Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:02 AM GMT

PDB ID	:	2VOE
Title	:	Crystal structure of Rv2780 from M. tuberculosis H37Rv
Authors	:	Tripathi, S.M.; Ramachandran, R.
Deposited on	:	2008-02-17
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:

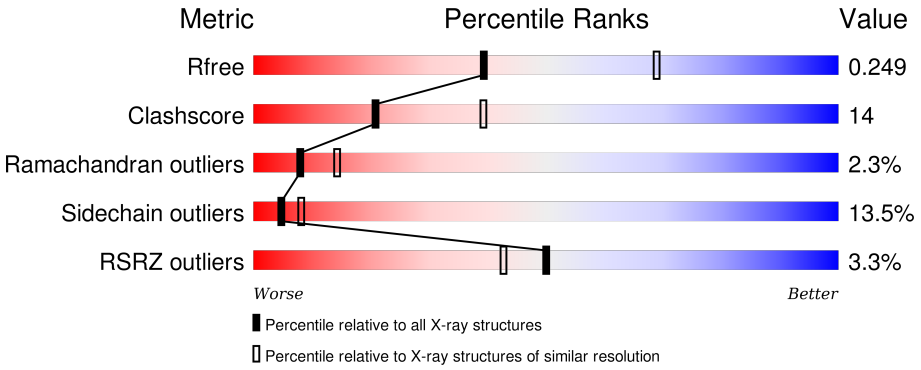
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	371	2% 70% 22% 7%
1	B	371	% 75% 16% 8%
1	C	371	8% 70% 22% 7%
1	D	371	3% 71% 21% 8%
1	E	371	3% 72% 21% 6%

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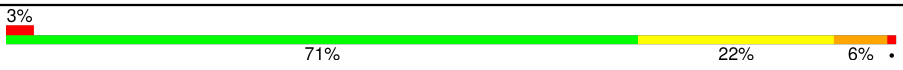
Mol	Chain	Length	Quality of chain
1	F	371	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16386 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 ALANINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2691	1691	473	514	13			
1	B	371	Total	C	N	O	S	0	0	0
			2699	1693	476	517	13			
1	C	371	Total	C	N	O	S	0	0	0
			2687	1688	470	516	13			
1	D	371	Total	C	N	O	S	0	0	0
			2699	1695	476	515	13			
1	E	371	Total	C	N	O	S	0	0	0
			2695	1693	473	516	13			
1	F	371	Total	C	N	O	S	0	0	0
			2691	1689	473	516	13			

- Molecule 2 is water.

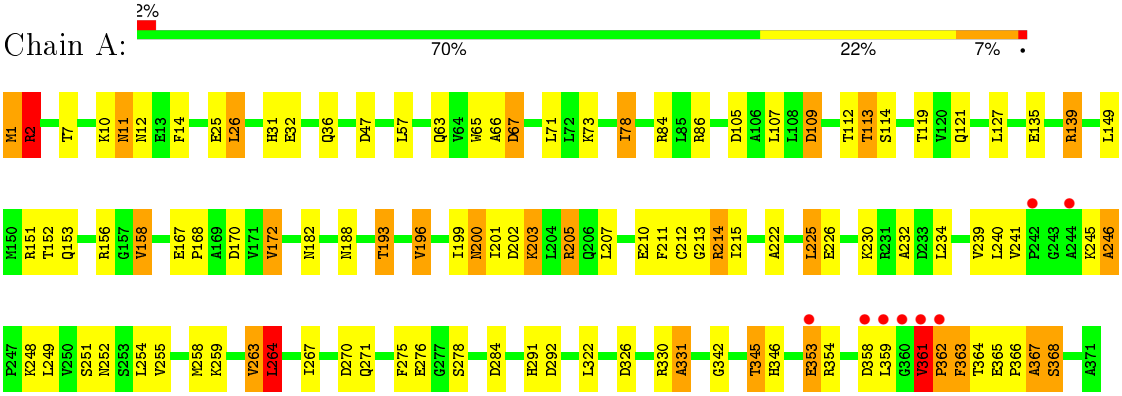
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	31	Total	O	0	0
			31	31		
2	B	49	Total	O	0	0
			49	49		
2	C	39	Total	O	0	0
			39	39		
2	D	30	Total	O	0	0
			30	30		
2	E	36	Total	O	0	0
			36	36		
2	F	39	Total	O	0	0
			39	39		

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.

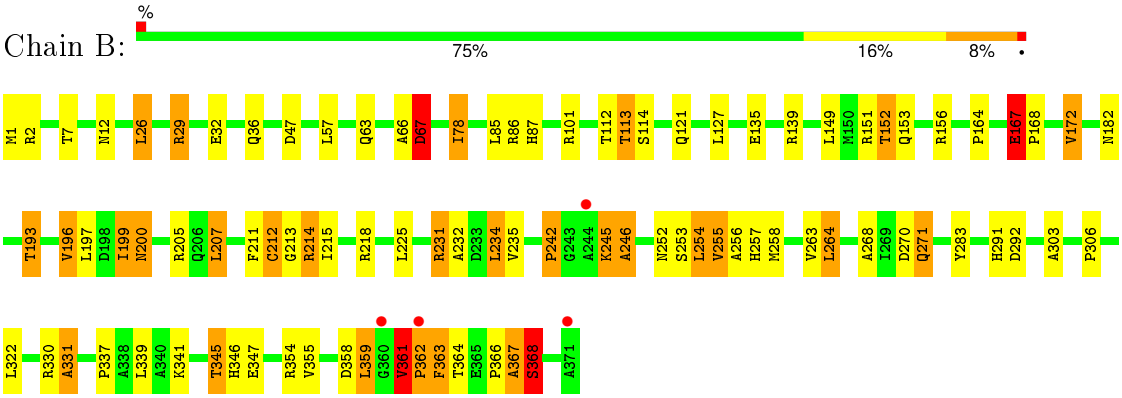
- Molecule 1: ALANINE DEHYDROGENASE

Chain A:



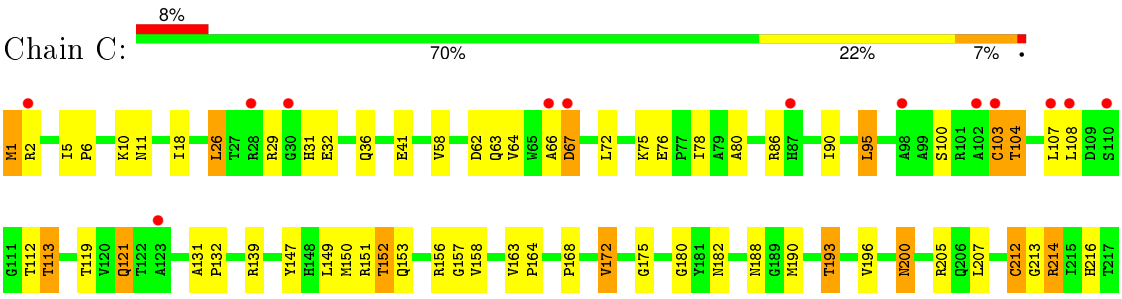
- Molecule 1: ALANINE DEHYDROGENASE

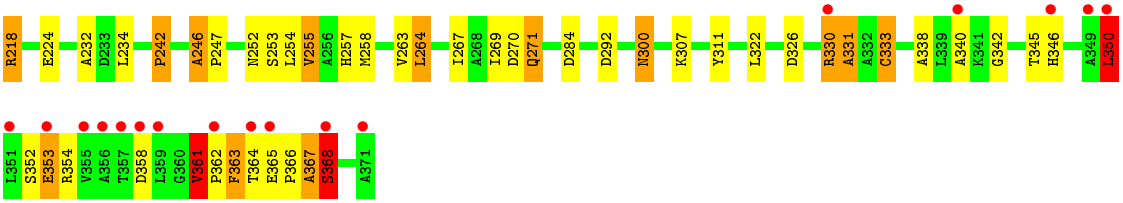
Chain B:



