Full wwPDB X-ray Structure Validation Report (i)

Sep 25, 2023 – 08:04 AM EDT

PDB ID	:	5WA4
Title	:	Pyridine synthase, TbtD, from thiomuracin biosynthesis bound to an N-terminal leader peptide fragment
Authors	:	Cogan, D.P.; Nair, S.K.
Deposited on	:	2017-06-24
Resolution	:	2.65 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:

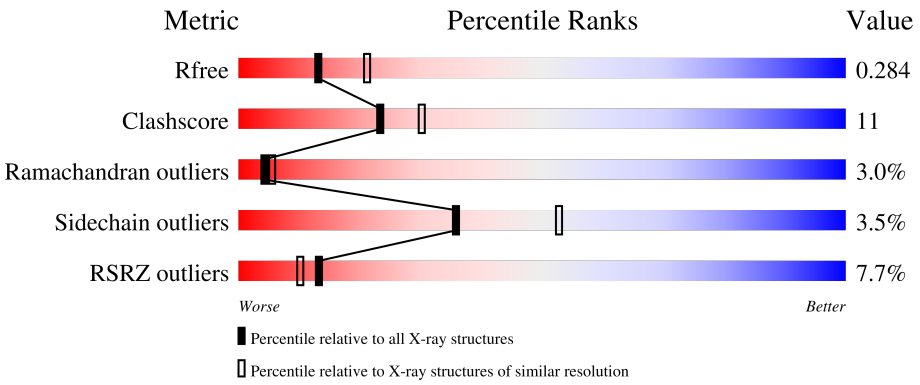
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.65 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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	361	6% 64% 20% • 14%
1	B	361	5% 62% 20% • 15%
1	C	361	3% 67% 17% • 15%
1	D	361	5% 66% 17% • • 14%
1	E	361	6% 67% 16% • • 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	361	14% 51% 29% 5% • 15%
2	M	16	6% 50% 19% 31%
2	N	16	6% 44% 12% 44%
2	O	16	56% 12% 31%
2	P	16	50% 6% 44%
2	Q	16	50% 50%
2	R	16	50% 19% 31%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15235 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 Pyridine synthase TbtD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	310	2447	1548	462	431	6	0	0	0
1	B	307	2431	1538	459	428	6	0	0	0
1	C	308	2438	1542	460	430	6	0	0	0
1	D	309	2445	1546	461	432	6	0	0	0
1	E	313	2479	1567	469	437	6	0	1	0
1	F	308	2439	1544	460	429	6	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP D6Y504
A	-1	GLY	-	expression tag	UNP D6Y504
A	0	SER	-	expression tag	UNP D6Y504
B	-2	SER	-	expression tag	UNP D6Y504
B	-1	GLY	-	expression tag	UNP D6Y504
B	0	SER	-	expression tag	UNP D6Y504
C	-2	SER	-	expression tag	UNP D6Y504
C	-1	GLY	-	expression tag	UNP D6Y504
C	0	SER	-	expression tag	UNP D6Y504
D	-2	SER	-	expression tag	UNP D6Y504
D	-1	GLY	-	expression tag	UNP D6Y504
D	0	SER	-	expression tag	UNP D6Y504
E	-2	SER	-	expression tag	UNP D6Y504
E	-1	GLY	-	expression tag	UNP D6Y504
E	0	SER	-	expression tag	UNP D6Y504
F	-2	SER	-	expression tag	UNP D6Y504
F	-1	GLY	-	expression tag	UNP D6Y504

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	0	SER	-	expression tag	UNP D6Y504

- Molecule 2 is a protein called TbtA 16-mer peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	11	90	59	12	18	1	0	0	0
2	N	9	74	47	10	16	1	0	0	0
2	O	11	90	59	12	18	1	0	0	0
2	P	9	74	47	10	16	1	0	0	0
2	Q	8	65	42	9	13	1	0	0	0
2	R	11	90	59	12	18	1	0	0	0

- Molecule 3 is water.

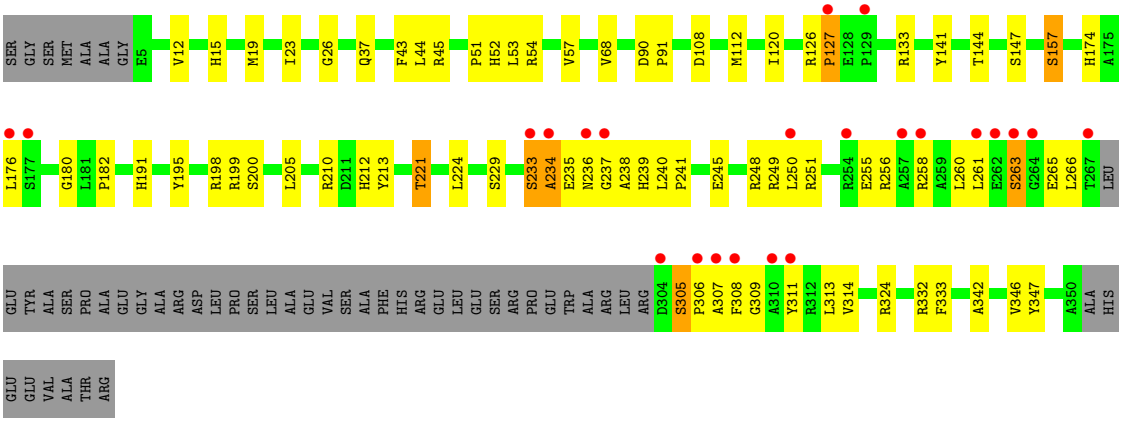
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	13	13	13	0	0
3	B	10	10	10	0	0
3	C	15	15	15	0	0
3	D	13	13	13	0	0
3	E	13	13	13	0	0
3	F	6	6	6	0	0
3	O	1	1	1	0	0
3	Q	2	2	2	0	0

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.

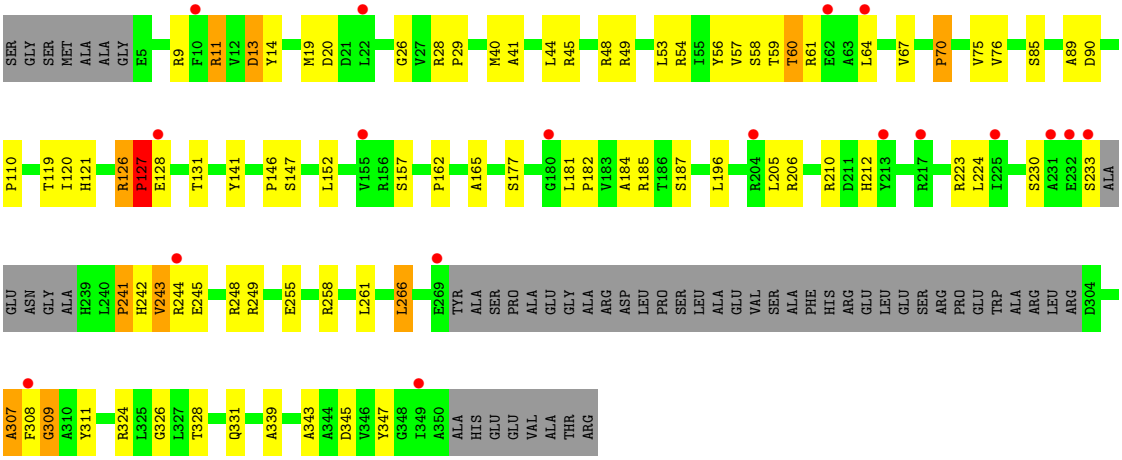
• Molecule 1: Pyridine synthase TbtD

Chain A:



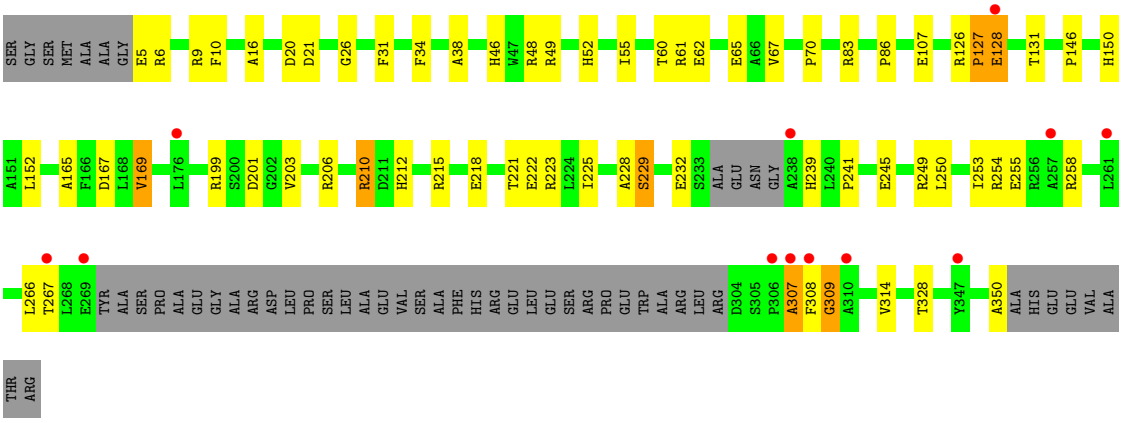
• Molecule 1: Pyridine synthase TbtD

Chain B:



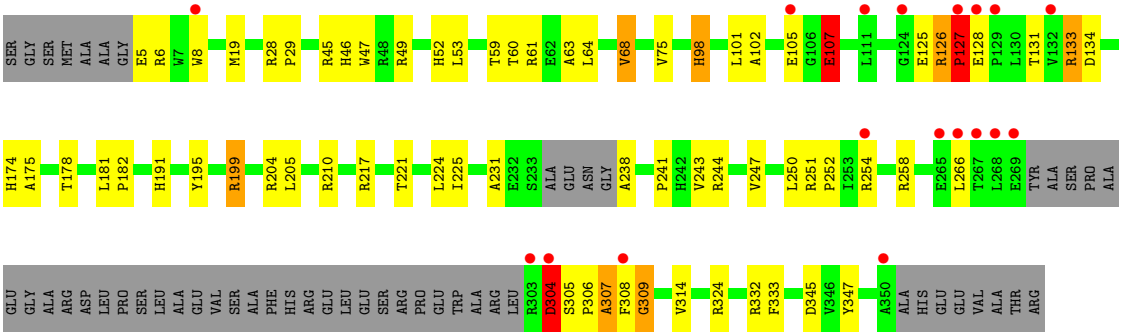
• Molecule 1: Pyridine synthase TbtD

Chain C:



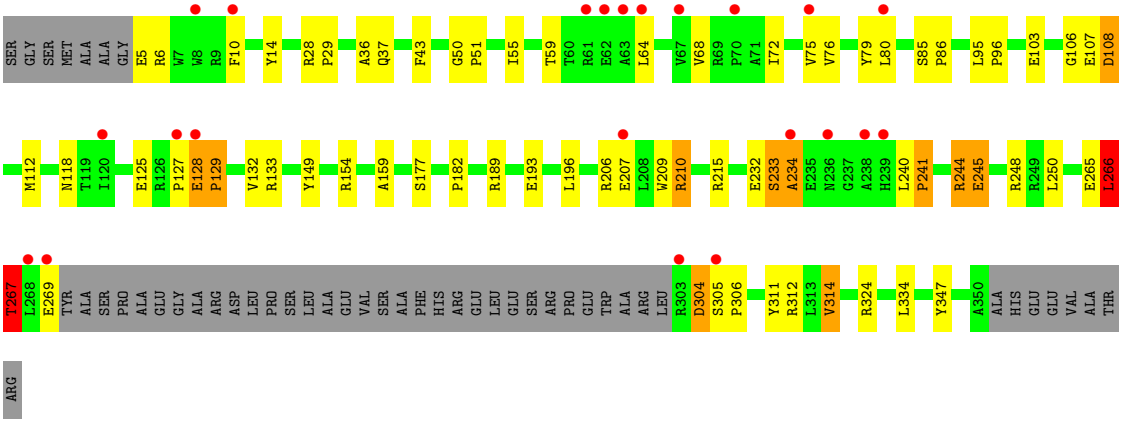
• Molecule 1: Pyridine synthase TbtD

Chain D:



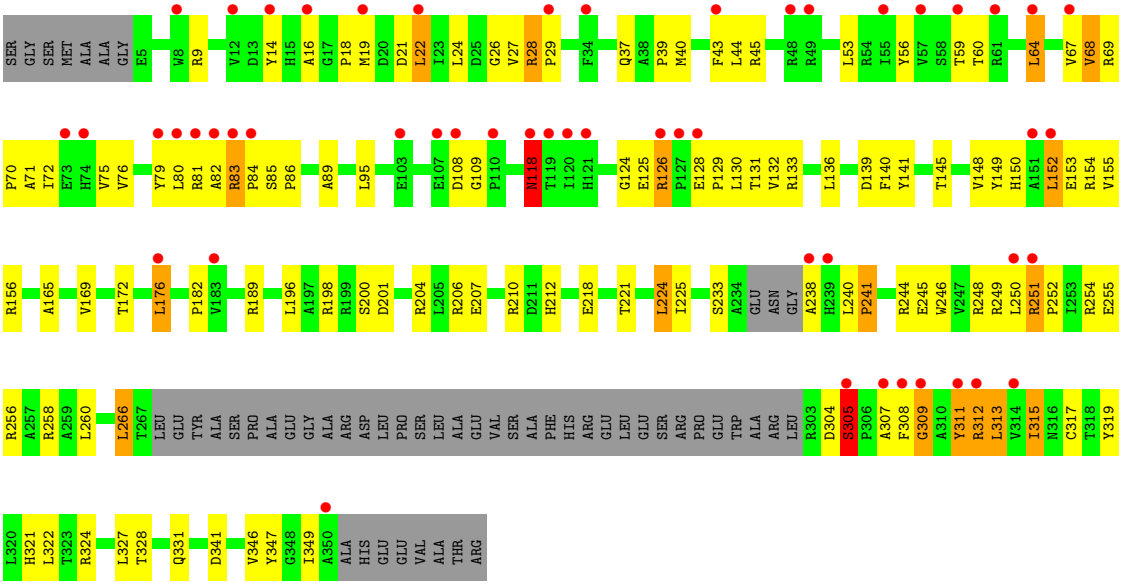
• Molecule 1: Pyridine synthase TbtD

Chain E:



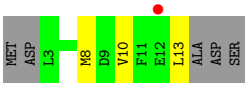
• Molecule 1: Pyridine synthase TbtD

Chain F:



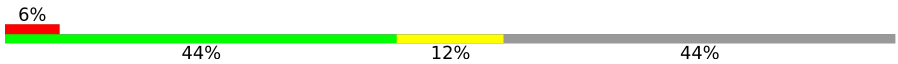
- Molecule 2: TbtA 16-mer peptide

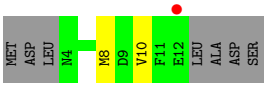
Chain M:



- Molecule 2: TbtA 16-mer peptide

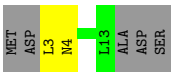
Chain N:





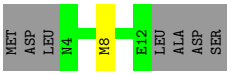
- Molecule 2: TbtA 16-mer peptide

Chain O:



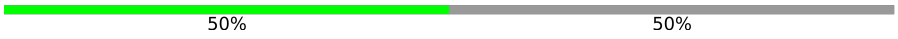
- Molecule 2: TbtA 16-mer peptide

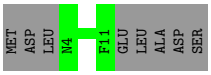
Chain P:



- Molecule 2: TbtA 16-mer peptide

Chain Q:





• Molecule 2: TbtA 16-mer peptide

Chain R:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.38Å 106.00Å 234.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.05 – 2.65 48.05 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.05-2.65) 98.8 (48.05-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.220 , 0.287 0.221 , 0.284	Depositor DCC
R_{free} test set	3735 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	59.6	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 56.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15235	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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	0.54	0/2514	0.68	0/3426
1	B	0.45	0/2496	0.63	0/3401
1	C	0.52	0/2503	0.67	1/3410 (0.0%)
1	D	0.51	0/2510	0.69	2/3420 (0.1%)
1	E	0.49	0/2546	0.69	3/3469 (0.1%)
1	F	0.48	0/2505	0.78	6/3413 (0.2%)
2	M	0.47	0/91	1.01	0/123
2	N	0.40	0/75	0.62	0/101
2	O	0.49	0/91	0.81	0/123
2	P	0.53	0/75	0.70	0/101
2	Q	0.48	0/66	0.71	0/89
2	R	0.40	0/91	0.61	0/123
All	All	0.50	0/15563	0.69	12/21199 (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	B	0	3
1	D	0	3
1	E	0	1
1	F	0	1
All	All	0	8

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	83	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	F	83	ARG	NE-CZ-NH1	7.17	123.88	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	266	LEU	CA-CB-CG	5.90	128.87	115.30
1	E	304	ASP	CB-CG-OD1	5.63	123.37	118.30
1	C	266	LEU	CA-CB-CG	5.59	128.15	115.30
1	D	107	GLU	CA-CB-CG	5.35	125.17	113.40
1	E	266	LEU	CA-CB-CG	5.32	127.53	115.30
1	F	22	LEU	CA-CB-CG	5.24	127.34	115.30
1	D	304	ASP	CB-CG-OD1	5.21	122.98	118.30
1	F	64	LEU	CA-CB-CG	-5.19	103.37	115.30
1	E	240	LEU	CA-CB-CG	5.18	127.21	115.30
1	F	176	LEU	CB-CG-CD2	5.03	119.56	111.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	126	ARG	Peptide
1	B	127	PRO	Peptide
1	B	266	LEU	Peptide
1	D	126	ARG	Peptide
1	D	127	PRO	Peptide
1	D	98	HIS	Sidechain
1	E	266	LEU	Peptide
1	F	305	SER	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	2447	0	2398	48	0
1	B	2431	0	2390	51	0
1	C	2438	0	2394	44	0
1	D	2445	0	2401	52	0
1	E	2479	0	2429	51	0
1	F	2439	0	2396	113	0
2	M	90	0	86	3	0
2	N	74	0	64	2	0
2	O	90	0	86	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	74	0	64	0	0
2	Q	65	0	58	0	0
2	R	90	0	86	3	0
3	A	13	0	0	1	0
3	B	10	0	0	1	0
3	C	15	0	0	2	0
3	D	13	0	0	1	0
3	E	13	0	0	1	0
3	F	6	0	0	0	0
3	O	1	0	0	1	0
3	Q	2	0	0	0	0
All	All	15235	0	14852	340	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 11.

