:ALA:HA	2.34	0.57
1:B:564:ASN:ND2	1:D:140:TRP:O	2.37	0.57
1:A:175:ARG:NE	1:C:230:GLN:OE1	2.34	0.57
1:A:715:VAL:HG11	1:B:715:VAL:HG12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:CYS:SG	1:B:345:ILE:HG21	2.45	0.57
1:D:118:ILE:H	1:D:118:ILE:HD13	1.70	0.57
1:D:68:THR:O	1:D:83:LEU:HD22	2.05	0.57
1:D:151:LEU:CD2	1:D:181:ILE:HD12	2.34	0.57
1:A:336:ARG:N	1:A:336:ARG:HD2	2.20	0.57
1:B:601:ILE:HG23	1:B:703:LEU:HD21	1.87	0.57
1:A:244:TYR:CZ	1:A:272:VAL:HG11	2.40	0.57
1:B:652:ASP:OD2	1:B:672:ARG:NH2	2.38	0.56
1:A:37:LYS:HG2	1:A:40:ASP:HA	1.86	0.56
1:D:191:GLU:HG3	1:D:192:ARG:HG3	1.85	0.56
1:D:192:ARG:HA	1:D:276:SER:O	2.05	0.56
1:D:191:GLU:HA	1:D:279:ALA:HB2	1.87	0.56
1:B:355:ASP:CB	1:B:356:TRP:HA	2.33	0.56
1:A:627:VAL:HG23	1:A:628:GLU:HG2	1.85	0.56
1:A:49:LYS:HD3	1:A:64:ARG:HD3	1.86	0.56
1:A:598:TYR:O	1:A:601:ILE:HG22	2.06	0.56
1:D:662:VAL:HG12	1:D:664:PRO:HD3	1.88	0.56
1:D:31:PRO:HD3	1:D:151:LEU:HD12	1.87	0.56
1:B:98:GLN:HG3	1:B:99:PHE:N	2.21	0.56
1:B:323:PHE:O	1:B:324:SER:CB	2.47	0.56
1:D:315:VAL:HG22	1:D:342:CYS:HA	1.86	0.56
1:A:69:LEU:HD11	1:A:81:LEU:HD12	1.88	0.56
1:C:191:GLU:CG	1:C:192:ARG:HE	2.17	0.56
1:D:75:ASN:ND2	1:D:105:ARG:O	2.38	0.56
1:D:97:LEU:HD23	1:D:98:GLN:CG	2.37	0.55
1:A:123:ASP:OD1	1:A:125:THR:HG21	2.05	0.55
1:B:435:TYR:CG	1:B:472:LYS:HD2	2.41	0.55
1:A:211:ARG:NH1	1:A:237:THR:OG1	2.36	0.55
1:D:35:TYR:CD2	1:D:119:LEU:HD23	2.42	0.55
1:D:52:LEU:HD22	1:D:57:VAL:HG11	1.88	0.55
1:C:26:TRP:NE1	1:C:185:LYS:HD3	2.21	0.55
1:D:362:PHE:HB3	1:D:363:ASN:CB	2.36	0.55
1:B:315:VAL:CG1	1:B:342:CYS:HA	2.36	0.55
1:D:354:THR:O	1:D:356:TRP:HA	2.06	0.55
1:A:686:THR:O	1:A:686:THR:OG1	2.10	0.55
1:C:583:SER:OG	1:C:584:HIS:ND1	2.38	0.55
1:C:192:ARG:HA	1:C:276:SER:O	2.07	0.55
1:A:332:CYS:SG	1:A:345:ILE:HG13	2.47	0.55
1:C:474:MET:HE2	1:C:479:LEU:HD13	1.88	0.55
1:B:171:PHE:HB3	1:B:175:ARG:HB3	1.89	0.54
1:C:161:ARG:O	1:C:162:GLU:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LYS:HD3	1:B:50:GLN:CB	2.37	0.54
1:C:43:VAL:HG13	1:C:68:THR:CG2	2.37	0.54
1:D:329:ASN:O	1:D:333:ASP:HB2	2.07	0.54
1:D:49:LYS:CD	1:D:64:ARG:HE	2.20	0.54
1:A:37:LYS:CB	1:A:39:GLY:H	2.11	0.54
1:B:178:GLY:O	1:B:179:LEU:HD23	2.08	0.54
1:C:525:CYS:O	1:C:527:SER:N	2.41	0.54
1:D:122:GLN:HG2	1:D:123:ASP:H	1.73	0.54
1:C:635:GLN:HB2	1:C:655:TYR:HB2	1.90	0.54
1:C:184:CYS:HB2	1:C:192:ARG:HB2	1.89	0.54
1:D:211:ARG:NH2	1:D:240:ASN:OD1	2.35	0.54
1:D:25:LEU:HD23	1:D:56:MET:HE3	1.89	0.53
1:C:53:ALA:CA	1:C:54:ASN:HB2	2.38	0.53
1:A:338:GLU:O	1:A:339:HIS:HB2	2.08	0.53
1:C:32:THR:N	1:C:45:VAL:O	2.39	0.53
1:C:106:VAL:N	1:C:107:PRO:CD	2.72	0.53
1:D:73:GLN:N	1:D:111:GLU:OE1	2.37	0.53
1:D:25:LEU:HD23	1:D:56:MET:HE1	1.89	0.53
1:A:31:PRO:HG2	1:A:130:ILE:HG21	1.91	0.53
1:A:580:VAL:O	1:A:612:ARG:NH1	2.41	0.53
1:B:691:GLN:OE1	1:B:691:GLN:N	2.37	0.53
1:A:474:MET:CG	1:A:479:LEU:HB2	2.37	0.53
1:B:507:ARG:HB2	1:B:520:TRP:CH2	2.44	0.53
1:C:193:ALA:HB2	1:C:279:ALA:HA	1.91	0.53
1:B:658:ASN:ND2	1:B:711:ARG:HH22	2.06	0.53
1:C:144:LEU:HG	1:C:172:SER:CB	2.39	0.53
1:B:465:ILE:HD12	1:B:480:ASN:HA	1.91	0.53
1:C:688:GLU:HG2	1:C:690:LEU:CD2	2.39	0.53
1:D:53:ALA:HA	1:D:54:ASN:HB3	1.90	0.53
1:A:69:LEU:HD11	1:A:81:LEU:CD1	2.39	0.53
1:B:432:ASP:OD2	1:B:472:LYS:HE2	2.09	0.53
1:D:53:ALA:CA	1:D:54:ASN:HB3	2.38	0.53
1:B:31:PRO:O	1:B:33:ALA:N	2.42	0.53
1:B:122:GLN:HB3	1:B:125:THR:HG23	1.90	0.53
1:C:358:CYS:O	1:C:360:TRP:N	2.42	0.53
1:B:30:LYS:O	1:B:32:THR:N	2.42	0.52
1:C:327:GLU:O	1:C:331:ILE:HG13	2.09	0.52
1:A:212:PHE:CE1	1:A:232:VAL:HG22	2.45	0.52