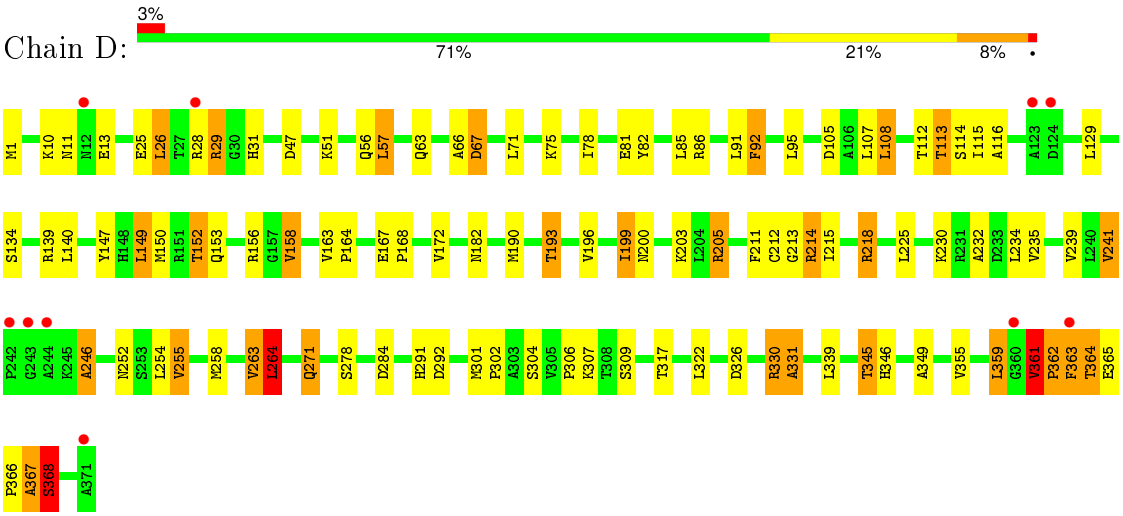
- Molecule 1: ALANINE DEHYDROGENASE

Chain C:

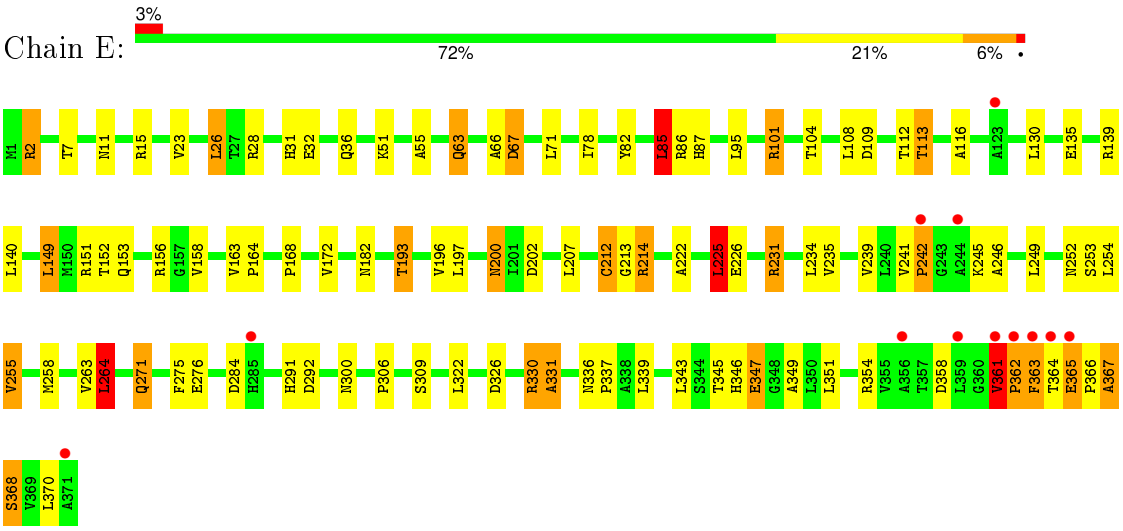




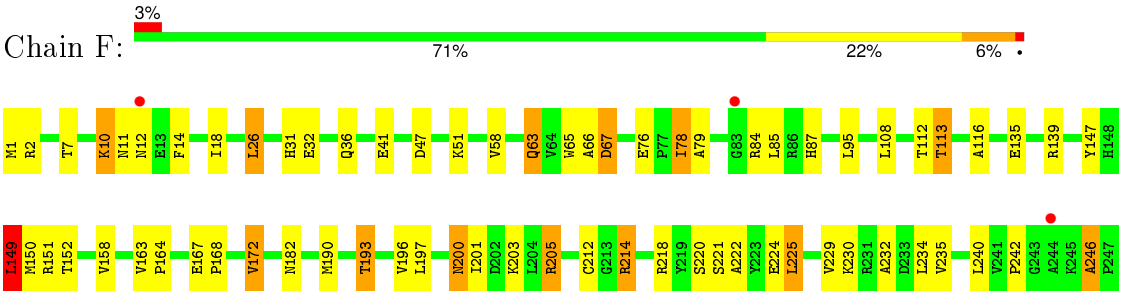
• Molecule 1: ALANINE DEHYDROGENASE



• Molecule 1: ALANINE DEHYDROGENASE



• Molecule 1: ALANINE DEHYDROGENASE




K248
L254
V255
M258
V263
L264
I267
Q271
E276
Y283
H291
D292
V305
D326
W329
R330
A331
A332
G333
R334
T345
H346
E347
G348
E353
R354
V355
A356
T357
D358
L359
G360
V361
P362
F363
T364
E365
P366
A367
S368
V369
L370
A371

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	173.89Å 127.08Å 135.95Å 90.00° 115.04° 90.00°	Depositor
Resolution (Å)	123.09 – 2.60 40.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.2 (123.09-2.60) 97.3 (40.00-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.196 , 0.251 0.195 , 0.249	Depositor DCC
R_{free} test set	4005 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 43.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	1 of 79672 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16386	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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	0.77	0/2740	0.88	5/3736 (0.1%)
1	B	0.79	3/2747 (0.1%)	0.89	5/3743 (0.1%)
1	C	0.88	1/2735 (0.0%)	0.91	6/3729 (0.2%)
1	D	0.79	0/2748	0.90	5/3746 (0.1%)
1	E	0.82	1/2744 (0.0%)	0.92	5/3741 (0.1%)
1	F	0.81	3/2739 (0.1%)	0.90	7/3733 (0.2%)
All	All	0.81	8/16453 (0.0%)	0.90	33/22428 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	1
1	D	0	4
1	E	0	1
1	F	0	1
All	All	0	10

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	167	GLU	CG-CD	6.96	1.62	1.51
1	F	333	CYS	CB-SG	-6.74	1.70	1.82
1	C	212	CYS	CB-SG	6.20	1.92	1.82
1	E	212	CYS	CB-SG	6.12	1.92	1.82
1	B	167	GLU	CB-CG	5.64	1.62	1.52
1	F	158	VAL	CA-CB	5.54	1.66	1.54
1	F	212	CYS	CB-SG	5.28	1.91	1.82
1	B	196	VAL	CB-CG2	-5.01	1.42	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	264	LEU	CA-CB-CG	7.67	132.93	115.30
1	C	264	LEU	CA-CB-CG	7.62	132.81	115.30
1	F	225	LEU	CA-CB-CG	7.42	132.38	115.30
1	F	264	LEU	CA-CB-CG	7.38	132.29	115.30
1	D	205	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	F	242	PRO	N-CA-CB	6.45	111.05	103.30
1	E	140	LEU	CB-CG-CD1	-6.40	100.12	111.00
1	E	225	LEU	CA-CB-CG	6.31	129.81	115.30
1	F	214	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	2	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	E	264	LEU	CA-CB-CG	5.94	128.97	115.30
1	D	368	SER	N-CA-C	-5.78	95.39	111.00
1	D	190	MET	CG-SD-CE	-5.74	91.02	100.20
1	B	234	LEU	CA-CB-CG	5.59	128.16	115.30
1	E	368	SER	N-CA-C	-5.51	96.11	111.00
1	A	368	SER	N-CA-C	-5.50	96.15	111.00
1	F	47	ASP	CB-CG-OD2	5.45	123.21	118.30
1	B	242	PRO	N-CA-CB	5.41	109.79	103.30
1	C	368	SER	N-CA-C	-5.39	96.45	111.00
1	B	225	LEU	CA-CB-CG	5.37	127.66	115.30
1	F	368	SER	N-CA-C	-5.36	96.54	111.00
1	B	368	SER	N-CA-C	-5.35	96.55	111.00
1	F	149	LEU	CA-CB-CG	5.33	127.56	115.30
1	C	350	LEU	CA-CB-CG	5.31	127.50	115.30
1	D	205	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	E	85	LEU	CA-CB-CG	5.25	127.38	115.30
1	A	205	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	C	95	LEU	CA-CB-CG	-5.21	103.32	115.30
1	C	242	PRO	N-CA-CB	5.17	109.51	103.30
1	C	190	MET	CG-SD-CE	-5.12	92.01	100.20
1	D	264	LEU	CA-CB-CG	5.10	127.03	115.30
1	A	139	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	207	LEU	CB-CG-CD2	-5.06	102.41	111.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	361	VAL	Peptide
1	B	361	VAL	Peptide
1	B	368	SER	Peptide

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Mol	Chain	Res	Type	Group
1	C	361	VAL	Peptide
1	D	241	VAL	Peptide
1	D	361	VAL	Peptide
1	D	364	THR	Peptide
1	D	368	SER	Peptide
1	E	361	VAL	Peptide
1	F	361	VAL	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	2691	0	2680	95	0
1	B	2699	0	2687	77	0
1	C	2687	0	2667	81	0
1	D	2699	0	2696	84	0
1	E	2695	0	2684	81	0
1	F	2691	0	2671	75	0
2	A	31	0	0	2	0
2	B	49	0	0	0	0
2	C	39	0	0	0	0
2	D	30	0	0	2	0
2	E	36	0	0	1	0
2	F	39	0	0	1	0
All	All	16386	0	16085	464	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 14.