All (340) 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:C:150:HIS:O	3:C:401:HOH:O	1.91	0.89
1:B:126:ARG:HG2	1:B:127:PRO:HD3	1.55	0.88
1:B:45:ARG:NH1	1:B:324:ARG:O	2.08	0.87
1:A:126:ARG:NH1	3:A:401:HOH:O	2.06	0.87
1:D:126:ARG:HG2	1:D:127:PRO:HD3	1.58	0.86
1:B:89:ALA:HB1	1:F:18:PRO:HD3	1.59	0.85
1:F:128:GLU:O	1:F:130:LEU:N	2.11	0.83
1:F:322:LEU:HB3	1:F:327:LEU:HD21	1.62	0.82
1:A:260:LEU:HG	1:A:265:GLU:HG2	1.60	0.81
1:A:263:SER:OG	1:A:265:GLU:OE2	1.96	0.81
1:D:175:ALA:HB2	1:D:231:ALA:HB1	1.63	0.80
1:C:5:GLU:N	3:C:402:HOH:O	2.13	0.80
1:A:258:ARG:HG3	1:A:306:PRO:HA	1.63	0.80
1:D:105:GLU:CD	1:D:107:GLU:HB2	2.02	0.80
1:E:64:LEU:HA	1:E:68:VAL:HG12	1.64	0.79
1:B:345:ASP:OD2	1:D:217:ARG:NH2	2.16	0.79
1:F:16:ALA:HB3	1:F:86:PRO:HD2	1.65	0.79
1:F:29:PRO:HB2	1:F:75:VAL:HG21	1.66	0.77
1:E:304:ASP:OD1	1:E:305:SER:N	2.18	0.77
1:F:118:ASN:N	1:F:118:ASN:HD22	1.83	0.77
1:D:131:THR:HG23	1:D:134:ASP:H	1.53	0.74
1:C:218:GLU:HA	1:C:221:THR:HG22	1.71	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:131:THR:HB	1:F:133:ARG:HH21	1.52	0.72
1:E:215:ARG:HG2	1:F:349:ILE:HA	1.71	0.72
1:F:311:TYR:CD2	1:F:312:ARG:N	2.57	0.72
1:B:328:THR:OG1	1:B:331:GLN:HG3	1.89	0.71
1:A:176:LEU:HD22	1:A:314:VAL:HG21	1.72	0.71
1:A:261:LEU:HB3	1:A:305:SER:HB3	1.73	0.71
1:E:266:LEU:O	1:E:267:THR:OG1	2.09	0.70
1:E:245:GLU:OE2	1:E:248:ARG:NH1	2.23	0.70
1:E:29:PRO:HB2	1:E:75:VAL:HG11	1.74	0.70
1:A:212:HIS:HD2	2:M:10:VAL:HG12	1.56	0.70
1:B:245:GLU:OE2	1:B:248:ARG:NH2	2.25	0.69
1:A:91:PRO:HB2	1:A:112:MET:HE1	1.74	0.68
1:D:105:GLU:HB3	1:D:107:GLU:H	1.58	0.68
1:C:167:ASP:OD2	1:C:223:ARG:NH2	2.25	0.68
1:F:139:ASP:OD1	1:F:140:PHE:N	2.26	0.68
1:A:245:GLU:OE1	1:A:248:ARG:NH2	2.27	0.67
1:D:238:ALA:HB3	1:D:244:ARG:HE	1.60	0.67
1:F:80:LEU:HD12	1:F:118:ASN:HB3	1.76	0.67
1:F:79:TYR:O	1:F:82:ALA:N	2.27	0.67
1:F:67:VAL:HG13	1:F:68:VAL:HG12	1.76	0.67
1:F:59:THR:HG21	1:F:64:LEU:HD13	1.77	0.66
1:C:16:ALA:HB3	1:C:86:PRO:HD2	1.77	0.66
1:D:307:ALA:O	1:D:309:GLY:N	2.30	0.65
1:F:260:LEU:HB3	1:F:266:LEU:HD13	1.79	0.64
1:F:305:SER:O	1:F:309:GLY:HA3	1.97	0.64
1:B:255:GLU:HG2	1:B:258:ARG:HH11	1.63	0.64
1:C:350:ALA:HB3	2:M:13:LEU:HD13	1.80	0.63
1:F:189:ARG:NH2	1:F:341:ASP:OD1	2.31	0.63
1:F:311:TYR:CE2	1:F:312:ARG:HB2	2.33	0.63
1:F:9:ARG:HH22	1:F:125:GLU:N	1.98	0.62
1:F:312:ARG:HA	1:F:315:ILE:HG22	1.82	0.62
1:E:210:ARG:HD2	1:F:210:ARG:CZ	2.29	0.62
1:F:21:ASP:HB3	1:F:83:ARG:HH22	1.63	0.62
1:F:9:ARG:NH1	1:F:124:GLY:O	2.32	0.62
1:C:10:PHE:HB2	1:C:55:ILE:HB	1.82	0.62
1:F:9:ARG:NE	1:F:126:ARG:HG2	2.15	0.62
1:F:21:ASP:HB3	1:F:83:ARG:NH2	2.15	0.61
1:E:43:PHE:H	1:E:324:ARG:HH21	1.48	0.61
1:A:198:ARG:O	1:A:198:ARG:HG2	1.99	0.61
1:C:199:ARG:NH2	1:E:103:GLU:HB2	2.13	0.61
1:C:9:ARG:HD3	1:C:126:ARG:HG3	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:GLU:OE1	1:A:258:ARG:NH2	2.34	0.60
1:E:133:ARG:HB2	1:E:133:ARG:CZ	2.31	0.60
1:D:6:ARG:NH1	1:D:125:GLU:OE2	2.35	0.60
1:E:132:VAL:HG21	1:E:265:GLU:HB3	1.84	0.60
1:B:212:HIS:HB2	2:N:10:VAL:HG23	1.83	0.60
1:B:146:PRO:HG2	1:B:249:ARG:HH21	1.66	0.59
1:F:251:ARG:O	1:F:255:GLU:HG2	2.01	0.59
1:F:45:ARG:NH1	1:F:324:ARG:O	2.35	0.59
1:D:45:ARG:HD2	1:D:324:ARG:O	2.03	0.59
1:F:118:ASN:N	1:F:118:ASN:ND2	2.47	0.59
1:A:251:ARG:O	1:A:255:GLU:HG2	2.03	0.59
1:D:101:LEU:O	1:D:105:GLU:HB2	2.01	0.58
1:F:255:GLU:O	1:F:258:ARG:HB3	2.02	0.58
1:A:256:ARG:O	1:A:260:LEU:HB2	2.03	0.58
1:F:128:GLU:O	1:F:128:GLU:HG3	2.02	0.58
1:F:59:THR:HG21	1:F:64:LEU:CD1	2.33	0.58
1:E:193:GLU:OE1	1:E:206:ARG:NH1	2.37	0.58
1:C:34:PHE:HD1	1:C:38:ALA:HB3	1.68	0.58
1:D:199:ARG:HE	1:D:205:LEU:HD11	1.69	0.58
1:B:110:PRO:HD3	2:R:11:PHE:HB2	1.86	0.57
1:F:176:LEU:HD22	1:F:251:ARG:NE	2.19	0.57
1:C:203:VAL:HA	1:C:206:ARG:HD2	1.86	0.57
1:C:146:PRO:HG2	1:C:249:ARG:HH12	1.70	0.57
1:B:41:ALA:HB2	1:B:57:VAL:HG23	1.87	0.57
1:E:5:GLU:N	3:E:403:HOH:O	2.36	0.57
1:E:196:LEU:HD13	1:E:206:ARG:HG3	1.86	0.57
1:F:22:LEU:HD11	1:F:53:LEU:HD12	1.86	0.57
1:B:181:LEU:HD21	1:B:224:LEU:HD11	1.85	0.56
1:D:64:LEU:HD12	1:D:68:VAL:HG13	1.86	0.56
1:A:265:GLU:OE1	1:A:265:GLU:N	2.39	0.56
1:B:243:VAL:HG23	1:B:244:ARG:H	1.69	0.56
1:F:22:LEU:HB3	1:F:79:TYR:HE2	1.69	0.56
1:D:102:ALA:HA	1:D:105:GLU:OE1	2.05	0.56
1:D:304:ASP:HA	1:D:307:ALA:HB3	1.87	0.56
1:B:185:ARG:HD2	1:B:343:ALA:HB1	1.87	0.55
1:E:207:GLU:CD	1:F:189:ARG:HD2	2.27	0.55
1:E:133:ARG:NE	1:E:269:GLU:HG2	2.21	0.55
1:E:250:LEU:HD13	1:E:314:VAL:HG22	1.88	0.55
1:D:250:LEU:HD13	1:D:314:VAL:HG13	1.89	0.55
1:E:133:ARG:HE	1:E:269:GLU:HG2	1.72	0.55
1:F:68:VAL:HA	1:F:71:ALA:HB3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:GLU:O	1:A:237:GLY:N	2.37	0.54
1:A:19:MET:SD	1:A:53:LEU:HD13	2.48	0.54
1:E:133:ARG:HE	1:E:269:GLU:CG	2.21	0.54
1:E:95:LEU:HD13	1:E:112:MET:HG2	1.89	0.54
1:E:28:ARG:HB2	1:E:149:TYR:CE1	2.43	0.53
1:E:128:GLU:HB2	1:E:129:PRO:HD3	1.89	0.53
1:F:328:THR:OG1	1:F:331:GLN:HG3	2.08	0.53
1:F:59:THR:OG1	1:F:60:THR:N	2.39	0.53
1:F:37:GLN:OE1	1:F:37:GLN:N	2.37	0.53
1:F:24:LEU:HD23	1:F:149:TYR:HD1	1.74	0.53
1:D:47:TRP:CZ3	1:D:98:HIS:HB3	2.43	0.53
1:D:64:LEU:HA	1:D:68:VAL:CG1	2.39	0.52
1:E:233:SER:OG	1:E:234:ALA:N	2.42	0.52