1:D:35:TYR:CE2	1:D:119:LEU:HB2	2.44	0.52
1:B:115:GLY:HA2	1:B:119:LEU:HD23	1.90	0.52
1:A:18:GLU:CD	1:A:18:GLU:H	2.11	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ASP:HA	1:A:19:LEU:HA	1.91	0.52
1:B:53:ALA:HB1	1:B:54:ASN:O	2.09	0.52
1:A:49:LYS:HD3	1:A:64:ARG:CD	2.40	0.52
1:A:474:MET:HE3	1:A:479:LEU:HD13	1.91	0.52
1:C:184:CYS:O	1:C:191:GLU:N	2.42	0.52
1:D:430:THR:HG1	1:D:466:HIS:HD1	1.41	0.52
1:D:136:ALA:O	1:D:138:ASP:N	2.40	0.52
1:A:26:TRP:CE2	1:A:50:GLN:HB2	2.45	0.52
1:A:82:PHE:CZ	1:A:89:GLU:HA	2.45	0.52
1:A:579:GLY:O	1:A:582:THR:OG1	2.25	0.52
1:C:328:VAL:HG13	1:C:345:ILE:HG21	1.91	0.52
1:B:185:LYS:NZ	1:B:188:GLY:O	2.25	0.52
1:D:570:ASP:OD2	1:D:668:SER:OG	2.15	0.52
1:A:475:LYS:HB3	1:A:475:LYS:HZ3	1.73	0.52
1:A:361:LYS:O	1:A:362:PHE:CB	2.58	0.52
1:A:138:ASP:O	1:A:139:ARG:HB2	2.10	0.52
1:D:478:LEU:N	1:D:478:LEU:HD22	2.25	0.52
1:C:54:ASN:O	1:C:55:ASP:HB2	2.10	0.52
1:A:292:GLU:HG3	1:A:631:TRP:CE2	2.45	0.52
1:A:16:ASP:HB2	1:A:19:LEU:HD13	1.92	0.51
1:C:358:CYS:C	1:C:360:TRP:H	2.13	0.51
1:C:474:MET:HG3	1:C:479:LEU:HB2	1.90	0.51
1:C:144:LEU:HG	1:C:172:SER:HB3	1.91	0.51
1:D:134:GLU:H	1:D:135:PRO:HD2	1.74	0.51
1:A:314:GLY:HA3	1:A:343:ASP:HB2	1.93	0.51
1:D:116:LYS:O	1:D:117:TRP:CB	2.51	0.51
1:C:25:LEU:HD13	1:C:26:TRP:N	2.25	0.51
1:D:600:ALA:HA	1:D:601:ILE:HB	1.91	0.51
1:D:53:ALA:HA	1:D:54:ASN:C	2.30	0.51
1:C:365:GLU:O	1:C:366:ARG:HB2	2.10	0.51
1:B:59:ASP:OD1	1:B:62:VAL:HG22	2.10	0.51
1:B:49:LYS:HZ2	1:B:50:GLN:N	2.07	0.51
1:C:191:GLU:OE1	1:C:192:ARG:NE	2.44	0.51
1:C:362:PHE:C	1:C:364:GLU:H	2.13	0.51
1:C:116:LYS:O	1:C:117:TRP:CB	2.52	0.51
1:A:317:MET:HB3	1:A:345:ILE:HD13	1.92	0.51
1:A:18:GLU:N	1:A:18:GLU:OE1	2.32	0.51
1:C:355:ASP:HB3	1:C:356:TRP:CD1	2.45	0.51
1:A:31:PRO:HB3	1:A:44:THR:CG2	2.40	0.51
1:C:37:LYS:HB2	1:C:113:GLN:CG	2.40	0.51
1:B:332:CYS:SG	1:B:345:ILE:HD12	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:CYS:SG	1:C:345:ILE:HG13	2.51	0.50
1:A:430:THR:OG1	1:A:466:HIS:ND1	2.26	0.50
1:C:331:ILE:HG23	1:C:596:TRP:HH2	1.72	0.50
1:D:35:TYR:CB	1:D:119:LEU:HG	2.40	0.50
1:A:576:THR:HG22	1:A:587:TYR:OH	2.12	0.50
1:B:189:LYS:HB2	1:B:189:LYS:NZ	2.27	0.50
1:B:225:LYS:NZ	1:B:226:ASN:O	2.43	0.50
1:D:31:PRO:HB3	1:D:44:THR:CG2	2.41	0.50
1:C:689:ARG:NH2	1:C:712:GLU:HB2	2.27	0.50
1:D:29:CYS:HB3	1:D:149:GLU:CB	2.39	0.50
1:A:244:TYR:CE2	1:A:272:VAL:HG11	2.46	0.50
1:C:351:TRP:H	1:C:351:TRP:HD1	1.56	0.50
1:A:430:THR:HG1	1:A:466:HIS:CE1	2.30	0.50
1:B:348:ASP:O	1:B:350:GLY:N	2.43	0.50
1:B:614:SER:O	1:B:718:ILE:HG23	2.11	0.50
1:D:119:LEU:HD13	1:D:120:PHE:CA	2.41	0.50
1:B:49:LYS:CE	1:B:58:ALA:HB1	2.37	0.50
1:C:116:LYS:HZ3	1:C:120:PHE:HD2	1.59	0.50
1:A:573:MET:SD	1:A:601:ILE:HG13	2.51	0.50
1:B:563:MET:HG2	1:D:142:GLU:H	1.77	0.50
1:A:21:ARG:HH12	1:A:186:ARG:NH1	2.02	0.49
1:B:53:ALA:HA	1:B:54:ASN:CB	2.35	0.49
1:B:118:ILE:CG1	1:B:133:GLU:HG3	2.41	0.49
1:B:99:PHE:HB3	1:B:485:LEU:CD2	2.41	0.49
1:D:693:GLY:O	1:D:694:ARG:HD3	2.11	0.49
1:A:137:LEU:O	1:A:138:ASP:HB2	2.13	0.49
1:C:355:ASP:C	1:C:356:TRP:CD1	2.85	0.49
1:A:51:LEU:HD13	1:A:58:ALA:HA	1.95	0.49
1:A:82:PHE:CE2	1:A:89:GLU:HA	2.47	0.49
1:D:238:TYR:HD2	1:D:507:ARG:HD3	1.75	0.49
1:B:477:GLU:O	1:B:478:LEU:HD22	2.13	0.49
1:B:158:ASP:OD2	1:B:161:ARG:HB2	2.12	0.49
1:B:31:PRO:HD2	1:B:132:VAL:HG12	1.93	0.49
1:D:97:LEU:CB	1:D:98:GLN:CA	2.91	0.49
1:B:122:GLN:HB3	1:B:125:THR:HG22	1.94	0.49
1:C:331:ILE:HG23	1:C:596:TRP:CZ2	2.48	0.49
1:B:465:ILE:H	1:B:465:ILE:HD13	1.77	0.49
1:D:189:LYS:N	1:D:189:LYS:HD2	2.27	0.49
1:D:473:GLY:O	1:D:474:MET:HB3	2.13	0.49