All (464) 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:E:231:ARG:HG3	1:E:231:ARG:HH11	1.17	1.08
1:C:213:GLY:HA3	1:F:214:ARG:NH2	1.71	1.06
1:A:214:ARG:HH22	1:E:213:GLY:HA3	1.16	1.03
1:F:113:THR:HB	1:F:346:HIS:HD2	1.23	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ALA:O	1:B:67:ASP:HB2	1.55	1.01
1:B:47:ASP:HB3	1:B:57:LEU:HD11	1.41	1.01
1:A:252:ASN:ND2	1:A:276:GLU:HG3	1.80	0.97
1:A:66:ALA:O	1:A:67:ASP:HB2	1.64	0.96
1:C:29:ARG:HH11	1:C:29:ARG:HG3	1.31	0.94
1:A:11:ASN:H	1:A:11:ASN:ND2	1.61	0.94
1:D:291:HIS:O	1:D:292:ASP:HB2	1.66	0.94
1:F:113:THR:HB	1:F:346:HIS:CD2	2.02	0.94
1:A:156:ARG:HD3	2:A:2026:HOH:O	1.67	0.93
1:C:66:ALA:O	1:C:67:ASP:HB2	1.69	0.92
1:E:112:THR:O	1:E:345:THR:HG22	1.68	0.92
1:B:29:ARG:HH11	1:B:29:ARG:HG3	1.34	0.90
1:F:66:ALA:O	1:F:67:ASP:HB2	1.70	0.90
1:D:66:ALA:O	1:D:67:ASP:HB2	1.71	0.89
1:C:152:THR:HG22	1:C:153:GLN:HE21	1.37	0.89
1:D:139:ARG:HE	1:D:182:ASN:ND2	1.71	0.88
1:A:112:THR:O	1:A:345:THR:HG23	1.73	0.87
1:B:231:ARG:HG3	1:B:231:ARG:HH11	1.38	0.87
1:D:29:ARG:HG3	1:D:29:ARG:HH11	1.40	0.86
1:A:11:ASN:HD22	1:A:11:ASN:H	1.26	0.84
1:A:291:HIS:O	1:A:292:ASP:HB2	1.76	0.84
1:D:349:ALA:HB1	1:D:365:GLU:OE2	1.79	0.83
1:B:354:ARG:O	1:B:358:ASP:HB2	1.78	0.82
1:E:231:ARG:CG	1:E:231:ARG:HH11	1.91	0.82
1:C:139:ARG:HE	1:C:182:ASN:HD22	1.27	0.82
1:D:139:ARG:HE	1:D:182:ASN:HD22	1.23	0.82
1:D:152:THR:HG22	1:D:153:GLN:HE21	1.42	0.82
1:D:112:THR:O	1:D:345:THR:HG22	1.81	0.81
1:E:66:ALA:O	1:E:67:ASP:HB2	1.81	0.81
1:F:201:ILE:HG22	1:F:205:ARG:HH21	1.44	0.81
1:B:362:PRO:O	1:B:363:PHE:CB	2.28	0.80
1:E:149:LEU:HD13	1:E:263:VAL:HG13	1.64	0.80
1:E:214:ARG:CG	1:E:214:ARG:HH11	1.93	0.79
1:B:214:ARG:HH22	1:D:213:GLY:HA3	1.47	0.79
1:B:29:ARG:CG	1:B:29:ARG:HH11	1.95	0.79
1:A:214:ARG:NH2	1:E:213:GLY:HA3	1.97	0.79
1:F:355:VAL:HG13	1:F:359:LEU:HD12	1.64	0.79
1:F:31:HIS:HE1	1:F:326:ASP:OD1	1.65	0.79
1:D:66:ALA:HA	1:D:86:ARG:HE	1.47	0.79
1:E:271:GLN:O	1:E:271:GLN:HG2	1.83	0.78
1:C:253:SER:O	1:C:257:HIS:HD2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:GLY:HA3	1:F:214:ARG:HH22	1.46	0.77
1:A:330:ARG:O	1:A:331:ALA:CB	2.33	0.77
1:C:139:ARG:HE	1:C:182:ASN:ND2	1.82	0.76
1:A:353:GLU:OE2	1:A:364:THR:HG21	1.84	0.76
1:C:213:GLY:CA	1:F:214:ARG:NH2	2.49	0.76
1:E:291:HIS:O	1:E:292:ASP:HB2	1.84	0.76
1:B:330:ARG:O	1:B:331:ALA:CB	2.33	0.75
1:D:112:THR:O	1:D:345:THR:CG2	2.35	0.75
1:A:213:GLY:HA3	1:E:214:ARG:NH2	2.02	0.75
1:B:330:ARG:O	1:B:331:ALA:HB3	1.86	0.75
1:A:31:HIS:HE1	1:A:326:ASP:OD1	1.70	0.75
1:A:112:THR:O	1:A:345:THR:CG2	2.35	0.75
1:E:139:ARG:HE	1:E:182:ASN:ND2	1.84	0.74
1:E:2:ARG:HG3	1:E:32:GLU:HB3	1.69	0.74
1:A:330:ARG:O	1:A:331:ALA:HB3	1.88	0.74
1:E:200:ASN:HD22	1:E:200:ASN:C	1.91	0.74
1:A:66:ALA:O	1:A:67:ASP:CB	2.36	0.74
1:C:353:GLU:OE2	1:C:364:THR:HG21	1.87	0.73
1:A:149:LEU:HD13	1:A:263:VAL:CG1	2.19	0.72
1:C:330:ARG:O	1:C:331:ALA:HB3	1.90	0.72
1:D:330:ARG:O	1:D:331:ALA:HB3	1.88	0.72
1:A:200:ASN:HD22	1:A:203:LYS:H	1.37	0.71
1:B:139:ARG:HE	1:B:182:ASN:ND2	1.88	0.71
1:D:149:LEU:HD13	1:D:263:VAL:HG13	1.71	0.71
1:F:354:ARG:O	1:F:358:ASP:HB2	1.91	0.71
1:B:258:MET:CE	1:B:264:LEU:HD11	2.21	0.71
1:E:104:THR:O	1:E:108:LEU:HG	1.91	0.70
1:F:201:ILE:CG2	1:F:205:ARG:HH21	2.03	0.70
1:E:152:THR:HG22	1:E:153:GLN:HE21	1.56	0.70
1:C:10:LYS:HE3	1:C:76:GLU:OE2	1.92	0.70
1:C:29:ARG:NH1	1:C:29:ARG:HG3	2.00	0.69
1:F:355:VAL:O	1:F:359:LEU:HB2	1.91	0.69
1:F:334:ARG:HG2	1:F:370:LEU:HD23	1.75	0.69
1:D:47:ASP:HB3	1:D:57:LEU:HD11	1.74	0.69
1:C:152:THR:HG22	1:C:153:GLN:NE2	2.08	0.68
1:B:255:VAL:HA	1:B:258:MET:HG3	1.76	0.68
1:B:235:VAL:HB	1:B:264:LEU:HD13	1.75	0.68
1:C:255:VAL:HB	1:C:258:MET:HE3	1.76	0.68
1:B:271:GLN:HG3	1:B:271:GLN:O	1.93	0.67
1:E:139:ARG:HE	1:E:182:ASN:HD22	1.42	0.67
1:A:240:LEU:HD11	1:A:267:ILE:HG22	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:ILE:H	1:D:199:ILE:HD13	1.59	0.67
1:D:330:ARG:O	1:D:331:ALA:CB	2.42	0.66
1:B:258:MET:HE1	1:B:264:LEU:HD11	1.76	0.66
1:E:255:VAL:HB	1:E:258:MET:HE3	1.78	0.66
1:A:114:SER:H	1:A:345:THR:HG22	1.60	0.66
1:B:218:ARG:HH21	1:D:167:GLU:CD	1.99	0.66
1:B:66:ALA:O	1:B:67:ASP:CB	2.37	0.66
1:D:114:SER:OG	1:D:345:THR:HB	1.96	0.66
1:B:113:THR:HB	1:B:346:HIS:HD2	1.61	0.66
1:D:205:ARG:HD3	1:F:135:GLU:OE2	1.96	0.66
1:A:252:ASN:ND2	1:A:276:GLU:CG	2.58	0.65
1:F:291:HIS:O	1:F:292:ASP:HB2	1.96	0.65
1:C:100:SER:OG	1:C:103:CYS:HB2	1.96	0.65
1:D:152:THR:CG2	1:D:153:GLN:HE21	2.10	0.65
1:F:200:ASN:HD22	1:F:200:ASN:C	2.00	0.65
1:C:364:THR:HG22	1:C:365:GLU:N	2.12	0.65
1:D:66:ALA:O	1:D:67:ASP:CB	2.44	0.65
1:B:113:THR:HB	1:B:346:HIS:CD2	2.32	0.65
1:F:271:GLN:CG	1:F:271:GLN:O	2.45	0.65
1:A:11:ASN:HD22	1:A:11:ASN:N	1.93	0.64
1:C:119:THR:OG1	1:C:342:GLY:HA2	1.97	0.64
1:F:330:ARG:O	1:F:331:ALA:HB3	1.97	0.64
1:E:214:ARG:HH11	1:E:214:ARG:HG2	1.62	0.64
1:A:200:ASN:ND2	1:A:203:LYS:H	1.95	0.64
1:A:31:HIS:CE1	1:A:326:ASP:OD1	2.50	0.64
1:C:152:THR:CG2	1:C:153:GLN:HE21	2.09	0.64
1:C:330:ARG:O	1:C:331:ALA:CB	2.44	0.64
1:A:149:LEU:HD13	1:A:263:VAL:HG13	1.79	0.64
1:C:267:ILE:HG22	1:C:267:ILE:O	1.98	0.64
1:A:152:THR:HG22	1:A:153:GLN:NE2	2.13	0.64
1:D:291:HIS:O	1:D:292:ASP:CB	2.37	0.63