1:F:64:LEU:HA	1:F:68:VAL:HG13	1.92	0.52
1:F:9:ARG:HH12	1:F:125:GLU:CA	2.23	0.52
1:F:72:ILE:O	1:F:76:VAL:HB	2.09	0.52
1:C:46:HIS:HB3	1:C:52:HIS:CE1	2.45	0.52
1:D:29:PRO:HB2	1:D:75:VAL:HG11	1.91	0.51
1:B:11:ARG:NH2	1:B:49:ARG:HB2	2.26	0.51
1:D:217:ARG:NH1	1:D:345:ASP:OD2	2.39	0.51
1:F:27:VAL:HG11	1:F:43:PHE:CD2	2.46	0.51
1:B:44:LEU:HD21	1:B:141:TYR:CE2	2.45	0.51
1:F:9:ARG:CZ	1:F:126:ARG:HG2	2.41	0.51
1:E:6:ARG:HD2	1:E:125:GLU:OE1	2.11	0.51
1:F:69:ARG:HB3	1:F:70:PRO:HD3	1.92	0.51
1:F:311:TYR:CG	1:F:312:ARG:N	2.78	0.51
1:A:12:VAL:HG12	1:A:120:ILE:HG12	1.92	0.51
1:E:210:ARG:HB3	1:F:210:ARG:NH2	2.26	0.51
1:F:79:TYR:HE1	1:F:83:ARG:HB2	1.75	0.51
1:F:201:ASP:OD1	1:F:201:ASP:N	2.43	0.51
1:D:126:ARG:NH1	3:D:402:HOH:O	2.43	0.51
1:E:209:TRP:NE1	1:E:334:LEU:HD13	2.26	0.50
1:F:9:ARG:HH12	1:F:125:GLU:HA	1.76	0.50
1:F:176:LEU:O	1:F:251:ARG:NH2	2.43	0.50
1:E:206:ARG:HD2	1:E:210:ARG:CZ	2.42	0.50
1:D:254:ARG:HB2	1:D:314:VAL:HG21	1.93	0.50
1:F:140:PHE:CZ	1:F:317:CYS:HB3	2.47	0.50
1:F:233:SER:HB2	1:F:244:ARG:NH2	2.27	0.50
1:D:221:THR:O	1:D:225:ILE:HG13	2.11	0.50
1:D:243:VAL:O	1:D:247:VAL:HG23	2.12	0.50
1:B:59:THR:HG23	1:B:60:THR:O	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:HIS:HB3	1:D:52:HIS:CE1	2.47	0.49
1:D:199:ARG:NE	1:D:205:LEU:HD11	2.26	0.49
1:F:9:ARG:CD	1:F:126:ARG:HG2	2.43	0.49
1:B:233:SER:H	1:B:244:ARG:HE	1.61	0.49
1:A:311:TYR:O	1:A:314:VAL:HG12	2.13	0.48
1:C:48:ARG:HG2	1:C:49:ARG:HG3	1.95	0.48
1:A:250:LEU:HD22	1:A:314:VAL:CG2	2.43	0.48
1:E:177:SER:HB3	1:E:311:TYR:CE1	2.48	0.48
1:B:48:ARG:HG2	1:B:49:ARG:HG3	1.96	0.48
1:F:246:TRP:NE1	1:F:250:LEU:HD11	2.27	0.48
2:O:3:LEU:N	3:O:101:HOH:O	2.46	0.48
1:A:238:ALA:O	1:A:240:LEU:N	2.47	0.48
1:E:10:PHE:HB2	1:E:55:ILE:HB	1.96	0.48
1:C:255:GLU:HB2	1:C:258:ARG:NH2	2.29	0.48
1:E:232:GLU:C	1:E:244:ARG:HH22	2.16	0.48
1:B:40:MET:HB3	1:B:58:SER:HB3	1.94	0.48
1:B:19:MET:SD	1:B:53:LEU:HD13	2.54	0.47
1:D:251:ARG:HB3	1:D:252:PRO:HD3	1.96	0.47
1:A:52:HIS:NE2	1:A:54:ARG:HD2	2.30	0.47
1:A:44:LEU:HD21	1:A:141:TYR:CE2	2.49	0.47
1:E:207:GLU:OE2	1:F:189:ARG:HD2	2.15	0.47
1:F:148:VAL:O	1:F:152:LEU:HB2	2.15	0.47
1:B:245:GLU:O	1:B:249:ARG:HB2	2.15	0.47
1:D:59:THR:OG1	1:D:63:ALA:HB3	2.15	0.47
1:F:18:PRO:HB2	1:F:21:ASP:HB2	1.96	0.47
1:B:119:THR:HG22	1:B:121:HIS:CD2	2.49	0.47
1:B:177:SER:HB3	1:B:311:TYR:CE1	2.50	0.47
1:C:222:GLU:O	1:C:225:ILE:HG13	2.15	0.47
1:B:76:VAL:HG12	1:B:120:ILE:HD11	1.97	0.47
1:D:5:GLU:OE1	1:D:60:THR:HA	2.15	0.47
1:D:181:LEU:HD23	1:D:224:LEU:HD21	1.96	0.47
1:C:250:LEU:HA	1:C:253:ILE:HD13	1.97	0.46
1:A:133:ARG:HB2	1:A:266:LEU:HD22	1.96	0.46
1:C:146:PRO:HG2	1:C:249:ARG:NH1	2.29	0.46
1:D:28:ARG:HB3	1:D:29:PRO:HD3	1.98	0.46
1:F:79:TYR:HE1	1:F:83:ARG:CB	2.27	0.46
1:D:174:HIS:HB2	1:D:181:LEU:HD13	1.97	0.46
1:E:80:LEU:HD23	1:E:118:ASN:O	2.15	0.46
1:F:79:TYR:CD1	1:F:79:TYR:C	2.88	0.46
1:C:60:THR:HB	1:C:62:GLU:OE1	2.16	0.46
1:D:19:MET:SD	1:D:53:LEU:HD13	2.56	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ARG:HD3	1:C:210:ARG:HH21	1.80	0.46
1:D:133:ARG:HB2	1:D:266:LEU:HD22	1.97	0.46
1:A:157:SER:O	1:A:157:SER:OG	2.33	0.46
1:F:256:ARG:O	1:F:260:LEU:HG	2.15	0.46
1:A:57:VAL:HG11	1:A:68:VAL:HG11	1.98	0.46
1:E:107:GLU:O	1:E:108:ASP:HB2	2.16	0.46
1:A:108:ASP:OD2	1:D:204:ARG:NH2	2.49	0.46
1:F:154:ARG:HE	1:F:154:ARG:HB3	1.66	0.46
1:A:15:HIS:O	1:A:51:PRO:HG2	2.16	0.46
1:B:162:PRO:HB2	2:N:8:MET:HG3	1.98	0.46
1:C:212:HIS:HA	1:C:215:ARG:NH1	2.31	0.45
1:D:195:TYR:CG	1:D:333:PHE:CD2	3.05	0.45
1:C:48:ARG:NE	1:C:107:GLU:OE2	2.49	0.45
1:F:59:THR:CG2	1:F:64:LEU:HD13	2.46	0.45
1:F:82:ALA:O	1:F:84:PRO:HD3	2.16	0.45
1:C:61:ARG:NH1	1:C:65:GLU:OE1	2.49	0.45
1:E:245:GLU:HG2	1:E:248:ARG:CZ	2.47	0.45
1:F:28:ARG:HG2	1:F:29:PRO:HD3	1.99	0.45
1:A:43:PHE:HA	1:A:54:ARG:O	2.17	0.45
1:A:261:LEU:CB	1:A:305:SER:HB3	2.45	0.45
1:D:61:ARG:HG3	1:D:61:ARG:HH11	1.81	0.45
1:D:305:SER:OG	1:D:306:PRO:HD3	2.17	0.45
1:F:176:LEU:HB3	1:F:251:ARG:NH2	2.32	0.45
1:F:224:LEU:HD22	1:F:346:VAL:HG21	1.97	0.45
1:B:90:ASP:HB2	1:F:18:PRO:HA	1.98	0.45
1:C:5:GLU:C	1:C:6:ARG:HD3	2.37	0.45
1:C:225:ILE:O	1:C:229:SER:N	2.39	0.45
1:D:8:TRP:CD2	1:D:64:LEU:HD22	2.51	0.45
1:A:195:TYR:OH	1:A:199:ARG:NH1	2.50	0.45
1:B:9:ARG:HG2	1:B:56:TYR:CD1	2.52	0.45
1:B:181:LEU:HD23	1:B:347:TYR:HE2	1.82	0.45
1:B:261:LEU:HD23	1:B:261:LEU:HA	1.60	0.45
1:E:6:ARG:NH1	1:E:128:GLU:OE1	2.49	0.45
1:F:182:PRO:HG3	1:F:347:TYR:HB3	2.00	0.45
1:F:196:LEU:HD13	1:F:206:ARG:HB2	1.98	0.45
1:F:238:ALA:HB2	1:F:244:ARG:HH11	1.80	0.45
1:A:245:GLU:OE2	1:A:249:ARG:NH1	2.50	0.44
1:B:29:PRO:HB2	1:B:75:VAL:HG11	1.99	0.44
1:E:215:ARG:CG	1:F:349:ILE:HA	2.44	0.44
1:B:307:ALA:O	1:B:309:GLY:N	2.48	0.44
1:E:210:ARG:HD2	1:F:210:ARG:NH2	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:ARG:HH21	1:E:103:GLU:HB2	1.82	0.44
1:C:250:LEU:HD13	1:C:314:VAL:HG22	1.99	0.44
1:F:309:GLY:N	1:F:311:TYR:CD2	2.85	0.44
1:B:339:ALA:O	1:B:343:ALA:N	2.39	0.44
1:F:67:VAL:O	1:F:71:ALA:N	2.48	0.44
1:F:245:GLU:HA	1:F:248:ARG:NH1	2.32	0.44
1:D:101:LEU:HD23	1:D:101:LEU:HA	1.86	0.44
1:E:189:ARG:HD2	1:F:207:GLU:OE2	2.18	0.44