1:B:350:GLY:CA	1:B:351:TRP:CB	2.91	0.49
1:D:27:LYS:HG2	1:D:50:GLN:CG	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:THR:HB	1:C:128:ALA:HB3	1.94	0.49
1:A:299:ARG:NH1	1:A:629:SER:O	2.46	0.49
1:D:97:LEU:CD2	1:D:98:GLN:HG3	2.40	0.49
1:B:118:ILE:N	1:B:118:ILE:HD12	2.28	0.49
1:B:69:LEU:HD13	1:B:83:LEU:HB2	1.95	0.49
1:A:551:HIS:CD2	1:A:578:PHE:CE2	3.01	0.49
1:B:163:ILE:HD11	1:B:197:PHE:CG	2.48	0.49
1:A:144:LEU:HD23	1:C:562:PHE:CG	2.47	0.49
1:A:338:GLU:HB3	1:A:340:TYR:CE2	2.48	0.49
1:B:186:ARG:CD	1:B:187:THR:HG23	2.42	0.49
1:D:573:MET:HG2	1:D:601:ILE:HD12	1.95	0.49
1:D:480:ASN:HB3	2:D:805:HOH:O	2.11	0.49
1:C:658:ASN:O	1:C:711:ARG:NH2	2.46	0.49
1:C:22:ASP:O	1:C:186:ARG:HA	2.12	0.48
1:D:576:THR:O	1:D:580:VAL:HG23	2.12	0.48
1:A:37:LYS:HD2	1:A:38:ASP:HA	1.95	0.48
1:B:30:LYS:HE2	1:B:149:GLU:OE2	2.14	0.48
1:D:583:SER:OG	1:D:584:HIS:ND1	2.42	0.48
1:B:667:ASN:O	1:B:668:SER:CB	2.61	0.48
1:C:475:LYS:HB3	1:C:477:GLU:CD	2.34	0.48
1:A:124:GLY:N	1:A:125:THR:OG1	2.46	0.48
1:C:123:ASP:N	1:C:125:THR:N	2.62	0.48
1:A:474:MET:CE	1:A:479:LEU:HD13	2.44	0.48
1:D:588:HIS:N	1:D:593:ARG:HD2	2.29	0.48
1:D:211:ARG:HD3	1:D:222:LEU:HD22	1.94	0.48
1:A:560:PRO:O	1:A:561:ASN:CB	2.62	0.48
1:D:144:LEU:HG	1:D:172:SER:OG	2.14	0.48
1:C:37:LYS:HE3	1:C:38:ASP:O	2.13	0.48
1:D:216:ASP:OD1	1:D:218:SER:OG	2.31	0.48
1:B:551:HIS:CD2	1:B:575:TRP:HE1	2.31	0.48
1:D:221:THR:HA	1:D:263:SER:HA	1.94	0.48
1:A:37:LYS:HB3	1:A:41:ILE:O	2.14	0.48
1:B:31:PRO:HG3	1:B:151:LEU:CD1	2.44	0.48
1:D:318:SER:OG	1:D:319:ARG:N	2.45	0.48
1:D:25:LEU:HD12	1:D:26:TRP:H	1.79	0.48
1:A:691:GLN:HB3	1:A:694:ARG:NE	2.23	0.48
1:B:635:GLN:HB2	1:B:655:TYR:HB2	1.96	0.48
1:C:160:LYS:HB3	1:C:160:LYS:NZ	2.29	0.48
1:B:594:GLU:HG2	1:B:596:TRP:CZ2	2.49	0.48
1:A:37:LYS:HB3	1:A:41:ILE:H	1.79	0.48
1:B:184:CYS:HB2	1:B:192:ARG:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:PRO:O	1:B:672:ARG:NH1	2.44	0.48
1:A:617:PRO:HB2	1:A:717:PRO:HB2	1.96	0.48
1:B:629:SER:OG	1:B:630:GLY:N	2.47	0.48
1:C:35:TYR:CE1	1:C:119:LEU:HG	2.48	0.48
1:A:35:TYR:CZ	1:A:43:VAL:HG22	2.49	0.48
1:D:326:ASP:OD2	1:D:326:ASP:N	2.47	0.48
1:C:577:GLN:CB	1:C:706:MET:HE3	2.44	0.48
1:C:254:TYR:O	1:C:256:THR:N	2.46	0.48
1:A:221:THR:HA	1:A:263:SER:HA	1.95	0.48
1:D:49:LYS:CE	1:D:64:ARG:HH21	2.26	0.47
1:A:33:ALA:HB3	1:A:45:VAL:HG11	1.92	0.47
1:D:45:VAL:O	1:D:45:VAL:HG13	2.13	0.47
1:C:40:ASP:O	1:C:111:GLU:HB2	2.13	0.47
1:A:144:LEU:HD22	1:C:563:MET:HE1	1.96	0.47
1:C:309:PRO:HG3	1:C:501:ASP:HB3	1.96	0.47
1:A:583:SER:OG	1:A:584:HIS:ND1	2.46	0.47
1:C:53:ALA:HA	1:C:54:ASN:C	2.34	0.47
1:D:113:GLN:CG	1:D:114:GLY:HA2	2.44	0.47
1:D:215:MET:CE	1:D:636:ALA:HB1	2.44	0.47
1:C:570:ASP:OD2	1:C:668:SER:OG	2.16	0.47
1:D:355:ASP:HA	1:D:356:TRP:HA	1.58	0.47
1:B:616:ILE:N	1:B:617:PRO:HD2	2.29	0.47
1:B:686:THR:OG1	1:B:687:GLY:N	2.46	0.47
1:D:326:ASP:HA	1:D:327:GLU:C	2.35	0.47
1:D:327:GLU:HA	1:D:331:ILE:HD13	1.97	0.47
1:A:302:THR:OG1	1:A:514:GLN:NE2	2.47	0.47
1:A:126:LYS:O	1:A:126:LYS:HD2	2.14	0.47
1:B:57:VAL:HG12	1:B:58:ALA:N	2.22	0.47
1:D:432:ASP:OD1	1:D:471:TYR:HB3	2.14	0.47
1:C:349:THR:HG21	1:C:356:TRP:CH2	2.50	0.47
1:C:191:GLU:CA	1:C:279:ALA:HB2	2.43	0.47
1:C:102:ARG:C	1:C:103:ILE:HG12	2.35	0.47
1:D:247:SER:HA	1:D:648:TRP:CZ2	2.50	0.47
1:A:49:LYS:HB3	1:A:49:LYS:NZ	2.29	0.47
1:B:30:LYS:HB2	1:B:149:GLU:HB2	1.97	0.47
1:D:35:TYR:HD2	1:D:119:LEU:HD23	1.77	0.46
1:A:572:TYR:O	1:A:576:THR:HG23	2.15	0.46
1:C:592:LYS:HD3	1:C:597:HIS:HB3	1.97	0.46
1:C:599:PRO:HA	1:C:602:ALA:CB	2.45	0.46
1:A:87:GLU:HB3	1:A:88:TYR:CD1	2.51	0.46