1:C:255:VAL:HA	1:C:258:MET:HE2	1.78	0.63
1:B:7:THR:H	1:B:36:GLN:NE2	1.96	0.63
1:A:251:SER:HA	1:A:276:GLU:HG2	1.81	0.63
1:B:366:PRO:O	1:B:367:ALA:HB2	1.99	0.63
1:D:31:HIS:HE1	1:D:326:ASP:OD1	1.80	0.63
1:E:26:LEU:CD1	1:E:322:LEU:HD23	2.28	0.63
1:D:26:LEU:HD13	1:D:322:LEU:HD23	1.79	0.63
1:B:112:THR:O	1:B:345:THR:CG2	2.46	0.63
1:C:271:GLN:HG3	1:C:271:GLN:O	1.96	0.63
1:A:107:LEU:HD22	1:A:112:THR:HG21	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:TYR:O	1:D:150:MET:HG3	1.99	0.62
1:D:235:VAL:HB	1:D:264:LEU:HD13	1.81	0.62
1:F:10:LYS:HE3	1:F:76:GLU:OE2	1.98	0.62
1:A:196:VAL:HG11	1:A:207:LEU:HD23	1.81	0.62
1:A:86:ARG:HB3	1:A:86:ARG:HH11	1.65	0.62
1:C:188:ASN:HD21	1:C:214:ARG:HD2	1.65	0.61
1:E:152:THR:HG22	1:E:153:GLN:NE2	2.15	0.61
1:F:330:ARG:O	1:F:331:ALA:CB	2.48	0.61
1:F:95:LEU:HD12	1:F:116:ALA:HB2	1.82	0.61
1:E:112:THR:O	1:E:345:THR:CG2	2.44	0.61
1:F:87:HIS:HE1	1:F:347:GLU:OE2	1.82	0.61
1:B:211:PHE:CD1	1:B:215:ILE:HD12	2.36	0.61
1:A:354:ARG:O	1:A:358:ASP:HB2	2.00	0.61
1:A:113:THR:HB	1:A:346:HIS:HD2	1.64	0.61
1:B:231:ARG:NH1	1:B:231:ARG:HG3	2.08	0.61
1:A:152:THR:HG22	1:A:153:GLN:HE21	1.65	0.61
1:E:82:TYR:HA	1:E:85:LEU:HD22	1.83	0.61
1:B:139:ARG:HE	1:B:182:ASN:HD22	1.46	0.61
1:D:113:THR:HB	1:D:346:HIS:HD2	1.64	0.61
1:C:75:LYS:NZ	1:C:300:ASN:HD21	1.99	0.60
1:A:139:ARG:HE	1:A:182:ASN:ND2	1.98	0.60
1:C:149:LEU:HD13	1:C:263:VAL:HG13	1.83	0.60
1:A:168:PRO:HG2	1:A:193:THR:HG22	1.83	0.60
1:F:271:GLN:HG3	1:F:271:GLN:O	2.02	0.60
1:C:254:LEU:HD13	1:C:254:LEU:C	2.22	0.60
1:D:271:GLN:HG3	1:D:271:GLN:O	2.01	0.60
1:B:29:ARG:NH1	1:B:29:ARG:HG3	2.07	0.60
1:E:168:PRO:HG2	1:E:193:THR:HG22	1.84	0.60
1:B:152:THR:CG2	1:B:153:GLN:HE21	2.14	0.60
1:F:139:ARG:HE	1:F:182:ASN:ND2	1.99	0.59
1:E:362:PRO:O	1:E:363:PHE:CB	2.50	0.59
1:C:252:ASN:HA	1:C:255:VAL:HG13	1.83	0.59
1:D:29:ARG:HG3	1:D:29:ARG:NH1	2.12	0.59
1:A:105:ASP:O	1:A:109:ASP:HB2	2.03	0.59
1:F:230:LYS:HE2	2:F:2031:HOH:O	2.02	0.59
1:E:66:ALA:O	1:E:67:ASP:CB	2.48	0.59
1:A:291:HIS:O	1:A:292:ASP:CB	2.47	0.59
1:B:168:PRO:HG2	1:B:193:THR:HG22	1.83	0.58
1:C:333:CYS:SG	1:C:340:ALA:HA	2.43	0.58
1:A:135:GLU:OE2	1:B:205:ARG:HD3	2.02	0.58
1:A:205:ARG:HG2	1:E:164:PRO:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:VAL:HG13	1:D:232:ALA:HB2	1.85	0.58
1:C:253:SER:O	1:C:257:HIS:CD2	2.54	0.58
1:E:366:PRO:O	1:E:367:ALA:HB2	2.04	0.58
1:F:31:HIS:CE1	1:F:326:ASP:OD1	2.53	0.58
1:F:139:ARG:HE	1:F:182:ASN:HD22	1.50	0.58
1:A:26:LEU:CD1	1:A:322:LEU:HD23	2.34	0.58
1:E:235:VAL:HB	1:E:264:LEU:HD13	1.85	0.57
1:A:10:LYS:HG3	1:A:78:ILE:HD11	1.85	0.57
1:B:26:LEU:HD13	1:B:322:LEU:HD23	1.85	0.57
1:D:241:VAL:HG11	1:D:246:ALA:H	1.68	0.57
1:F:168:PRO:HG2	1:F:193:THR:HG22	1.85	0.57
1:F:334:ARG:CG	1:F:370:LEU:HD23	2.34	0.57
1:C:2:ARG:HG3	1:C:32:GLU:HB2	1.86	0.57
1:B:291:HIS:O	1:B:292:ASP:HB2	2.03	0.57
1:C:267:ILE:O	1:C:267:ILE:CG2	2.51	0.57
1:D:366:PRO:O	1:D:367:ALA:HB2	2.04	0.57
1:E:7:THR:H	1:E:36:GLN:NE2	2.03	0.57
1:E:349:ALA:HB1	1:E:365:GLU:HG3	1.86	0.57
1:E:330:ARG:O	1:E:331:ALA:HB3	2.05	0.57
1:C:168:PRO:HG2	1:C:193:THR:HG22	1.86	0.57
1:B:87:HIS:NE2	1:B:347:GLU:HG2	2.19	0.57
1:A:107:LEU:CD2	1:A:112:THR:HG21	2.35	0.57
1:C:103:CYS:O	1:C:107:LEU:HD23	2.05	0.57
1:E:31:HIS:HE1	1:E:326:ASP:OD1	1.87	0.57
1:E:200:ASN:HD21	1:E:202:ASP:HB2	1.70	0.57
1:A:26:LEU:HD13	1:A:322:LEU:HD23	1.87	0.57
1:A:7:THR:H	1:A:36:GLN:NE2	2.02	0.57
1:E:214:ARG:HG3	1:E:214:ARG:HH11	1.69	0.56
1:F:87:HIS:CE1	1:F:347:GLU:OE2	2.58	0.56
1:E:330:ARG:O	1:E:331:ALA:CB	2.53	0.56
1:A:2:ARG:NH2	1:A:32:GLU:CB	2.69	0.56
1:D:355:VAL:O	1:D:359:LEU:HB2	2.05	0.56
1:B:213:GLY:HA3	1:D:214:ARG:NH2	2.21	0.56
1:A:139:ARG:HE	1:A:182:ASN:HD22	1.51	0.56
1:F:255:VAL:HB	1:F:258:MET:HE3	1.87	0.56
1:C:31:HIS:HE1	1:C:326:ASP:OD1	1.89	0.56
1:E:252:ASN:HA	1:E:255:VAL:HG13	1.88	0.56
1:F:113:THR:CB	1:F:346:HIS:HD2	2.10	0.56
1:A:107:LEU:HD22	1:A:112:THR:CG2	2.36	0.55
1:A:113:THR:HB	1:A:346:HIS:CD2	2.40	0.55
1:F:354:ARG:O	1:F:358:ASP:CB	2.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:LYS:HG3	1:A:78:ILE:CD1	2.37	0.55
1:C:66:ALA:O	1:C:67:ASP:CB	2.49	0.55
1:A:114:SER:N	1:A:345:THR:HG22	2.21	0.55
1:E:26:LEU:HD13	1:E:322:LEU:HD23	1.88	0.55
1:E:284:ASP:N	1:E:284:ASP:OD1	2.27	0.55
1:B:199:ILE:H	1:B:199:ILE:HD13	1.71	0.55
1:A:362:PRO:O	1:A:363:PHE:CB	2.55	0.55
1:F:364:THR:HG22	1:F:365:GLU:N	2.22	0.54
1:F:149:LEU:HD13	1:F:263:VAL:CG1	2.36	0.54
1:D:271:GLN:O	1:D:271:GLN:CG	2.55	0.54
1:B:12:ASN:HB3	1:B:283:TYR:CE1	2.43	0.54
1:A:252:ASN:HD22	1:A:276:GLU:CD	2.10	0.54
1:E:271:GLN:O	1:E:271:GLN:CG	2.56	0.54
1:B:152:THR:HG23	1:B:153:GLN:HE21	1.73	0.54
1:A:364:THR:HG22	1:A:365:GLU:N	2.22	0.54
1:C:200:ASN:HD22	1:C:200:ASN:C	2.10	0.54
1:F:7:THR:H	1:F:36:GLN:NE2	2.06	0.53
1:E:354:ARG:O	1:E:358:ASP:HB2	2.08	0.53
1:A:158:VAL:HG12	1:D:307:LYS:HG2	1.90	0.53
1:F:172:VAL:CG1	1:F:232:ALA:HB2	2.38	0.53
1:D:218:ARG:NH1	2:D:2023:HOH:O	2.40	0.53
1:C:364:THR:CG2	1:C:365:GLU:N	2.72	0.53
1:B:114:SER:OG	1:B:345:THR:HB	2.09	0.53
1:D:113:THR:HB	1:D:346:HIS:CD2	2.44	0.52
1:D:252:ASN:HA	1:D:255:VAL:HG13	1.89	0.52
1:C:32:GLU:N	1:C:32:GLU:OE1	2.42	0.52