1:A:90:ASP:HA	1:A:91:PRO:HD2	1.82	0.44
1:B:67:VAL:C	1:B:70:PRO:HD2	2.37	0.44
1:F:132:VAL:O	1:F:136:LEU:HB3	2.17	0.44
1:A:213:TYR:OH	1:A:342:ALA:HA	2.17	0.44
1:A:45:ARG:HD2	1:A:324:ARG:O	2.18	0.44
1:B:9:ARG:HG2	1:B:56:TYR:HD1	1.82	0.44
1:B:28:ARG:HB3	1:B:29:PRO:HD3	2.00	0.44
1:B:210:ARG:CZ	1:D:210:ARG:HE	2.31	0.44
1:B:210:ARG:CD	1:D:210:ARG:HH21	2.31	0.44
1:D:105:GLU:OE1	1:D:107:GLU:HB2	2.18	0.44
1:F:136:LEU:CD2	1:F:266:LEU:HD21	2.48	0.44
1:F:218:GLU:HA	1:F:221:THR:OG1	2.16	0.44
1:B:11:ARG:HD3	1:B:13:ASP:OD1	2.17	0.43
1:F:212:HIS:ND1	2:R:10:VAL:HA	2.32	0.43
1:F:321:HIS:O	1:F:324:ARG:N	2.49	0.43
1:A:221:THR:HG22	1:A:346:VAL:HG23	2.01	0.43
1:C:223:ARG:NH1	2:O:4:ASN:O	2.50	0.43
1:E:36:ALA:HB3	1:E:37:GLN:NE2	2.33	0.43
1:B:230:SER:OG	1:B:243:VAL:HG21	2.18	0.43
1:F:22:LEU:HB3	1:F:79:TYR:CE2	2.50	0.43
1:C:20:ASP:CG	1:C:152:LEU:HD22	2.38	0.43
1:C:165:ALA:O	1:C:169:VAL:HG13	2.19	0.43
1:D:59:THR:OG1	1:D:60:THR:N	2.51	0.43
1:E:210:ARG:HD2	1:F:210:ARG:NE	2.33	0.43
1:A:126:ARG:CG	1:A:127:PRO:HD2	2.48	0.43
1:F:308:PHE:HA	1:F:311:TYR:CG	2.53	0.43
1:C:34:PHE:CD1	1:C:38:ALA:HB3	2.52	0.43
1:C:126:ARG:O	1:C:127:PRO:C	2.57	0.43
1:F:145:THR:HG22	1:F:149:TYR:CE2	2.53	0.43
1:B:241:PRO:HD2	1:B:242:HIS:ND1	2.33	0.43
1:E:85:SER:HA	1:E:86:PRO:HD3	1.88	0.43
1:F:165:ALA:O	1:F:169:VAL:HG23	2.19	0.43
1:A:144:THR:O	1:A:147:SER:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ARG:HD3	1:C:107:GLU:HG2	2.01	0.42
2:R:6:LEU:HD23	2:R:6:LEU:HA	1.82	0.42
1:F:64:LEU:HD12	1:F:68:VAL:HG13	2.01	0.42
1:F:153:GLU:HA	1:F:156:ARG:HB2	2.01	0.42
1:C:228:ALA:O	1:C:232:GLU:HG3	2.20	0.42
1:B:196:LEU:HD13	1:B:206:ARG:HG2	2.02	0.42
1:C:199:ARG:HG2	1:C:201:ASP:OD1	2.19	0.42
1:E:241:PRO:O	1:E:244:ARG:N	2.52	0.42
1:F:108:ASP:OD1	1:F:109:GLY:N	2.53	0.42
1:F:152:LEU:O	1:F:155:VAL:HB	2.19	0.42
1:C:31:PHE:HA	1:C:34:PHE:CE2	2.54	0.42
1:D:182:PRO:HG3	1:D:347:TYR:CD1	2.55	0.42
1:F:176:LEU:HA	1:F:251:ARG:CZ	2.50	0.42
1:B:162:PRO:O	1:B:165:ALA:HB3	2.20	0.42
1:F:304:ASP:HB2	1:F:308:PHE:CE2	2.55	0.42
1:A:212:HIS:CD2	2:M:10:VAL:HG12	2.45	0.42
1:B:20:ASP:OD1	1:B:152:LEU:HD22	2.20	0.42
1:F:245:GLU:O	1:F:249:ARG:HG3	2.20	0.42
1:F:85:SER:HA	1:F:86:PRO:HD3	1.90	0.41
1:A:174:HIS:O	1:A:180:GLY:HA2	2.20	0.41
1:A:205:LEU:HD23	1:A:205:LEU:HA	1.91	0.41
1:B:210:ARG:CG	1:D:210:ARG:HH21	2.33	0.41
1:E:182:PRO:HG3	1:E:347:TYR:CD1	2.55	0.41
1:F:95:LEU:HD23	1:F:95:LEU:HA	1.80	0.41
1:A:233:SER:OG	1:A:234:ALA:N	2.53	0.41
1:C:229:SER:OG	1:C:239:HIS:CE1	2.73	0.41
1:A:191:HIS:NE2	1:A:332:ARG:HD2	2.34	0.41
1:C:245:GLU:O	1:C:249:ARG:HG2	2.20	0.41
1:E:250:LEU:HD23	1:E:250:LEU:HA	1.83	0.41
1:C:328:THR:HG22	1:E:96:PRO:HG3	2.03	0.41
1:D:217:ARG:HD3	1:D:345:ASP:OD2	2.20	0.41
1:E:14:TYR:CZ	1:E:79:TYR:HE1	2.38	0.41
1:F:221:THR:O	1:F:225:ILE:HG13	2.21	0.41
1:D:131:THR:HG22	1:D:134:ASP:CG	2.41	0.41
1:A:182:PRO:HD3	1:A:347:TYR:CE2	2.55	0.41
1:C:218:GLU:HA	1:C:221:THR:CG2	2.47	0.41
1:D:49:ARG:HH11	1:D:49:ARG:HD2	1.76	0.41
1:F:132:VAL:HG12	1:F:133:ARG:NH2	2.35	0.41
1:F:240:LEU:HA	1:F:241:PRO:HD3	1.88	0.41
1:A:250:LEU:HD22	1:A:314:VAL:HG22	2.02	0.41
1:B:184:ALA:O	1:B:187:SER:OG	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:LEU:O	1:B:266:LEU:HD12	2.20	0.41
1:F:14:TYR:CD2	1:F:19:MET:HE3	2.56	0.41
1:F:84:PRO:HB3	1:F:118:ASN:OD1	2.21	0.41
1:F:319:TYR:O	1:F:322:LEU:HB2	2.21	0.41
1:A:191:HIS:CE1	1:A:333:PHE:HE1	2.39	0.41
1:C:229:SER:HG	1:C:239:HIS:CE1	2.38	0.41
1:E:72:ILE:O	1:E:76:VAL:HB	2.20	0.41
1:F:79:TYR:O	1:F:81:ARG:N	2.54	0.41
1:F:248:ARG:O	1:F:252:PRO:HD2	2.20	0.41
1:F:256:ARG:HE	1:F:256:ARG:HB2	1.59	0.41
1:C:67:VAL:C	1:C:70:PRO:HD2	2.41	0.41
1:C:307:ALA:O	1:C:309:GLY:N	2.50	0.41
1:D:258:ARG:NH1	1:D:306:PRO:HB3	2.35	0.41
1:E:95:LEU:HB3	1:E:96:PRO:HD3	2.03	0.41
1:B:326:GLY:O	3:B:401:HOH:O	2.20	0.40
1:C:21:ASP:OD2	1:C:83:ARG:NH2	2.54	0.40
1:E:50:GLY:HA2	1:E:51:PRO:HD3	1.94	0.40
1:F:9:ARG:HB3	1:F:56:TYR:CD2	2.56	0.40
1:F:22:LEU:CD1	1:F:53:LEU:HD12	2.49	0.40
1:F:44:LEU:HD11	1:F:141:TYR:CE2	2.57	0.40
1:A:23:ILE:HG12	1:A:53:LEU:HD21	2.03	0.40
1:E:154:ARG:O	1:E:159:ALA:HB3	2.21	0.40
1:F:14:TYR:OH	1:F:18:PRO:HD2	2.21	0.40
1:A:37:GLN:N	1:A:37:GLN:OE1	2.54	0.40
1:B:182:PRO:HG3	1:B:347:TYR:CD1	2.55	0.40
1:B:210:ARG:HD2	1:D:210:ARG:HH21	1.86	0.40
1:D:191:HIS:NE2	1:D:332:ARG:NH1	2.68	0.40
1:F:172:THR:HG23	1:F:176:LEU:HD12	2.02	0.40
1:B:61:ARG:O	1:B:64:LEU:HB3	2.21	0.40
1:F:313:LEU:HA	1:F:313:LEU:HD22	1.67	0.40
1:F:322:LEU:O	1:F:327:LEU:HD23	2.21	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	306/361 (85%)	279 (91%)	14 (5%)	13 (4%)	3	2
1	B	301/361 (83%)	271 (90%)	21 (7%)	9 (3%)	4	5
1	C	302/361 (84%)	274 (91%)	20 (7%)	8 (3%)	5	7
1	D	303/361 (84%)	278 (92%)	19 (6%)	6 (2%)	7	10
1	E	310/361 (86%)	288 (93%)	12 (4%)	10 (3%)	4	5
1	F	302/361 (84%)	263 (87%)	29 (10%)	10 (3%)	4	4
2	M	9/16 (56%)	7 (78%)	2 (22%)	0	100	100
2	N	7/16 (44%)	6 (86%)	1 (14%)	0	100	100
2	O	9/16 (56%)	7 (78%)	2 (22%)	0	100	100
2	P	7/16 (44%)	7 (100%)	0	0	100	100
2	Q	6/16 (38%)	4 (67%)	2 (33%)	0	100	100
2	R	9/16 (56%)	8 (89%)	1 (11%)	0	100	100
All	All	1871/2262 (83%)	1692 (90%)	123 (7%)	56 (3%)	4	5