1:D:680:GLN:HB2	1:D:712:GLU:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LEU:O	1:B:53:ALA:HB3	2.15	0.46
1:C:26:TRP:CE2	1:C:185:LYS:HD3	2.50	0.46
1:B:477:GLU:C	1:B:478:LEU:HD22	2.35	0.46
1:C:686:THR:CG2	1:C:688:GLU:HB2	2.46	0.46
1:A:171:PHE:HB3	1:A:175:ARG:HB3	1.98	0.46
1:A:552:ASP:OD1	1:A:586:ARG:NH1	2.47	0.46
1:A:328:VAL:HG21	1:A:347:LEU:HD11	1.98	0.46
1:C:44:THR:HG23	1:C:69:LEU:O	2.16	0.46
1:D:53:ALA:N	1:D:54:ASN:HB3	2.30	0.46
1:C:134:GLU:HB2	1:C:135:PRO:C	2.36	0.46
1:A:151:LEU:CD2	1:A:181:ILE:HD12	2.45	0.46
1:B:456:CYS:SG	1:B:457:ILE:N	2.88	0.46
1:B:562:PHE:CE1	1:B:590:THR:HG21	2.51	0.46
1:A:15:PHE:O	1:A:16:ASP:HB3	2.15	0.46
1:C:434:THR:HG21	1:C:474:MET:HE2	1.98	0.46
1:B:223:PHE:O	1:B:225:LYS:N	2.49	0.46
1:B:517:PRO:HA	1:B:518:LEU:HA	1.79	0.46
1:A:200:ARG:HB3	1:A:201:PRO:HD2	1.98	0.46
1:A:36:GLU:HA	1:A:37:LYS:HA	1.66	0.46
1:A:211:ARG:HH11	1:A:211:ARG:HG3	1.81	0.46
1:A:616:ILE:HB	1:A:617:PRO:HD3	1.96	0.46
1:D:574:ARG:NH2	1:D:670:ASN:OD1	2.45	0.46
1:A:618:TYR:CD1	1:A:716:ILE:HG23	2.51	0.46
1:A:54:ASN:CA	1:A:55:ASP:HB3	2.45	0.45
1:B:445:LEU:O	1:B:448:GLN:HG2	2.16	0.45
1:A:475:LYS:HE2	1:A:477:GLU:OE2	2.17	0.45
1:D:563:MET:HA	1:D:590:THR:HB	1.98	0.45
1:B:316:TRP:CE3	1:B:344:VAL:HG11	2.51	0.45
1:A:613:TYR:HA	1:A:616:ILE:HG12	1.98	0.45
1:D:717:PRO:O	1:D:718:ILE:HG23	2.17	0.45
1:A:505:TRP:CD1	1:A:520:TRP:CE3	3.04	0.45
1:B:573:MET:SD	1:B:601:ILE:HG21	2.57	0.45
1:D:118:ILE:HG12	1:D:118:ILE:O	2.14	0.45
1:A:212:PHE:CD1	1:A:232:VAL:HG22	2.52	0.45
1:C:31:PRO:O	1:C:33:ALA:N	2.50	0.45
1:A:347:LEU:N	1:A:347:LEU:HD22	2.32	0.45
1:B:49:LYS:HB3	1:B:64:ARG:CB	2.47	0.45
1:C:191:GLU:HG3	1:C:192:ARG:NE	2.26	0.45
1:C:46:PRO:HD2	1:C:67:TYR:O	2.15	0.45
1:A:567:VAL:O	1:A:568:ALA:HB3	2.17	0.45
1:A:37:LYS:N	1:A:38:ASP:HA	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:ALA:HB2	1:B:279:ALA:HA	1.98	0.45
1:D:446:LEU:HD12	1:D:494:ILE:HG21	1.99	0.45
1:D:208:THR:HG21	1:D:222:LEU:HD13	1.98	0.45
1:C:211:ARG:NH1	1:C:237:THR:HG21	2.32	0.45
1:D:55:ASP:HA	1:D:56:MET:HA	1.55	0.45
1:D:474:MET:SD	1:D:479:LEU:HA	2.56	0.45
1:B:177:ASP:OD1	1:B:267:HIS:NE2	2.50	0.45
1:D:613:TYR:HA	1:D:616:ILE:HG12	1.98	0.45
1:C:181:ILE:HG12	1:C:195:LEU:HD23	1.99	0.45
1:A:190:LYS:HE3	1:A:190:LYS:HB2	1.53	0.45
1:A:319:ARG:O	1:A:321:THR:HA	2.17	0.45
1:A:32:THR:O	1:A:33:ALA:HB2	2.17	0.45
1:B:118:ILE:HG13	1:B:133:GLU:HG2	1.96	0.45
1:D:348:ASP:OD1	1:D:458:LYS:NZ	2.34	0.45
1:B:350:GLY:CA	1:B:352:PHE:H	2.23	0.44
1:A:232:VAL:O	1:A:232:VAL:HG13	2.17	0.44
1:C:475:LYS:HB3	1:C:477:GLU:OE1	2.17	0.44
1:D:153:ILE:O	1:D:164:ARG:HB2	2.18	0.44
1:C:22:ASP:HB3	1:C:187:THR:CA	2.47	0.44
1:B:38:ASP:O	1:B:40:ASP:N	2.50	0.44
1:A:599:PRO:C	1:A:601:ILE:H	2.20	0.44
1:C:434:THR:CG2	1:C:474:MET:HE2	2.47	0.44
1:C:125:THR:N	1:C:126:LYS:HA	2.31	0.44
1:D:158:ASP:OD1	1:D:159:GLY:N	2.51	0.44
1:D:49:LYS:CG	1:D:64:ARG:HG2	2.47	0.44
1:D:40:ASP:CB	1:D:110:VAL:HG12	2.47	0.44
1:D:133:GLU:O	1:D:134:GLU:HB2	2.17	0.44
1:A:18:GLU:CD	1:A:18:GLU:N	2.71	0.44
1:D:97:LEU:HB3	1:D:98:GLN:CA	2.48	0.44
1:B:83:LEU:HB3	1:B:281:LEU:HD11	2.00	0.44
1:D:676:LEU:O	1:D:693:GLY:HA2	2.18	0.44
1:C:475:LYS:HB3	1:C:477:GLU:OE2	2.18	0.44
1:D:616:ILE:N	1:D:617:PRO:CD	2.81	0.44
1:B:239:LYS:HE2	1:B:519:HIS:HB3	2.00	0.44
1:C:49:LYS:HD3	1:C:64:ARG:HG2	1.99	0.44
1:A:88:TYR:O	1:A:89:GLU:HB2	2.17	0.44
1:D:352:PHE:CE2	1:D:358:CYS:HA	2.53	0.44
1:B:49:LYS:HB2	1:B:49:LYS:HZ3	1.83	0.44
1:D:119:LEU:HB3	1:D:130:ILE:HB	2.00	0.44
1:D:339:HIS:HB2	1:D:606:LYS:HE3	1.98	0.44
