Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 12:32 PM GMT

PDB ID	:	3RFR
Title	:	Crystal Structure of particulate methane monooxygenase (pMMO) from Methylocystis sp. strain M
Authors	:	Smith, S.M.; Rosenzweig, A.C.
Deposited on	:	2011-04-06
Resolution	:	2.68 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:

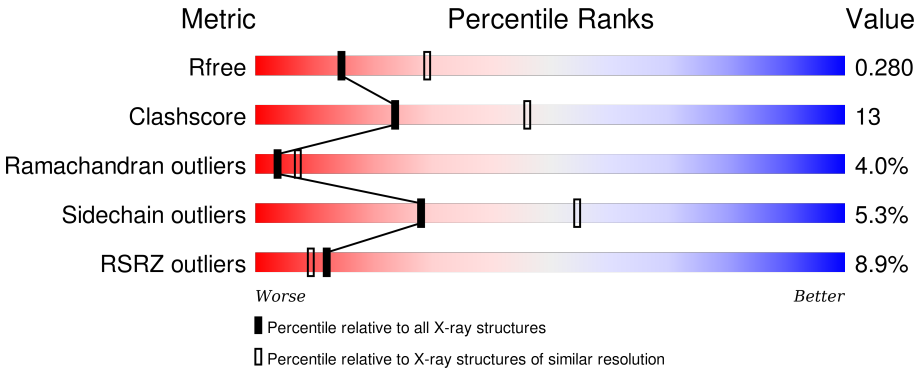
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.68 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	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

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	419	9% 68% 19% • • 8%
1	E	419	9% 68% 19% • • 8%
1	I	419	12% 56% 31% • • 8%
2	D	19	11% 74% 26%
2	H	19	26% 68% 16% 16%

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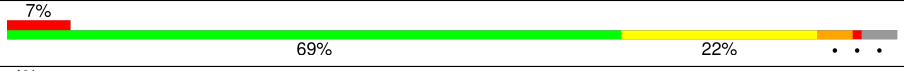
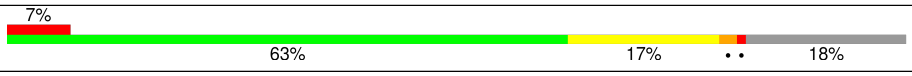
Mol	Chain	Length	Quality of chain
3	B	252	
3	F	252	
3	J	252	
4	C	256	
4	G	256	
4	K	256	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 20224 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 PmoB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			3012	1937	521	551	3			
1	E	386	Total	C	N	O	S	0	0	0
			3012	1937	521	551	3			
1	I	386	Total	C	N	O	S	0	0	0
			3012	1937	521	551	3			

- Molecule 2 is a protein called peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	19	Total	C	N	O	0	0	0
			94	57	19	18			
2	H	16	Total	C	N	O	0	0	0
			79	48	16	15			

- Molecule 3 is a protein called PmoA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	242	Total	C	N	O	S	0	0	0
			1964	1326	312	313	13			
3	B	242	Total	C	N	O	S	0	0	0
			1964	1326	312	313	13			
3	F	242	Total	C	N	O	S	0	0	0
			1964	1326	312	313	13			

- Molecule 4 is a protein called PmoC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	210	Total	C	N	O	S	0	0	0
			1695	1137	271	280	7			
4	G	211	Total	C	N	O	S	0	0	0
			1706	1146	272	281	7			

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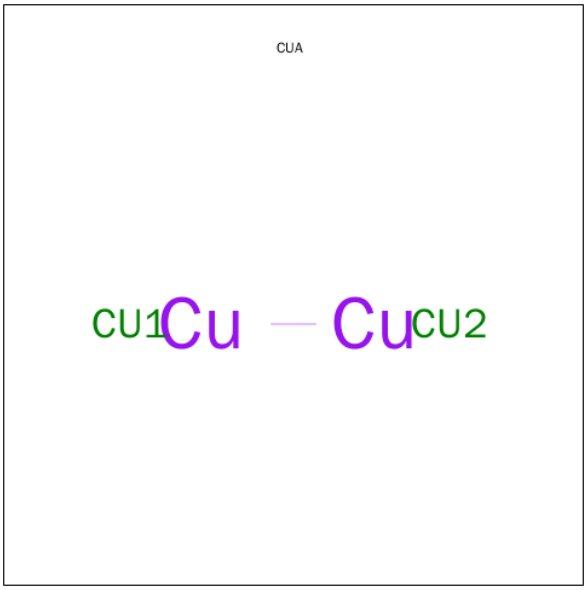
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	211	Total	C	N	O	S	0	0	0
			1706	1146	272	281	7			