1:A:270:ASP:O	1:A:271:GLN:HG2	2.09	0.52
1:D:349:ALA:CB	1:D:365:GLU:OE2	2.56	0.52
1:F:108:LEU:HD22	1:F:348:GLY:O	2.10	0.52
1:A:172:VAL:HG13	1:A:232:ALA:HB2	1.92	0.52
1:D:362:PRO:O	1:D:363:PHE:CB	2.58	0.52
1:B:164:PRO:HG2	1:D:205:ARG:HG2	1.92	0.52
1:D:26:LEU:CD1	1:D:322:LEU:HD23	2.38	0.52
1:F:12:ASN:HD22	1:F:283:TYR:HD1	1.58	0.52
1:E:149:LEU:HD13	1:E:263:VAL:CG1	2.36	0.52
1:C:205:ARG:HG2	1:F:164:PRO:HG2	1.92	0.52
1:E:87:HIS:NE2	1:E:347:GLU:HG3	2.24	0.51
1:F:366:PRO:O	1:F:367:ALA:HB2	2.10	0.51
1:B:214:ARG:NH2	1:D:213:GLY:HA3	2.20	0.51
1:E:2:ARG:HG3	1:E:32:GLU:CB	2.38	0.51
1:F:63:GLN:O	1:F:66:ALA:O	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ALA:HB2	1:B:291:HIS:CD2	2.46	0.50
1:F:149:LEU:HD13	1:F:263:VAL:HG13	1.91	0.50
1:E:231:ARG:CG	1:E:231:ARG:NH1	2.58	0.50
1:E:231:ARG:HG3	1:E:231:ARG:NH1	1.98	0.50
1:C:270:ASP:O	1:C:271:GLN:HG2	2.12	0.50
1:C:366:PRO:O	1:C:367:ALA:HB2	2.12	0.50
1:B:112:THR:O	1:B:345:THR:HG22	2.11	0.50
1:B:366:PRO:O	1:B:367:ALA:CB	2.59	0.50
1:E:135:GLU:OE2	1:F:205:ARG:HD3	2.12	0.50
1:B:214:ARG:HH12	1:D:213:GLY:H	1.59	0.49
1:E:214:ARG:NH1	1:E:214:ARG:HG2	2.27	0.49
1:E:78:ILE:HG13	2:E:2014:HOH:O	2.12	0.49
1:A:214:ARG:HH22	1:E:213:GLY:CA	2.06	0.49
1:C:29:ARG:NH1	1:C:29:ARG:CG	2.73	0.49
1:F:201:ILE:CG2	1:F:205:ARG:NH2	2.75	0.49
1:C:350:LEU:HD12	1:C:352:SER:H	1.77	0.49
1:C:254:LEU:HD13	1:C:254:LEU:O	2.12	0.49
1:F:361:VAL:O	1:F:363:PHE:N	2.45	0.49
1:A:365:GLU:O	1:A:366:PRO:C	2.51	0.49
1:E:15:ARG:NH2	1:E:300:ASN:HD21	2.10	0.49
1:A:255:VAL:HA	1:A:258:MET:HE2	1.94	0.49
1:D:255:VAL:HB	1:D:258:MET:HE3	1.95	0.49
1:D:26:LEU:HD13	1:D:322:LEU:CD2	2.42	0.48
1:E:364:THR:C	1:E:365:GLU:HG2	2.33	0.48
1:F:201:ILE:HG22	1:F:205:ARG:NH2	2.21	0.48
1:C:112:THR:O	1:C:345:THR:HG22	2.13	0.48
1:A:200:ASN:HD21	1:A:202:ASP:HB2	1.78	0.48
1:E:95:LEU:HD12	1:E:116:ALA:HB2	1.94	0.48
1:C:58:VAL:CG1	1:C:63:GLN:HB3	2.44	0.48
1:D:113:THR:HA	1:D:345:THR:O	2.13	0.48
1:F:362:PRO:O	1:F:363:PHE:CB	2.61	0.48
1:A:47:ASP:HB3	1:A:57:LEU:CD1	2.43	0.48
1:E:255:VAL:HA	1:E:258:MET:HG3	1.96	0.48
1:F:65:TRP:CD1	1:F:84:ARG:HD3	2.49	0.48
1:C:164:PRO:HG2	1:F:205:ARG:HG3	1.96	0.48
1:D:149:LEU:HD13	1:D:263:VAL:CG1	2.42	0.48
1:D:47:ASP:CB	1:D:57:LEU:HD11	2.41	0.48
1:D:366:PRO:O	1:D:367:ALA:CB	2.61	0.48
1:B:121:GLN:HB2	1:B:127:LEU:HD23	1.96	0.48
1:B:47:ASP:HB3	1:B:57:LEU:CD1	2.28	0.47
1:B:172:VAL:HG13	1:B:232:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:ALA:HA	1:E:86:ARG:HE	1.79	0.47
1:E:241:VAL:CG2	1:E:242:PRO:HD2	2.44	0.47
1:B:200:ASN:HD22	1:B:200:ASN:C	2.17	0.47
1:E:200:ASN:ND2	1:E:200:ASN:C	2.65	0.47
1:A:225:LEU:C	1:A:225:LEU:HD12	2.35	0.47
1:F:229:VAL:HG11	1:F:254:LEU:HD13	1.96	0.47
1:B:303:ALA:O	1:B:306:PRO:HD3	2.15	0.47
1:B:245:LYS:HG3	1:B:245:LYS:O	2.14	0.47
1:F:329:TRP:CZ2	1:F:346:HIS:CE1	3.03	0.47
1:B:253:SER:O	1:B:257:HIS:HD2	1.98	0.47
1:A:366:PRO:O	1:A:367:ALA:HB2	2.14	0.47
1:B:86:ARG:O	1:B:112:THR:HB	2.15	0.47
1:C:1:MET:HG3	1:C:2:ARG:N	2.30	0.47
1:B:214:ARG:HG2	1:D:214:ARG:HG3	1.98	0.46
1:E:15:ARG:HH22	1:E:300:ASN:HD21	1.63	0.46
1:F:2:ARG:HG2	1:F:32:GLU:HB3	1.97	0.46
1:C:152:THR:CG2	1:C:153:GLN:NE2	2.74	0.46
1:C:255:VAL:HA	1:C:258:MET:CE	2.43	0.46
1:E:361:VAL:O	1:E:363:PHE:N	2.49	0.46
1:E:241:VAL:HG23	1:E:242:PRO:HD2	1.98	0.46
1:F:58:VAL:HG11	1:F:63:GLN:HB3	1.97	0.46
1:C:307:LYS:O	1:C:311:TYR:HD1	1.99	0.46
1:C:218:ARG:HG2	1:C:224:GLU:HG3	1.98	0.46
1:F:355:VAL:CG1	1:F:359:LEU:HD12	2.41	0.46
1:F:112:THR:O	1:F:345:THR:HG22	2.15	0.46
1:D:78:ILE:HG22	1:D:81:GLU:HG3	1.98	0.46
1:D:105:ASP:HA	1:D:108:LEU:HD11	1.98	0.46
1:D:82:TYR:HA	1:D:85:LEU:HD13	1.97	0.46
1:B:361:VAL:O	1:B:363:PHE:N	2.48	0.45
1:A:121:GLN:HG3	1:A:127:LEU:CD2	2.46	0.45
1:C:121:GLN:O	1:C:338:ALA:HA	2.16	0.45
1:B:212:CYS:HB3	1:B:213:GLY:H	1.65	0.45
1:D:241:VAL:CG1	1:D:246:ALA:H	2.29	0.45
1:C:1:MET:HG3	1:C:2:ARG:H	1.82	0.45
1:F:163:VAL:O	1:F:164:PRO:C	2.52	0.45
1:D:85:LEU:CD2	1:D:107:LEU:HD23	2.46	0.45
1:D:304:SER:C	1:D:306:PRO:HD3	2.37	0.45
1:C:131:ALA:HB3	1:C:132:PRO:HD3	1.98	0.45
1:A:264:LEU:HB3	1:A:275:PHE:CE1	2.51	0.45
1:A:188:ASN:HD21	1:A:214:ARG:HD3	1.81	0.45
1:A:255:VAL:HA	1:A:258:MET:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:GLN:HB2	1:C:64:VAL:HG21	1.98	0.45
1:D:25:GLU:HA	1:D:25:GLU:OE1	2.17	0.45
1:C:104:THR:O	1:C:107:LEU:HB2	2.17	0.45
1:D:28:ARG:HB2	1:D:28:ARG:HE	1.59	0.45
1:A:211:PHE:CD1	1:A:215:ILE:HD12	2.52	0.45
1:B:245:LYS:O	1:B:246:ALA:HB3	2.16	0.45
1:D:211:PHE:CD1	1:D:215:ILE:HD12	2.52	0.45
1:E:222:ALA:O	1:E:226:GLU:HG3	2.17	0.45
1:B:213:GLY:H	1:D:214:ARG:HH12	1.65	0.44
1:B:337:PRO:O	1:B:341:LYS:HG2	2.17	0.44
1:B:152:THR:HG22	1:B:153:GLN:HE21	1.82	0.44
1:C:269:ILE:HG23	1:C:270:ASP:H	1.82	0.44
1:A:121:GLN:HG3	1:A:127:LEU:HD23	2.00	0.44
1:F:78:ILE:CG2	1:F:79:ALA:N	2.79	0.44
1:D:239:VAL:O	1:D:239:VAL:HG12	2.18	0.44
1:C:271:GLN:CG	1:C:271:GLN:O	2.65	0.44
1:A:119:THR:OG1	1:A:342:GLY:HA2	2.17	0.44
1:B:214:ARG:CG	1:D:214:ARG:HG3	2.47	0.44
1:D:13:GLU:HG2	1:D:75:LYS:HG3	1.98	0.44
1:A:361:VAL:O	1:A:363:PHE:N	2.50	0.44
1:D:129:LEU:HD13	1:D:317:THR:HG22	1.99	0.44
1:F:235:VAL:HB	1:F:264:LEU:HD13	1.99	0.44