1:C:430:THR:HG22	1:C:431:ILE:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:ASN:HD21	1:B:711:ARG:HH22	1.66	0.44
1:C:688:GLU:HG2	1:C:690:LEU:HD22	2.00	0.43
1:C:434:THR:CG2	1:C:479:LEU:HD13	2.47	0.43
1:D:53:ALA:CA	1:D:54:ASN:CB	2.96	0.43
1:C:599:PRO:HA	1:C:602:ALA:HB2	2.00	0.43
1:D:62:VAL:HG23	1:D:63:PRO:HD2	2.00	0.43
1:D:160:LYS:HE2	1:D:160:LYS:HB3	1.78	0.43
1:B:212:PHE:CE1	1:B:232:VAL:HG23	2.53	0.43
1:B:211:ARG:HD2	1:B:237:THR:HG21	1.99	0.43
1:B:113:GLN:HG3	1:B:120:PHE:O	2.18	0.43
1:C:115:GLY:O	1:C:116:LYS:HB3	2.17	0.43
1:C:665:VAL:HG21	1:C:701:VAL:CG2	2.49	0.43
1:D:362:PHE:CB	1:D:363:ASN:CB	2.96	0.43
1:B:49:LYS:HB2	1:B:49:LYS:NZ	2.33	0.43
1:D:188:GLY:C	1:D:189:LYS:HD2	2.38	0.43
1:D:314:GLY:HA3	1:D:343:ASP:HB2	2.00	0.43
1:A:223:PHE:O	1:A:225:LYS:N	2.52	0.43
1:B:135:PRO:O	1:B:137:LEU:HD22	2.18	0.43
1:B:83:LEU:C	1:B:83:LEU:HD23	2.38	0.43
1:A:358:CYS:O	1:A:359:GLU:HB3	2.18	0.43
1:C:474:MET:CE	1:C:479:LEU:HD13	2.48	0.43
1:D:583:SER:HG	1:D:584:HIS:HD1	1.58	0.43
1:B:441:TRP:O	1:B:445:LEU:N	2.46	0.43
1:A:316:TRP:CE2	1:A:344:VAL:HG21	2.53	0.43
1:B:291:MET:HB3	1:B:639:LEU:HD23	2.00	0.43
1:D:359:GLU:O	1:D:360:TRP:CB	2.67	0.43
1:C:318:SER:OG	1:C:319:ARG:N	2.52	0.43
1:B:72:ARG:NH2	1:B:108:LEU:HD22	2.34	0.43
1:D:212:PHE:CZ	1:D:232:VAL:HG23	2.54	0.43
1:D:364:GLU:O	1:D:365:GLU:HB2	2.19	0.43
1:B:116:LYS:O	1:B:118:ILE:N	2.52	0.43
1:D:215:MET:HE3	1:D:636:ALA:HB1	2.00	0.43
1:A:316:TRP:CE3	1:A:344:VAL:HG11	2.54	0.43
1:A:350:GLY:HA2	1:A:355:ASP:HA	2.00	0.43
1:A:37:LYS:HB3	1:A:41:ILE:N	2.34	0.42
1:C:54:ASN:HB3	1:C:55:ASP:H	1.62	0.42
1:A:211:ARG:HH12	1:A:237:THR:CB	2.32	0.42
1:A:602:ALA:N	1:A:603:PRO:CD	2.82	0.42
1:D:52:LEU:CD1	1:D:59:ASP:HB2	2.49	0.42
1:C:154:THR:HG23	1:C:164:ARG:HB3	2.02	0.42
1:C:549:TRP:CZ3	1:C:551:HIS:HD2	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:561:ASN:OD1	1:C:564:ASN:HB2	2.19	0.42
1:B:601:ILE:H	1:B:601:ILE:HG13	1.71	0.42
1:B:465:ILE:HD11	1:B:467:MET:SD	2.60	0.42
1:D:30:LYS:NZ	1:D:132:VAL:O	2.52	0.42
1:A:37:LYS:H	1:A:38:ASP:HA	1.85	0.42
1:B:191:GLU:CA	1:B:279:ALA:HB2	2.49	0.42
1:B:118:ILE:HD12	1:B:118:ILE:H	1.83	0.42
1:A:245:LEU:HD13	1:A:291:MET:HE2	2.00	0.42
1:B:175:ARG:NE	1:D:230:GLN:OE1	2.52	0.42
1:D:321:THR:HG21	1:D:350:GLY:H	1.84	0.42
1:B:592:LYS:H	1:B:592:LYS:HD2	1.85	0.42
1:A:224:LEU:HB2	1:A:260:SER:HB2	2.02	0.42
1:D:28:ALA:HB2	1:D:48:GLN:NE2	2.34	0.42
1:A:144:LEU:HD21	1:A:172:SER:HB3	2.01	0.42
1:B:190:LYS:HD3	1:B:190:LYS:H	1.85	0.42
1:B:352:PHE:C	1:B:354:THR:H	2.23	0.42
1:D:130:ILE:HD12	1:D:130:ILE:N	2.34	0.42
1:C:688:GLU:HG2	1:C:690:LEU:HD21	2.02	0.42
1:D:211:ARG:NH1	1:D:237:THR:OG1	2.52	0.42
1:A:551:HIS:HE1	1:A:579:GLY:HA2	1.84	0.42
1:A:309:PRO:HG3	1:A:501:ASP:HB3	2.01	0.42
1:A:676:LEU:HD11	1:A:690:LEU:HD13	2.01	0.42
1:A:118:ILE:O	1:A:119:LEU:HD23	2.19	0.42
1:C:505:TRP:CD1	1:C:520:TRP:CE3	3.08	0.42
1:C:53:ALA:H	1:C:54:ASN:HB2	1.85	0.42
1:D:48:GLN:HG2	1:D:183:PHE:HE2	1.85	0.42
1:D:76:ILE:HD12	1:D:106:VAL:HG12	2.01	0.42
1:C:616:ILE:N	1:C:617:PRO:HD2	2.33	0.42
1:D:635:GLN:HB2	1:D:655:TYR:HB2	2.02	0.42
1:C:567:VAL:O	1:C:568:ALA:HB3	2.20	0.42
1:A:517:PRO:HA	1:A:518:LEU:HA	1.84	0.42
1:C:463:GLU:OE1	1:C:507:ARG:NH2	2.53	0.42
1:A:23:GLU:HA	1:A:185:LYS:O	2.19	0.42
1:C:232:VAL:HG13	1:C:232:VAL:O	2.20	0.42
1:C:158:ASP:HB2	1:C:287:ALA:HB1	2.01	0.42
1:C:602:ALA:HB3	1:C:603:PRO:HD3	2.01	0.42
1:A:173:PRO:O	1:A:176:TYR:HE1	2.03	0.42
1:A:27:LYS:O	1:A:48:GLN:HA	2.20	0.41
1:B:465:ILE:HD12	1:B:480:ASN:HD22	1.85	0.41
1:A:561:ASN:CG	1:A:564:ASN:HB2	2.40	0.41