- Molecule 5 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cu	0	0
			2	2		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	2	Total	Zn	0	0
			2	2		
6	K	2	Total	Zn	0	0
			2	2		
6	E	1	Total	Zn	0	0
			1	1		
6	I	1	Total	Zn	0	0
			1	1		
6	C	2	Total	Zn	0	0
			2	2		
6	A	1	Total	Zn	0	0
			1	1		

- Molecule 7 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	I	1	Total Cu 1 1	0	0
7	E	1	Total Cu 1 1	0	0

- Molecule 8 is water.

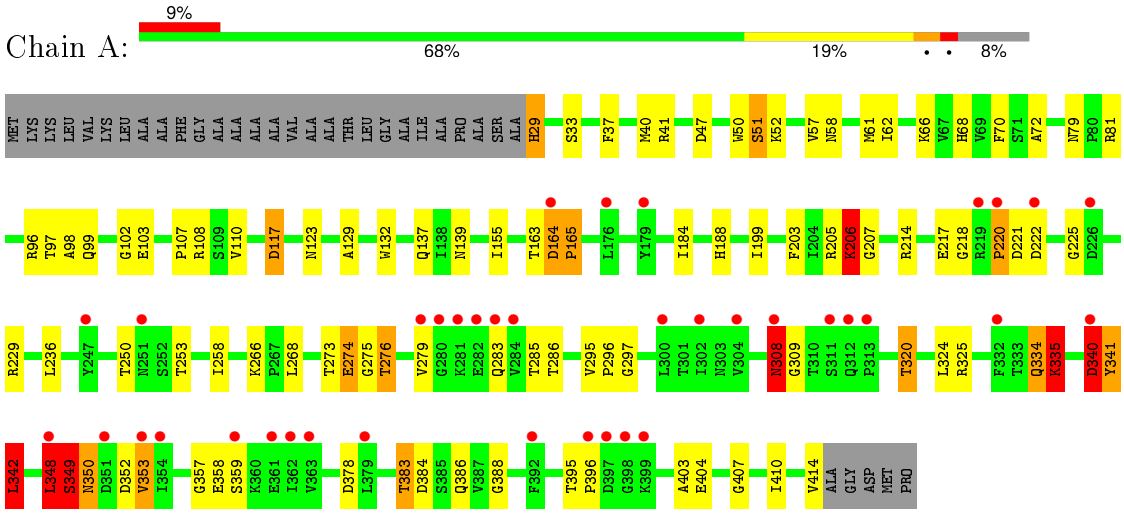
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total O 1 1	0	0
8	G	1	Total O 1 1	0	0
8	K	1	Total O 1 1	0	0

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.