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	PRO
1	A	239	HIS
1	A	308	PHE
1	C	127	PRO
1	C	128	GLU
1	C	267	THR
1	D	127	PRO
1	D	308	PHE
1	E	127	PRO
1	E	233	SER
1	E	234	ALA
1	E	267	THR
1	E	306	PRO
1	A	236	ASN
1	A	263	SER
1	A	307	ALA
1	B	127	PRO
1	B	241	PRO
1	C	307	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	309	GLY
1	D	307	ALA
1	F	118	ASN
1	F	129	PRO
1	F	241	PRO
1	A	234	ALA
1	B	128	GLU
1	B	307	ALA
1	B	309	GLY
1	C	241	PRO
1	E	128	GLU
1	F	26	GLY
1	F	39	PRO
1	F	305	SER
1	F	307	ALA
1	A	26	GLY
1	A	200	SER
1	A	233	SER
1	A	241	PRO
1	A	309	GLY
1	B	308	PHE
1	C	308	PHE
1	D	128	GLU
1	D	309	GLY
1	E	106	GLY
1	E	108	ASP
1	F	89	ALA
1	F	150	HIS
1	E	129	PRO
1	F	309	GLY
1	A	305	SER
1	B	26	GLY
1	B	70	PRO
1	C	26	GLY
1	D	241	PRO
1	E	241	PRO
1	B	243	VAL