1:C:517:PRO:HA	1:C:518:LEU:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:TYR:CZ	1:C:272:VAL:HG11	2.54	0.41
1:C:651:ASP:OD2	1:C:651:ASP:N	2.52	0.41
1:B:55:ASP:N	1:B:55:ASP:OD1	2.53	0.41
1:D:292:GLU:HG3	1:D:631:TRP:CE2	2.54	0.41
1:A:57:VAL:HG22	1:A:58:ALA:N	2.35	0.41
1:C:353:ARG:HA	1:C:362:PHE:HD2	1.83	0.41
1:C:115:GLY:HA2	1:C:119:LEU:HD13	2.02	0.41
1:A:51:LEU:HD22	1:A:51:LEU:N	2.34	0.41
1:B:49:LYS:C	1:B:49:LYS:HD3	2.41	0.41
1:D:26:TRP:HA	1:D:50:GLN:HB2	2.02	0.41
1:C:686:THR:HG21	1:C:688:GLU:HB2	2.03	0.41
1:A:144:LEU:HD22	1:C:563:MET:CE	2.50	0.41
1:A:367:PHE:CD2	1:A:368:PRO:HD2	2.55	0.41
1:A:326:ASP:O	1:A:330:GLU:HG3	2.19	0.41
1:B:31:PRO:HD2	1:B:132:VAL:CG1	2.49	0.41
1:D:113:GLN:CB	1:D:114:GLY:CA	2.97	0.41
1:A:126:LYS:C	1:A:126:LYS:HD2	2.41	0.41
1:C:212:PHE:CE1	1:C:232:VAL:HG22	2.55	0.41
1:A:163:ILE:HD11	1:A:197:PHE:CD2	2.54	0.41
1:A:553:VAL:HA	1:A:554:PRO:HA	1.89	0.41
1:B:125:THR:HA	1:B:126:LYS:HA	1.89	0.41
1:B:601:ILE:O	1:B:602:ALA:CB	2.67	0.41
1:A:614:SER:O	1:A:718:ILE:HB	2.19	0.41
1:D:135:PRO:O	1:D:136:ALA:HB2	2.20	0.41
1:C:348:ASP:C	1:C:350:GLY:H	2.23	0.41
1:B:450:LEU:CB	1:B:498:VAL:HG21	2.51	0.41
1:B:594:GLU:HA	1:B:595:PRO:HD3	1.83	0.41
1:C:134:GLU:HB2	1:C:135:PRO:CA	2.51	0.41
1:B:139:ARG:HD2	1:B:139:ARG:HA	1.69	0.41
1:A:241:ILE:CG2	1:A:243:PHE:HB3	2.51	0.41
1:B:493:GLU:O	1:B:497:GLU:HB2	2.20	0.41
1:A:17:THR:HA	1:A:18:GLU:HA	1.79	0.41
1:A:27:LYS:HG3	1:A:179:LEU:HD22	2.02	0.41
1:C:357:LEU:HD23	1:C:359:GLU:H	1.86	0.41
1:A:361:LYS:O	1:A:362:PHE:HB2	2.21	0.41
1:B:224:LEU:N	1:B:260:SER:O	2.54	0.41
1:D:37:LYS:HA	1:D:42:CYS:HA	2.03	0.41
1:C:319:ARG:HG2	1:C:320:MET:N	2.36	0.41
1:D:347:LEU:N	1:D:347:LEU:HD22	2.35	0.41
1:C:242:PRO:HD2	1:C:511:ALA:HB2	2.03	0.41
1:D:134:GLU:N	1:D:135:PRO:CD	2.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:LEU:HB3	1:B:281:LEU:CD1	2.50	0.41
1:A:616:ILE:N	1:A:617:PRO:CD	2.84	0.41
1:B:701:VAL:HG11	1:B:707:PRO:HD3	2.03	0.41
1:A:594:GLU:HA	1:A:595:PRO:HD3	1.87	0.41
1:A:30:LYS:HD3	1:A:133:GLU:CD	2.41	0.40
1:A:315:VAL:HA	1:A:585:ILE:HG23	2.02	0.40
1:C:461:PHE:H	1:C:507:ARG:NH1	2.19	0.40
1:B:27:LYS:O	1:B:48:GLN:HA	2.21	0.40
1:D:72:ARG:HH11	1:D:108:LEU:HD13	1.86	0.40
1:B:600:ALA:HA	1:B:601:ILE:C	2.42	0.40
1:A:717:PRO:C	1:A:718:ILE:HG22	2.42	0.40
1:A:173:PRO:N	1:A:174:PRO:CD	2.84	0.40
1:D:96:MET:HB3	1:D:97:LEU:H	1.65	0.40
1:A:338:GLU:HB3	1:A:340:TYR:CD2	2.55	0.40
1:D:315:VAL:HA	1:D:585:ILE:HG23	2.04	0.40
1:D:75:ASN:N	1:D:75:ASN:OD1	2.53	0.40
1:D:292:GLU:OE1	1:D:296:ARG:NH2	2.53	0.40
1:B:204:CYS:HB2	1:B:648:TRP:CE3	2.56	0.40
1:A:30:LYS:HE3	1:A:149:GLU:HG2	2.03	0.40
1:C:349:THR:HG21	1:C:356:TRP:CZ2	2.56	0.40
1:C:505:TRP:CZ2	1:C:586:ARG:HD2	2.56	0.40
1:D:173:PRO:N	1:D:174:PRO:CD	2.84	0.40
1:D:51:LEU:O	1:D:52:LEU:HB2	2.21	0.40
1:A:144:LEU:CD2	1:A:172:SER:HB3	2.51	0.40
1:B:207:GLY:O	1:B:208:THR:OG1	2.27	0.40
1:C:41:ILE:HG21	1:C:72:ARG:HE	1.86	0.40
1:D:49:LYS:NZ	1:D:64:ARG:HH21	2.20	0.40
1:B:435:TYR:CD2	1:B:438:ALA:HB2	2.55	0.40
1:A:458:LYS:HA	1:A:505:TRP:HB3	2.03	0.40
1:A:54:ASN:HA	1:A:55:ASP:HA	1.98	0.40
1:D:352:PHE:N	1:D:352:PHE:CD1	2.89	0.40
1:C:41:ILE:HG22	1:C:72:ARG:HD3	2.02	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	619/761 (81%)	518 (84%)	71 (12%)	30 (5%)	3	3
1	B	605/761 (80%)	523 (86%)	59 (10%)	23 (4%)	4	5
1	C	626/761 (82%)	537 (86%)	66 (10%)	23 (4%)	4	5
1	D	617/761 (81%)	532 (86%)	55 (9%)	30 (5%)	3	3
All	All	2467/3044 (81%)	2110 (86%)	251 (10%)	106 (4%)	3	4

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	GLU
1	A	133	GLU
1	A	137	LEU