1:B:258:MET:HE3	1:B:264:LEU:HD11	1.98	0.44
1:E:366:PRO:O	1:E:367:ALA:CB	2.66	0.44
1:A:225:LEU:O	1:A:225:LEU:HD12	2.17	0.44
1:F:221:SER:OG	1:F:224:GLU:HB2	2.18	0.44
1:E:101:ARG:HD2	1:E:101:ARG:HA	1.39	0.44
1:A:239:VAL:HG21	1:A:249:LEU:HD11	1.99	0.44
1:E:291:HIS:O	1:E:292:ASP:CB	2.52	0.44
1:D:168:PRO:HG2	1:D:193:THR:CG2	2.48	0.44
1:C:361:VAL:O	1:C:363:PHE:N	2.50	0.44
1:A:156:ARG:HG2	1:A:158:VAL:HG13	2.00	0.44
1:C:269:ILE:HG23	1:C:270:ASP:N	2.32	0.44
1:C:246:ALA:HA	1:C:247:PRO:HD3	1.85	0.44
1:B:167:GLU:OE1	1:D:218:ARG:NE	2.51	0.43
1:B:355:VAL:O	1:B:359:LEU:HB2	2.18	0.43
1:C:5:ILE:HA	1:C:6:PRO:HD2	1.84	0.43
1:F:147:TYR:O	1:F:150:MET:HG3	2.18	0.43
1:F:200:ASN:C	1:F:200:ASN:ND2	2.71	0.43
1:D:163:VAL:HB	1:D:164:PRO:CD	2.49	0.43
1:A:170:ASP:C	1:A:170:ASP:OD2	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:23:VAL:HG11	1:E:55:ALA:HB2	2.00	0.43
1:C:113:THR:HB	1:C:346:HIS:CD2	2.53	0.43
1:A:222:ALA:O	1:A:226:GLU:HG3	2.18	0.43
1:B:135:GLU:CD	1:C:205:ARG:HH11	2.22	0.43
1:F:356:ALA:O	1:F:360:GLY:O	2.37	0.43
1:F:240:LEU:HD11	1:F:267:ILE:HG22	2.01	0.43
1:D:95:LEU:HD12	1:D:116:ALA:HB2	2.01	0.43
1:E:239:VAL:HG21	1:E:249:LEU:CD1	2.49	0.43
1:C:172:VAL:HG13	1:C:232:ALA:HB2	2.01	0.43
1:E:225:LEU:C	1:E:225:LEU:HD12	2.38	0.43
1:A:113:THR:HA	1:A:345:THR:O	2.18	0.42
1:C:5:ILE:HG13	1:C:72:LEU:HB2	2.00	0.42
1:B:2:ARG:HG3	1:B:32:GLU:HB2	2.00	0.42
1:A:1:MET:HE2	1:A:1:MET:HB2	1.95	0.42
1:B:29:ARG:CG	1:B:29:ARG:NH1	2.64	0.42
1:D:63:GLN:O	1:D:66:ALA:O	2.37	0.42
1:C:353:GLU:OE2	1:C:364:THR:CG2	2.64	0.42
1:B:139:ARG:HH21	1:B:182:ASN:HD21	1.67	0.42
1:C:354:ARG:O	1:C:358:ASP:HB2	2.18	0.42
1:A:210:GLU:HG2	1:A:211:PHE:CE1	2.54	0.42
1:D:168:PRO:HG2	1:D:193:THR:HG22	2.00	0.42
1:F:12:ASN:HA	1:F:14:PHE:CE2	2.55	0.42
1:A:255:VAL:HA	1:A:258:MET:CE	2.48	0.42
1:A:248:LYS:HD2	1:A:276:GLU:HA	2.02	0.42
1:F:246:ALA:HB2	1:F:271:GLN:HE21	1.84	0.42
1:E:82:TYR:HA	1:E:85:LEU:CD2	2.49	0.42
1:E:113:THR:HB	1:E:346:HIS:CD2	2.54	0.42
1:B:113:THR:HA	1:B:345:THR:O	2.20	0.42
1:D:75:LYS:HA	1:D:75:LYS:HE2	2.02	0.42
1:E:28:ARG:NH2	1:F:222:ALA:HB3	2.35	0.42
1:F:365:GLU:O	1:F:366:PRO:C	2.58	0.42
1:A:255:VAL:HB	1:A:258:MET:HE3	2.02	0.42
1:E:255:VAL:HA	1:E:258:MET:HE2	2.01	0.42
1:C:254:LEU:HA	1:C:254:LEU:HD22	1.87	0.42
1:E:365:GLU:O	1:E:366:PRO:C	2.58	0.42
1:A:239:VAL:HG21	1:A:249:LEU:CD1	2.50	0.42
1:A:241:VAL:HG23	1:A:246:ALA:HA	2.02	0.42
1:D:92:PHE:CD1	1:D:115:ILE:HB	2.55	0.42
1:D:301:MET:N	1:D:302:PRO:CD	2.83	0.41
1:B:78:ILE:HA	1:B:78:ILE:HD12	1.75	0.41
1:C:1:MET:O	1:C:31:HIS:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLN:O	1:A:66:ALA:O	2.38	0.41
1:B:205:ARG:HG2	1:D:164:PRO:HG2	2.01	0.41
1:A:26:LEU:HD13	1:A:322:LEU:CD2	2.49	0.41
1:E:343:LEU:HD23	1:E:343:LEU:HA	1.70	0.41
1:B:271:GLN:CG	1:B:271:GLN:O	2.67	0.41
1:D:211:PHE:HB2	2:D:2021:HOH:O	2.19	0.41
1:B:268:ALA:O	1:B:270:ASP:O	2.39	0.41
1:A:65:TRP:CD1	1:A:84:ARG:HD3	2.56	0.41
1:D:67:ASP:H	1:D:86:ARG:HH21	1.68	0.41
1:B:252:ASN:HA	1:B:255:VAL:HG13	2.01	0.41
1:C:100:SER:O	1:C:104:THR:OG1	2.37	0.41
1:E:336:ASN:HA	1:E:337:PRO:HD2	1.88	0.41
1:C:26:LEU:HD13	1:C:322:LEU:HD23	2.02	0.41
1:A:12:ASN:HA	1:A:14:PHE:CZ	2.56	0.41
1:A:66:ALA:HA	1:A:86:ARG:HE	1.84	0.41
1:F:331:ALA:H	1:F:334:ARG:HG3	1.86	0.41
1:E:7:THR:H	1:E:36:GLN:HE21	1.68	0.41
1:A:271:GLN:O	1:A:271:GLN:HG3	2.21	0.41
1:F:78:ILE:HG23	1:F:79:ALA:N	2.36	0.41
1:C:90:ILE:HA	1:C:113:THR:O	2.21	0.41
1:E:343:LEU:HD13	1:E:351:LEU:HD13	2.03	0.41
1:F:197:LEU:HD23	1:F:220:SER:HA	2.03	0.41
1:D:140:LEU:HD23	1:D:140:LEU:HA	1.91	0.41
1:C:147:TYR:O	1:C:150:MET:HG3	2.20	0.41
1:C:157:GLY:HA3	1:E:306:PRO:HD2	2.03	0.41
1:F:26:LEU:HA	1:F:26:LEU:HD12	1.94	0.41
1:F:248:LYS:HD3	1:F:276:GLU:HA	2.03	0.41
1:A:47:ASP:HB3	1:A:57:LEU:HD13	2.03	0.41
1:A:86:ARG:NH1	1:A:86:ARG:HB3	2.33	0.40
1:F:172:VAL:HG13	1:F:232:ALA:HB2	2.02	0.40
1:A:25:GLU:HG2	2:A:2006:HOH:O	2.21	0.40
1:D:156:ARG:HG2	1:D:158:VAL:HG12	2.03	0.40
1:C:175:GLY:O	1:C:180:GLY:HA3	2.20	0.40
1:C:350:LEU:HD12	1:C:350:LEU:C	2.42	0.40
1:C:95:LEU:HA	1:C:95:LEU:HD23	1.62	0.40
1:B:254:LEU:HD22	1:B:254:LEU:O	2.22	0.40
1:E:86:ARG:HH11	1:E:86:ARG:HB3	1.86	0.40
1:C:163:VAL:O	1:C:164:PRO:C	2.59	0.40
1:D:361:VAL:O	1:D:363:PHE:N	2.54	0.40
1:D:211:PHE:CE1	1:D:215:ILE:HD12	2.56	0.40
1:B:213:GLY:HA3	1:D:214:ARG:HH22	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ASN:HD22	1:A:200:ASN:C	2.25	0.40
1:B:63:GLN:O	1:B:66:ALA:O	2.40	0.40
1:A:11:ASN:ND2	1:A:11:ASN:N	2.40	0.40
1:E:63:GLN:O	1:E:66:ALA:O	2.40	0.40
1:E:163:VAL:O	1:E:164:PRO:C	2.58	0.40
1:F:255:VAL:HA	1:F:258:MET:HE2	2.03	0.40
1:D:105:ASP:O	1:D:108:LEU:HD12	2.21	0.40
1:B:101:ARG:NH2	1:B:359:LEU:O	2.54	0.40
1:E:275:PHE:CD2	1:E:275:PHE:N	2.88	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	369/371 (100%)	343 (93%)	18 (5%)	8 (2%)	8	15
1	B	369/371 (100%)	349 (95%)	11 (3%)	9 (2%)	7	13
1	C	369/371 (100%)	342 (93%)	17 (5%)	10 (3%)	6	10
1	D	369/371 (100%)	348 (94%)	13 (4%)	8 (2%)	8	15
1	E	369/371 (100%)	343 (93%)	17 (5%)	9 (2%)	7	13
1	F	369/371 (100%)	347 (94%)	14 (4%)	8 (2%)	8	15
All	All	2214/2226 (100%)	2072 (94%)	90 (4%)	52 (2%)	8	14