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	245/285 (86%)	240 (98%)	5 (2%)	55	72
1	B	245/285 (86%)	234 (96%)	11 (4%)	27	42
1	C	245/285 (86%)	239 (98%)	6 (2%)	49	67
1	D	246/285 (86%)	240 (98%)	6 (2%)	49	67
1	E	248/285 (87%)	241 (97%)	7 (3%)	43	61
1	F	245/285 (86%)	229 (94%)	16 (6%)	17	26
2	M	11/15 (73%)	10 (91%)	1 (9%)	9	13
2	N	9/15 (60%)	9 (100%)	0	100	100
2	O	11/15 (73%)	11 (100%)	0	100	100
2	P	9/15 (60%)	8 (89%)	1 (11%)	6	8
2	Q	8/15 (53%)	8 (100%)	0	100	100
2	R	11/15 (73%)	11 (100%)	0	100	100
All	All	1533/1800 (85%)	1480 (96%)	53 (4%)	36	53

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	SER
1	A	221	THR
1	A	224	LEU
1	A	229	SER
1	A	313	LEU
1	B	11	ARG
1	B	13	ASP
1	B	14	TYR
1	B	54	ARG
1	B	60	THR
1	B	85	SER
1	B	131	THR
1	B	147	SER
1	B	157	SER
1	B	205	LEU
1	B	223	ARG
1	C	128	GLU
1	C	131	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	169	VAL
1	C	210	ARG
1	C	229	SER
1	C	254	ARG
1	D	68	VAL
1	D	107	GLU
1	D	133	ARG
1	D	178	THR
1	D	199	ARG
1	D	304	ASP
1	E	59	THR
1	E	210	ARG
1	E	244	ARG
1	E	245	GLU
1	E	267	THR
1	E	312	ARG
1	E	314	VAL
1	F	28	ARG
1	F	40	MET
1	F	68	VAL
1	F	118	ASN
1	F	126	ARG
1	F	152	LEU
1	F	198	ARG
1	F	200	SER
1	F	204	ARG
1	F	224	LEU
1	F	251	ARG
1	F	254	ARG
1	F	311	TYR
1	F	312	ARG
1	F	313	LEU
1	F	315	ILE
2	M	8	MET
2	P	8	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	ASN
1	F	118	ASN
1	F	321	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 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	310/361 (85%)	0.32	23 (7%)	14	11	30, 53, 118, 141	0
1	B	307/361 (85%)	0.55	18 (5%)	22	19	47, 72, 118, 156	0
1	C	308/361 (85%)	0.23	12 (3%)	39	36	33, 57, 110, 136	0
1	D	309/361 (85%)	0.32	18 (5%)	23	20	32, 60, 111, 156	0
1	E	313/361 (86%)	0.38	22 (7%)	16	13	40, 61, 102, 133	0
1	F	308/361 (85%)	1.01	52 (16%)	1	1	53, 92, 121, 148	0
2	M	11/16 (68%)	0.64	1 (9%)	9	7	59, 83, 117, 118	0
2	N	9/16 (56%)	0.70	1 (11%)	5	3	78, 93, 107, 117	0
2	O	11/16 (68%)	-0.12	0	100	100	51, 61, 92, 96	0
2	P	9/16 (56%)	-0.33	0	100	100	55, 62, 75, 87	0
2	Q	8/16 (50%)	0.31	0	100	100	67, 83, 102, 115	0
2	R	11/16 (68%)	-0.18	0	100	100	64, 70, 88, 89	0
All	All	1914/2262 (84%)	0.46	147 (7%)	13	10	30, 66, 116, 156	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	308	PHE	8.2
1	F	308	PHE	6.7
1	D	105	GLU	5.9
1	F	82	ALA	5.6
1	F	120	ILE	5.3
1	F	8	TRP	5.2
1	D	303	ARG	5.1
1	F	251	ARG	5.0
1	A	257	ALA	4.8
1	C	269	GLU	4.8
1	E	128	GLU	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	83	ARG	4.6
1	F	80	LEU	4.6
1	F	110	PRO	4.5
1	A	176	LEU	4.4
1	F	64	LEU	4.4
1	A	234	ALA	4.3
1	A	261	LEU	4.3
1	D	128	GLU	4.3
1	D	267	THR	4.2
1	E	238	ALA	4.1
1	C	307	ALA	4.0
1	F	59	THR	3.9
1	F	79	TYR	3.8
1	F	350	ALA	3.7
1	C	267	THR	3.7
1	E	268	LEU	3.6
1	E	10	PHE	3.6
1	F	239	HIS	3.6
1	E	236	ASN	3.6
2	N	12	GLU	3.5
1	A	250	LEU	3.5
1	C	261	LEU	3.5
1	F	81	ARG	3.5
1	C	238	ALA	3.4
1	A	237	GLY	3.4
1	D	268	LEU	3.3
1	B	155	VAL	3.3
1	F	55	ILE	3.3
1	E	269	GLU	3.3
1	F	57	VAL	3.3
1	F	305	SER	3.3
1	A	236	ASN	3.3
1	F	118	ASN	3.3
1	F	73	GLU	3.3
1	D	350	ALA	3.3
1	E	305	SER	3.2
1	F	16	ALA	3.2
1	D	269	GLU	3.2
1	C	347	TYR	3.2
1	A	308	PHE	3.2
1	F	67	VAL	3.2
1	F	128	GLU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	43	PHE	3.2
1	E	234	ALA	3.2
1	F	74	HIS	3.1
1	B	308	PHE	3.1
1	E	62	GLU	3.1
1	F	238	ALA	3.1
1	F	176	LEU	3.0
1	E	80	LEU	3.0
1	A	310	ALA	3.0
1	A	258	ARG	3.0
1	A	306	PRO	3.0
1	B	204	ARG	2.9
1	A	233	SER	2.9
1	D	254	ARG	2.9
1	F	29	PRO	2.9
1	B	213	TYR	2.9
1	F	126	ARG	2.8
1	F	14	TYR	2.8
1	E	70	PRO	2.8
1	D	308	PHE	2.8
1	F	121	HIS	2.7
1	E	64	LEU	2.7
1	A	177	SER	2.7
1	B	62	GLU	2.7
1	F	152	LEU	2.7
1	F	48	ARG	2.7
1	E	207	GLU	2.7
1	B	64	LEU	2.7
1	D	266	LEU	2.7
1	B	225	ILE	2.6
1	F	12	VAL	2.6
1	A	262	GLU	2.6
1	F	103	GLU	2.6
1	E	8	TRP	2.6
1	D	8	TRP	2.6
1	A	254	ARG	2.6
1	F	19	MET	2.6
1	B	180	GLY	2.6
1	C	257	ALA	2.5
1	F	311	TYR	2.5
1	F	84	PRO	2.5
1	D	127	PRO	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	250	LEU	2.5
2	M	12	GLU	2.5
1	E	61	ARG	2.5
1	F	108	ASP	2.5
1	A	129	PRO	2.5
1	A	264	GLY	2.5
1	A	307	ALA	2.5
1	F	107	GLU	2.4
1	F	22	LEU	2.4
1	A	263	SER	2.4
1	E	75	VAL	2.4
1	D	132	VAL	2.4
1	B	128	GLU	2.4
1	D	129	PRO	2.4
1	E	303	ARG	2.4
1	B	269	GLU	2.4
1	B	233	SER	2.3
1	F	127	PRO	2.3
1	E	239	HIS	2.3
1	F	119	THR	2.3
1	B	244	ARG	2.3
1	F	61	ARG	2.3
1	A	304	ASP	2.3
1	F	312	ARG	2.3
1	F	309	GLY	2.2
1	E	127	PRO	2.2
1	F	49	ARG	2.2
1	A	267	THR	2.2
1	E	67	VAL	2.2
1	C	128	GLU	2.2
1	D	124	GLY	2.2
1	C	310	ALA	2.2
1	A	311	TYR	2.1
1	D	304	ASP	2.1
1	B	22	LEU	2.1
1	E	63	ALA	2.1
1	F	307	ALA	2.1
1	C	176	LEU	2.1
1	C	306	PRO	2.1
1	B	231	ALA	2.1
1	A	127	PRO	2.1
1	F	34	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	217	ARG	2.1
1	D	265	GLU	2.1
1	B	10	PHE	2.0
1	B	349	ILE	2.0
1	E	120	ILE	2.0
1	D	111	LEU	2.0
1	F	314	VAL	2.0
1	F	151	ALA	2.0
1	B	232	GLU	2.0
1	F	183	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.