1	A	142	GLU
1	A	162	GLU
1	A	355	ASP
1	A	359	GLU
1	A	360	TRP
1	A	361	LYS
1	A	362	PHE
1	A	687	GLY
1	A	713	ASN
1	B	31	PRO
1	B	32	THR
1	B	51	LEU
1	B	107	PRO
1	B	142	GLU
1	B	602	ALA
1	C	55	ASP
1	C	105	ARG
1	C	116	LYS
1	C	142	GLU
1	C	357	LEU
1	C	359	GLU
1	C	363	ASN
1	D	103	ILE
1	D	107	PRO
1	D	134	GLU

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Mol	Chain	Res	Type
1	D	136	ALA
1	D	137	LEU
1	D	142	GLU
1	D	351	TRP
1	D	359	GLU
1	D	360	TRP
1	A	15	PHE
1	A	54	ASN
1	A	86	GLY
1	A	123	ASP
1	A	124	GLY
1	A	138	ASP
1	A	437	LYS
1	A	561	ASN
1	B	39	GLY
1	B	349	THR
1	C	32	THR
1	C	39	GLY
1	C	57	VAL
1	C	98	GLN
1	C	143	LEU
1	C	366	ARG
1	C	526	SER
1	D	33	ALA
1	D	38	ASP
1	D	357	LEU
1	A	715	VAL
1	B	104	ARG
1	B	117	TRP
1	B	668	SER
1	C	351	TRP
1	C	356	TRP
1	D	51	LEU
1	D	53	ALA
1	D	113	GLN
1	D	323	PHE
1	D	362	PHE
1	D	568	ALA
1	D	601	ILE
1	D	686	THR
1	A	161	ARG
1	A	255	HIS

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Mol	Chain	Res	Type
1	A	568	ALA
1	B	34	VAL
1	B	55	ASP
1	B	123	ASP
1	B	140	TRP
1	B	160	LYS
1	B	324	SER
1	C	53	ALA
1	C	140	TRP
1	C	600	ALA
1	C	602	ALA
1	D	123	ASP
1	D	363	ASN
1	D	472	LYS
1	A	139	ARG
1	A	714	ALA
1	B	224	LEU
1	B	354	THR
1	C	102	ARG
1	D	57	VAL
1	D	718	ILE
1	A	85	PHE
1	B	599	PRO
1	D	39	GLY
1	D	77	GLY
1	D	692	GLY
1	B	76	ILE
1	A	367	PHE
1	A	554	PRO
1	D	115	GLY
1	A	436	PRO
1	C	473	GLY
1	B	57	VAL
1	B	554	PRO
1	C	554	PRO
1	D	554	PRO

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	512/663 (77%)	460 (90%)	52 (10%)	9 17
1	B	504/663 (76%)	460 (91%)	44 (9%)	13 24
1	C	527/663 (80%)	495 (94%)	32 (6%)	23 46
1	D	507/663 (76%)	464 (92%)	43 (8%)	13 25
All	All	2050/2652 (77%)	1879 (92%)	171 (8%)	14 27

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	13	PHE
1	A	15	PHE
1	A	18	GLU
1	A	20	LEU
1	A	21	ARG
1	A	43	VAL
1	A	48	GLN
1	A	52	LEU
1	A	68	THR
1	A	75	ASN
1	A	83	LEU
1	A	87	GLU
1	A	123	ASP
1	A	126	LYS
1	A	144	LEU
1	A	158	ASP
1	A	161	ARG
1	A	163	ILE
1	A	200	ARG
1	A	215	MET
1	A	232	VAL
1	A	241	ILE
1	A	249	MET
1	A	269	THR
1	A	278	GLN
1	A	280	MET
1	A	338	GLU
1	A	342	CYS
1	A	343	ASP

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Mol	Chain	Res	Type
1	A	362	PHE
1	A	367	PHE
1	A	449	LEU
1	A	474	MET
1	A	475	LYS
1	A	494	ILE
1	A	504	VAL
1	A	518	LEU
1	A	520	TRP
1	A	551	HIS
1	A	563	MET
1	A	574	ARG
1	A	583	SER
1	A	593	ARG
1	A	634	LEU
1	A	651	ASP
1	A	672	ARG
1	A	680	GLN
1	A	697	LYS
1	A	711	ARG
1	A	715	VAL
1	A	718	ILE
1	B	44	THR
1	B	48	GLN
1	B	49	LYS
1	B	72	ARG
1	B	79	THR
1	B	102	ARG
1	B	111	GLU
1	B	123	ASP
1	B	125	THR
1	B	137	LEU
1	B	160	LYS
1	B	163	ILE
1	B	177	ASP
1	B	186	ARG
1	B	189	LYS
1	B	190	LYS
1	B	195	LEU
1	B	200	ARG
1	B	281	LEU
1	B	310	LEU

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Mol	Chain	Res	Type
1	B	330	GLU
1	B	334	ARG
1	B	343	ASP
1	B	345	ILE
1	B	354	THR
1	B	430	THR
1	B	445	LEU
1	B	465	ILE
1	B	472	LYS
1	B	475	LYS
1	B	518	LEU
1	B	520	TRP
1	B	559	LEU
1	B	564	ASN
1	B	592	LYS
1	B	593	ARG
1	B	614	SER
1	B	625	LEU
1	B	634	LEU
1	B	651	ASP
1	B	667	ASN
1	B	669	GLU
1	B	710	VAL
1	B	713	ASN
1	C	35	TYR
1	C	44	THR
1	C	70	ILE
1	C	83	LEU
1	C	102	ARG
1	C	113	GLN
1	C	122	GLN
1	C	137	LEU
1	C	140	TRP
1	C	163	ILE
1	C	192	ARG
1	C	194	THR
1	C	195	LEU
1	C	208	THR
1	C	225	LYS
1	C	232	VAL
1	C	261	LYS
1	C	348	ASP

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Mol	Chain	Res	Type
1	C	351	TRP
1	C	356	TRP
1	C	454	VAL
1	C	463	GLU
1	C	475	LYS
1	C	497	GLU
1	C	504	VAL
1	C	518	LEU
1	C	520	TRP
1	C	583	SER
1	C	593	ARG
1	C	625	LEU
1	C	651	ASP
1	C	701	VAL
1	D	29	CYS
1	D	37	LYS