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ASP
1	A	331	ALA
1	A	362	PRO

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Mol	Chain	Res	Type
1	A	363	PHE
1	A	367	ALA
1	A	368	SER
1	B	242	PRO
1	B	331	ALA
1	B	362	PRO
1	B	363	PHE
1	B	367	ALA
1	B	368	SER
1	C	242	PRO
1	C	331	ALA
1	C	362	PRO
1	C	367	ALA
1	C	368	SER
1	D	67	ASP
1	D	331	ALA
1	D	362	PRO
1	D	367	ALA
1	D	368	SER
1	E	331	ALA
1	E	362	PRO
1	E	363	PHE
1	E	367	ALA
1	E	368	SER
1	F	331	ALA
1	F	362	PRO
1	F	367	ALA
1	F	368	SER
1	B	67	ASP
1	C	67	ASP
1	C	363	PHE
1	D	363	PHE
1	E	67	ASP
1	F	67	ASP
1	F	363	PHE
1	A	246	ALA
1	B	246	ALA
1	C	246	ALA
1	D	246	ALA
1	E	246	ALA
1	F	246	ALA
1	D	361	VAL

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Mol	Chain	Res	Type
1	C	80	ALA
1	B	361	VAL
1	C	361	VAL
1	E	361	VAL
1	A	361	VAL
1	E	242	PRO
1	F	361	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	269/276 (98%)	235 (87%)	34 (13%)	5 10
1	B	270/276 (98%)	237 (88%)	33 (12%)	6 11
1	C	268/276 (97%)	230 (86%)	38 (14%)	4 7
1	D	271/276 (98%)	230 (85%)	41 (15%)	3 6
1	E	270/276 (98%)	231 (86%)	39 (14%)	4 7
1	F	268/276 (97%)	235 (88%)	33 (12%)	6 11
All	All	1616/1656 (98%)	1398 (86%)	218 (14%)	5 8

All (218) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ARG
1	A	11	ASN
1	A	26	LEU
1	A	71	LEU
1	A	73	LYS
1	A	78	ILE
1	A	109	ASP
1	A	113	THR
1	A	151	ARG
1	A	158	VAL

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Mol	Chain	Res	Type
1	A	167	GLU
1	A	172	VAL
1	A	193	THR
1	A	196	VAL
1	A	199	ILE
1	A	200	ASN
1	A	201	ILE
1	A	203	LYS
1	A	212	CYS
1	A	214	ARG
1	A	225	LEU
1	A	230	LYS
1	A	234	LEU
1	A	245	LYS
1	A	254	LEU
1	A	259	LYS
1	A	263	VAL
1	A	264	LEU
1	A	278	SER
1	A	284	ASP
1	A	345	THR
1	A	353	GLU
1	A	359	LEU
1	B	1	MET
1	B	26	LEU
1	B	29	ARG
1	B	67	ASP
1	B	78	ILE
1	B	85	LEU
1	B	113	THR
1	B	149	LEU
1	B	151	ARG
1	B	152	THR
1	B	156	ARG
1	B	167	GLU
1	B	172	VAL
1	B	193	THR
1	B	196	VAL
1	B	197	LEU
1	B	199	ILE
1	B	200	ASN
1	B	207	LEU