1	D	41	ILE
1	D	48	GLN
1	D	56	MET
1	D	70	ILE
1	D	81	LEU
1	D	83	LEU
1	D	96	MET
1	D	97	LEU
1	D	102	ARG
1	D	113	GLN
1	D	118	ILE
1	D	126	LYS
1	D	162	GLU
1	D	163	ILE
1	D	189	LYS
1	D	194	THR
1	D	215	MET
1	D	225	LYS
1	D	272	VAL
1	D	310	LEU
1	D	343	ASP
1	D	348	ASP
1	D	352	PHE
1	D	357	LEU
1	D	359	GLU
1	D	514	GLN

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Mol	Chain	Res	Type
1	D	518	LEU
1	D	520	TRP
1	D	563	MET
1	D	567	VAL
1	D	586	ARG
1	D	591	ASN
1	D	593	ARG
1	D	607	LYS
1	D	628	GLU
1	D	633	LEU
1	D	634	LEU
1	D	651	ASP
1	D	697	LYS
1	D	701	VAL
1	D	704	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	148	GLN
1	B	255	HIS
1	B	551	HIS
1	B	591	ASN
1	B	649	HIS
1	D	113	GLN
1	D	259	HIS

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 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	625/761 (82%)	0.22	15 (2%) 62 56	22, 45, 78, 95	0
1	B	611/761 (80%)	0.69	67 (10%) 7 4	47, 64, 88, 96	0
1	C	632/761 (83%)	0.31	22 (3%) 48 40	25, 49, 83, 95	0
1	D	623/761 (81%)	0.38	32 (5%) 32 25	32, 53, 87, 101	0
All	All	2491/3044 (81%)	0.40	136 (5%) 29 21	22, 56, 85, 101	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	323	PHE	6.4
1	A	54	ASN	6.1
1	B	350	GLY	5.7
1	C	54	ASN	5.6
1	D	113	GLN	5.4
1	A	470	VAL	4.9
1	D	119	LEU	4.9
1	B	468	ASP	4.8
1	D	328	VAL	4.6
1	C	337	ALA	4.6
1	D	143	LEU	4.4
1	D	53	ALA	4.3
1	C	120	PHE	4.3
1	C	33	ALA	4.2
1	B	177	ASP	4.1
1	B	323	PHE	4.1
1	D	468	ASP	4.1
1	B	601	ILE	4.0
1	B	689	ARG	4.0
1	B	117	TRP	4.0
1	B	472	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	566	ILE	3.9
1	B	62	VAL	3.8
1	B	143	LEU	3.8
1	B	442	TYR	3.5
1	D	120	PHE	3.5
1	B	27	LYS	3.4
1	D	54	ASN	3.4
1	D	470	VAL	3.4
1	B	110	VAL	3.4
1	B	122	GLN	3.4
1	D	27	LYS	3.4
1	B	52	LEU	3.4
1	B	718	ILE	3.3
1	A	477	GLU	3.3
1	D	60	THR	3.3
1	C	35	TYR	3.2
1	B	120	PHE	3.2
1	B	69	LEU	3.2
1	B	142	GLU	3.2
1	B	140	TRP	3.2
1	D	601	ILE	3.2
1	B	65	GLU	3.1
1	C	99	PHE	3.1
1	A	720	PRO	3.1
1	B	29	CYS	3.1
1	A	13	PHE	3.0
1	D	130	ILE	3.0
1	B	627	VAL	3.0
1	C	110	VAL	3.0
1	B	116	LYS	3.0
1	B	313	PHE	3.0
1	B	186	ARG	3.0
1	B	439	THR	3.0
1	B	81	LEU	3.0
1	B	715	VAL	2.9
1	B	434	THR	2.9
1	D	188	GLY	2.9
1	D	471	TYR	2.9
1	B	68	THR	2.9
1	B	193	ALA	2.9
1	D	71	ILE	2.8
1	B	470	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	62	VAL	2.8
1	B	61	ALA	2.8
1	D	133	GLU	2.8
1	B	487	TYR	2.8
1	B	127	ARG	2.8
1	B	453	GLY	2.8
1	C	713	ASN	2.8
1	C	113	GLN	2.7
1	D	311	TRP	2.7
1	D	352	PHE	2.7
1	B	130	ILE	2.7
1	A	132	VAL	2.7
1	A	70	ILE	2.6
1	B	44	THR	2.6
1	D	76	ILE	2.6
1	B	435	TYR	2.6
1	A	140	TRP	2.6
1	B	694	ARG	2.6
1	B	59	ASP	2.5
1	B	231	GLY	2.5
1	B	548	PHE	2.5
1	C	32	THR	2.5
1	B	35	TYR	2.5
1	C	70	ILE	2.5
1	A	62	VAL	2.5
1	B	141	SER	2.5
1	B	454	VAL	2.5
1	B	451	ASP	2.5
1	B	719	TYR	2.5
1	D	324	SER	2.5
1	C	619	ILE	2.4
1	C	356	TRP	2.4
1	A	49	LYS	2.4
1	B	125	THR	2.4
1	B	137	LEU	2.4
1	D	590	THR	2.3
1	C	56	MET	2.3
1	B	667	ASN	2.3
1	D	50	GLN	2.3
1	B	455	THR	2.3
1	D	661	LEU	2.2
1	B	28	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	337	ALA	2.2
1	D	144	LEU	2.2
1	C	323	PHE	2.2
1	B	82	PHE	2.2
1	D	58	ALA	2.2
1	A	131	ASN	2.2
1	B	58	ALA	2.2
1	D	187	THR	2.2
1	B	671	ARG	2.2
1	B	34	VAL	2.2
1	C	143	LEU	2.1
1	C	720	PRO	2.1
1	D	703	LEU	2.1
1	B	351	TRP	2.1
1	A	368	PRO	2.1
1	C	712	GLU	2.1
1	B	619	ILE	2.1
1	B	136	ALA	2.1
1	B	36	GLU	2.1
1	C	121	THR	2.1
1	A	129	VAL	2.1
1	B	295	LEU	2.1
1	A	686	THR	2.1
1	B	181	ILE	2.1
1	C	53	ALA	2.1
1	C	566	ILE	2.0
1	D	431	ILE	2.0
1	A	181	ILE	2.0
1	D	560	PRO	2.0
1	B	688	GLU	2.0
1	C	633	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.