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Mol	Chain	Res	Type
1	B	212	CYS
1	B	214	ARG
1	B	231	ARG
1	B	234	LEU
1	B	245	LYS
1	B	254	LEU
1	B	255	VAL
1	B	263	VAL
1	B	264	LEU
1	B	271	GLN
1	B	339	LEU
1	B	345	THR
1	B	359	LEU
1	B	364	THR
1	C	1	MET
1	C	11	ASN
1	C	18	ILE
1	C	26	LEU
1	C	41	GLU
1	C	62	ASP
1	C	78	ILE
1	C	86	ARG
1	C	103	CYS
1	C	104	THR
1	C	108	LEU
1	C	113	THR
1	C	121	GLN
1	C	151	ARG
1	C	152	THR
1	C	156	ARG
1	C	158	VAL
1	C	172	VAL
1	C	193	THR
1	C	196	VAL
1	C	200	ASN
1	C	207	LEU
1	C	212	CYS
1	C	214	ARG
1	C	216	HIS
1	C	218	ARG
1	C	234	LEU
1	C	255	VAL

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Mol	Chain	Res	Type
1	C	264	LEU
1	C	271	GLN
1	C	284	ASP
1	C	292	ASP
1	C	300	ASN
1	C	330	ARG
1	C	333	CYS
1	C	350	LEU
1	C	353	GLU
1	C	368	SER
1	D	1	MET
1	D	10	LYS
1	D	11	ASN
1	D	26	LEU
1	D	29	ARG
1	D	51	LYS
1	D	56	GLN
1	D	57	LEU
1	D	71	LEU
1	D	91	LEU
1	D	92	PHE
1	D	108	LEU
1	D	113	THR
1	D	134	SER
1	D	149	LEU
1	D	152	THR
1	D	158	VAL
1	D	193	THR
1	D	196	VAL
1	D	199	ILE
1	D	200	ASN
1	D	203	LYS
1	D	212	CYS
1	D	214	ARG
1	D	218	ARG
1	D	225	LEU
1	D	230	LYS
1	D	234	LEU
1	D	254	LEU
1	D	255	VAL
1	D	263	VAL
1	D	264	LEU

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Mol	Chain	Res	Type
1	D	271	GLN
1	D	278	SER
1	D	284	ASP
1	D	309	SER
1	D	330	ARG
1	D	339	LEU
1	D	345	THR
1	D	359	LEU
1	D	364	THR
1	E	2	ARG
1	E	11	ASN
1	E	26	LEU
1	E	51	LYS
1	E	63	GLN
1	E	71	LEU
1	E	85	LEU
1	E	101	ARG
1	E	109	ASP
1	E	113	THR
1	E	130	LEU
1	E	149	LEU
1	E	151	ARG
1	E	156	ARG
1	E	158	VAL
1	E	172	VAL
1	E	193	THR
1	E	196	VAL
1	E	197	LEU
1	E	200	ASN
1	E	207	LEU
1	E	212	CYS
1	E	214	ARG
1	E	225	LEU
1	E	231	ARG
1	E	234	LEU
1	E	245	LYS
1	E	253	SER
1	E	254	LEU
1	E	255	VAL
1	E	264	LEU
1	E	271	GLN
1	E	276	GLU

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Mol	Chain	Res	Type
1	E	309	SER
1	E	330	ARG
1	E	339	LEU
1	E	347	GLU
1	E	365	GLU
1	E	370	LEU
1	F	1	MET
1	F	10	LYS
1	F	11	ASN
1	F	18	ILE
1	F	26	LEU
1	F	41	GLU
1	F	51	LYS
1	F	63	GLN
1	F	78	ILE
1	F	85	LEU
1	F	113	THR
1	F	149	LEU
1	F	151	ARG
1	F	152	THR
1	F	167	GLU
1	F	172	VAL
1	F	190	MET
1	F	193	THR
1	F	196	VAL
1	F	200	ASN
1	F	203	LYS
1	F	205	ARG
1	F	218	ARG
1	F	225	LEU
1	F	234	LEU
1	F	254	LEU
1	F	263	VAL
1	F	264	LEU
1	F	271	GLN
1	F	305	VAL
1	F	359	LEU
1	F	365	GLU
1	F	368	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	31	HIS
1	A	36	GLN
1	A	63	GLN
1	A	89	GLN
1	A	153	GLN
1	A	182	ASN
1	A	200	ASN
1	A	216	HIS
1	A	252	ASN
1	A	257	HIS
1	A	346	HIS
1	B	31	HIS
1	B	36	GLN
1	B	56	GLN
1	B	63	GLN
1	B	153	GLN
1	B	182	ASN
1	B	200	ASN
1	B	257	HIS
1	B	271	GLN
1	B	300	ASN
1	B	346	HIS
1	C	11	ASN
1	C	31	HIS
1	C	36	GLN
1	C	89	GLN
1	C	121	GLN
1	C	153	GLN
1	C	182	ASN
1	C	188	ASN
1	C	200	ASN
1	C	257	HIS
1	C	300	ASN
1	C	346	HIS
1	D	11	ASN
1	D	31	HIS
1	D	36	GLN
1	D	63	GLN
1	D	143	GLN
1	D	153	GLN
1	D	182	ASN
1	D	200	ASN

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Mol	Chain	Res	Type
1	D	300	ASN
1	D	346	HIS
1	E	31	HIS
1	E	36	GLN
1	E	153	GLN
1	E	182	ASN
1	E	200	ASN
1	E	300	ASN
1	E	346	HIS
1	F	31	HIS
1	F	36	GLN
1	F	87	HIS
1	F	89	GLN
1	F	182	ASN
1	F	200	ASN
1	F	257	HIS
1	F	271	GLN
1	F	300	ASN
1	F	346	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	371/371 (100%)	-0.28	8 (2%)	65	59	16, 37, 62, 77	0
1	B	371/371 (100%)	-0.21	4 (1%)	82	79	16, 36, 61, 77	0
1	C	371/371 (100%)	0.08	30 (8%)	15	10	15, 37, 62, 77	0
1	D	371/371 (100%)	-0.18	10 (2%)	58	51	16, 37, 62, 77	0
1	E	371/371 (100%)	-0.10	12 (3%)	51	44	15, 36, 62, 77	0
1	F	371/371 (100%)	-0.28	10 (2%)	58	51	15, 37, 62, 77	0
All	All	2226/2226 (100%)	-0.16	74 (3%)	50	43	15, 37, 62, 77	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	371	ALA	6.4
1	A	360	GLY	5.3
1	F	371	ALA	5.1
1	C	359	LEU	4.9
1	A	361	VAL	4.7
1	C	123	ALA	4.0
1	C	108	LEU	3.9
1	C	87	HIS	3.9
1	D	244	ALA	3.8
1	C	356	ALA	3.7
1	D	242	PRO	3.7
1	C	362	PRO	3.6
1	B	244	ALA	3.5
1	E	363	PHE	3.5
1	E	361	VAL	3.4
1	C	364	THR	3.4
1	F	356	ALA	3.3
1	C	355	VAL	3.3
1	C	368	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	349	ALA	3.1
1	C	351	LEU	3.0
1	E	362	PRO	3.0
1	C	2	ARG	3.0
1	A	362	PRO	2.9
1	C	365	GLU	2.9
1	C	110	SER	2.8
1	E	371	ALA	2.8
1	D	124	ASP	2.8
1	A	244	ALA	2.7
1	B	371	ALA	2.7
1	B	362	PRO	2.7
1	E	242	PRO	2.7
1	C	30	GLY	2.7
1	E	365	GLU	2.6
1	E	244	ALA	2.6
1	F	361	VAL	2.5
1	F	362	PRO	2.5
1	E	359	LEU	2.5
1	D	123	ALA	2.5
1	C	353	GLU	2.5
1	A	242	PRO	2.4
1	C	340	ALA	2.4
1	C	28	ARG	2.4
1	C	102	ALA	2.4
1	D	371	ALA	2.4
1	A	358	ASP	2.3
1	C	66	ALA	2.3
1	C	350	LEU	2.3
1	F	244	ALA	2.3
1	D	360	GLY	2.3
1	A	353	GLU	2.3
1	F	353	GLU	2.3
1	F	366	PRO	2.2
1	B	360	GLY	2.2
1	E	356	ALA	2.2
1	D	363	PHE	2.2
1	D	28	ARG	2.2
1	E	123	ALA	2.2
1	C	330	ARG	2.2
1	F	359	LEU	2.1
1	C	107	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	359	LEU	2.1
1	C	357	THR	2.1
1	C	346	HIS	2.1
1	F	83	GLY	2.1
1	C	98	ALA	2.1
1	D	12	ASN	2.1
1	F	12	ASN	2.1
1	C	103	CYS	2.1
1	C	358	ASP	2.1
1	D	243	GLY	2.0
1	E	285	HIS	2.0
1	C	67	ASP	2.0
1	E	364	THR	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 (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.