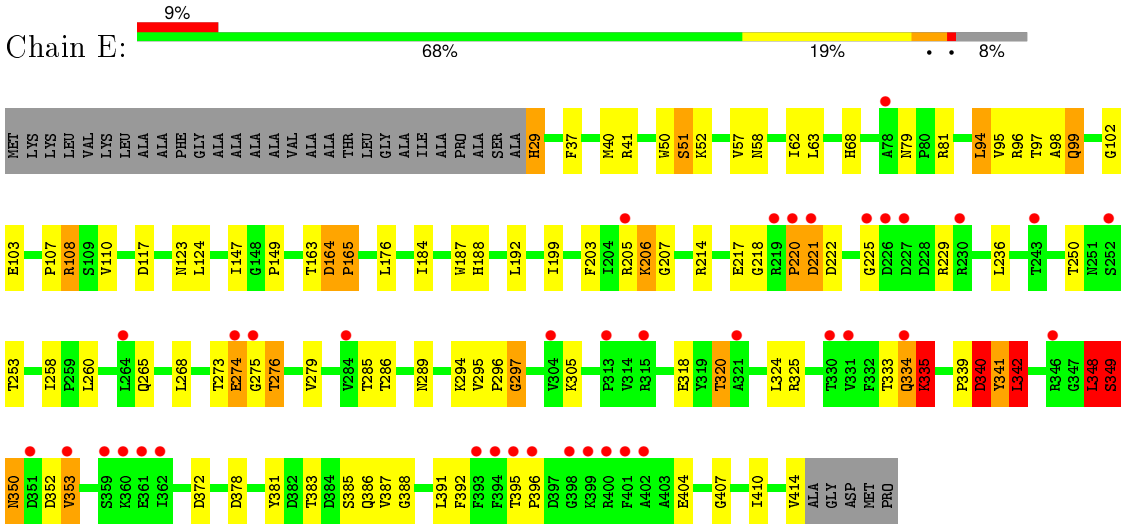
- Molecule 1: PmoB

Chain A:



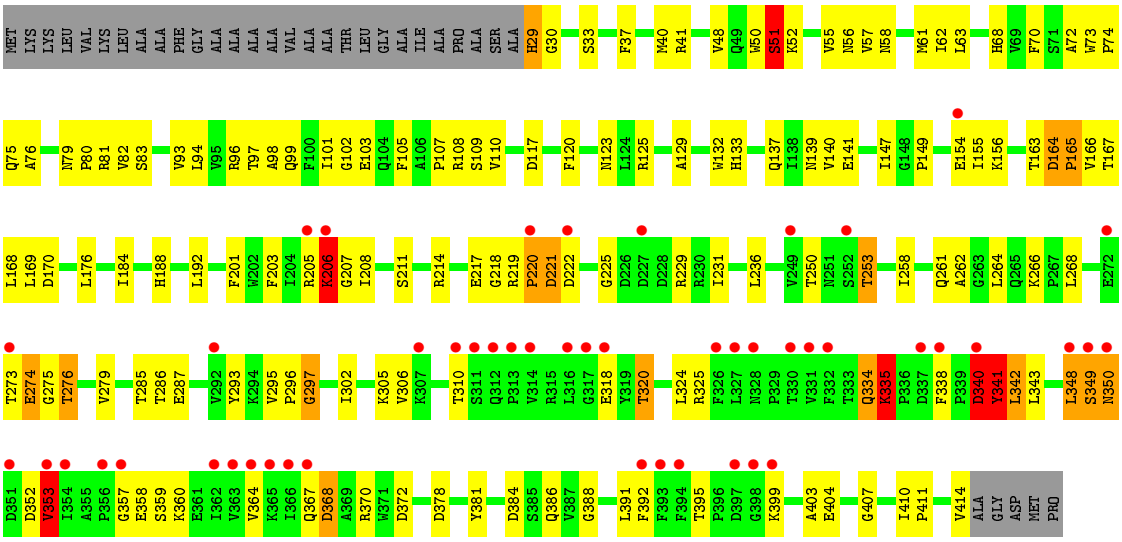
- Molecule 1: PmoB

Chain E:

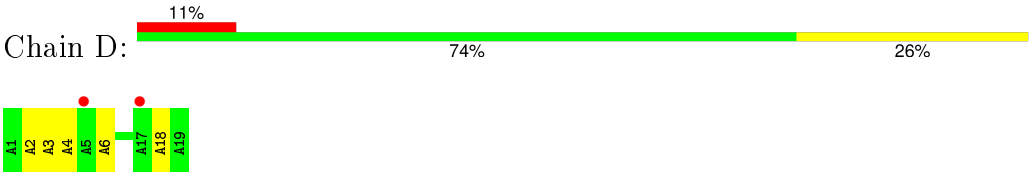


- Molecule 1: PmoB

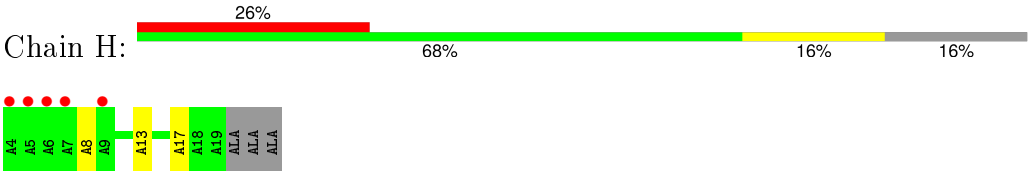
Chain I:



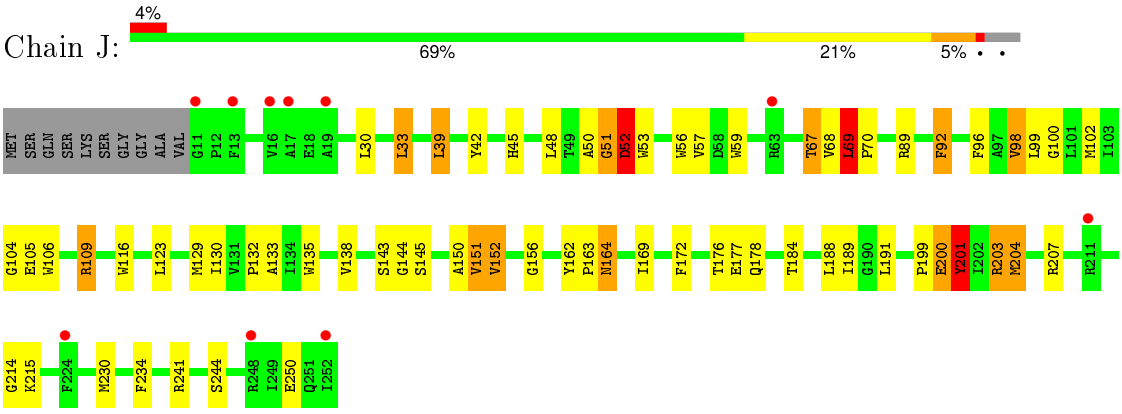
- Molecule 2: peptide



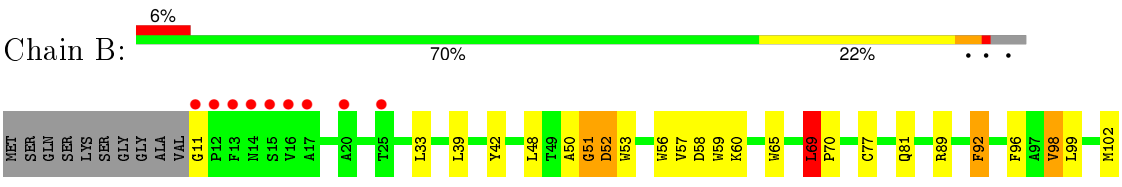
- Molecule 2: peptide

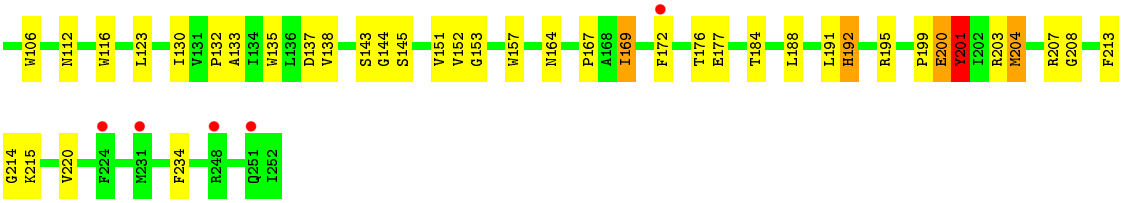


- Molecule 3: PmoA



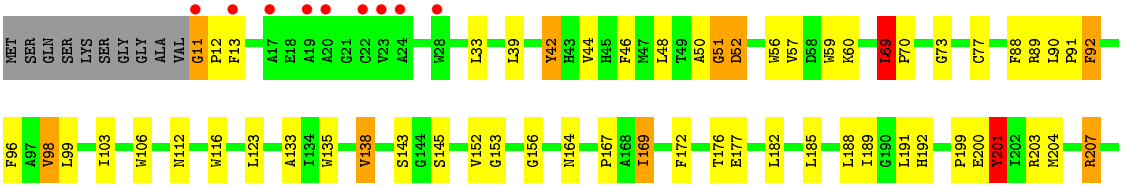
- Molecule 3: PmoA

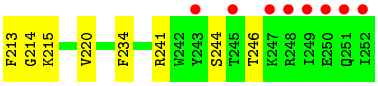




• Molecule 3: PmoA

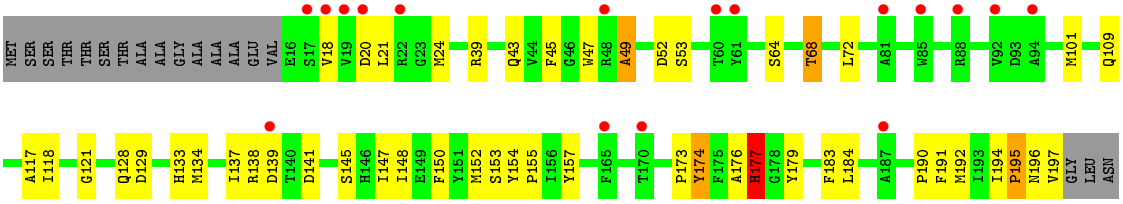
Chain F:

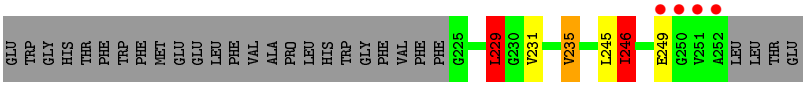




• Molecule 4: PmoC

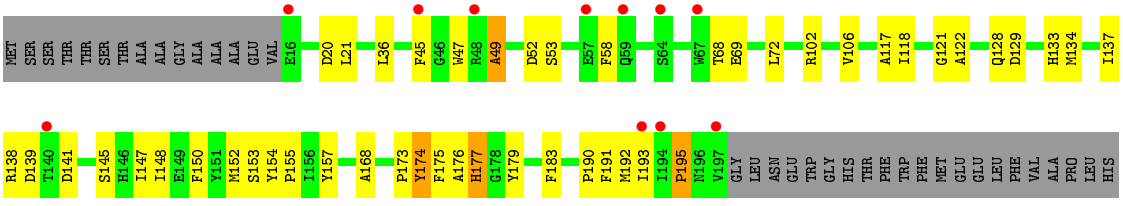
Chain C:

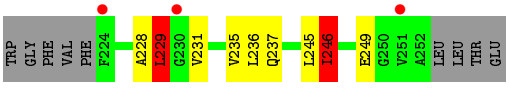




• Molecule 4: PmoC

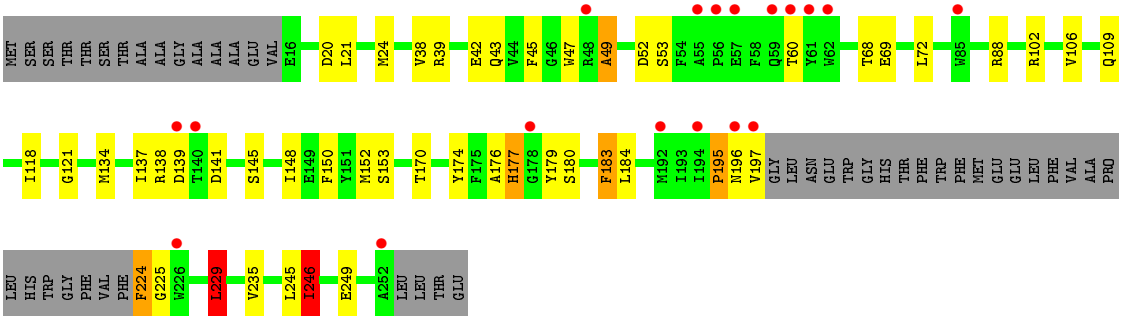
Chain G:





• Molecule 4: PmoC

Chain K:


MET SER SER THR THR SER THR ALA ALA GLY ALA ALA ALA GLU VAL E16 D20 L21 M24 V38 R39 E42 Q43 V44 F45 G46 W47 R48 A49 D52 S53 F54 A55 P56 E57 F58 Q59 T60 Y61 W62 T68 E69 L72 W85 R88 R102 V106 Q109
I118 G121 M134 I137 R138 D139 T140 D141 S145 I148 E149 F150 Y151 M152 S153 T170 Y174 F175 A176 H177 G178 Y179 S180 F183 L184 M192 I193 I194 P195 N196 V197 GLY LEU ASN GLU TRP GLY HIS THR PHE TRP PHE MET GLU GLU LEU PHE VAL ALA PRO
LEU HIS TRP GLY PHE VAL PHE F224 G225 W226 L229 V235 L245 I246 E249 A252 LEU LEU THR GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	107.72Å 178.31Å 183.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.79 – 2.68 45.79 – 2.68	Depositor EDS
% Data completeness (in resolution range)	88.9 (45.79-2.68) 88.9 (45.79-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.249 , 0.281 0.250 , 0.280	Depositor DCC
R_{free} test set	4440 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	61.2	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 52.6	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 88166 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	20224	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CUA, CU

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	0/3087	0.81	4/4205 (0.1%)
1	E	0.69	0/3087	0.81	5/4205 (0.1%)
1	I	1.04	1/3087 (0.0%)	0.94	4/4205 (0.1%)
2	D	1.00	0/93	1.02	0/129
2	H	0.84	0/78	0.67	0/108
3	B	0.79	0/2041	0.81	2/2795 (0.1%)
3	F	0.86	0/2041	0.86	2/2795 (0.1%)
3	J	0.92	0/2041	0.89	3/2795 (0.1%)
4	C	0.70	0/1749	0.70	1/2386 (0.0%)
4	G	0.66	0/1761	0.69	1/2402 (0.0%)
4	K	0.72	0/1761	0.72	2/2402 (0.1%)
All	All	0.80	1/20826 (0.0%)	0.82	24/28427 (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	4
1	E	0	3
1	I	0	4
3	B	0	3
3	F	0	3
3	J	0	2
4	G	0	1
4	K	0	1
All	All	0	21

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	154	GLU	CG-CD	5.42	1.60	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	69	LEU	CA-CB-CG	-7.86	97.23	115.30
3	F	69	LEU	CA-CB-CG	-7.58	97.87	115.30
3	J	69	LEU	CA-CB-CG	-7.37	98.34	115.30
4	G	229	LEU	CA-CB-CG	6.79	130.93	115.30
4	C	229	LEU	CA-CB-CG	6.76	130.85	115.30
3	J	200	GLU	OE1-CD-OE2	-6.22	115.83	123.30
1	E	348	LEU	CA-CB-CG	6.15	129.45	115.30
3	J	109	ARG	NE-CZ-NH1	6.09	123.34	120.30
3	F	207	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	E	342	LEU	N-CA-C	6.01	127.23	111.00
4	K	225	GLY	N-CA-C	5.97	128.03	113.10
1	I	192	LEU	CA-CB-CG	5.93	128.95	115.30
1	A	342	LEU	N-CA-C	5.92	126.98	111.00
1	A	348	LEU	CA-CB-CG	5.73	128.49	115.30
1	E	341	TYR	C-N-CA	5.54	135.56	121.70
3	B	195	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	341	TYR	C-N-CA	5.50	135.45	121.70
1	I	169	LEU	CA-CB-CG	5.30	127.50	115.30
1	I	63	LEU	CA-CB-CG	5.29	127.45	115.30
4	K	229	LEU	CA-CB-CG	5.24	127.35	115.30
1	E	192	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	308	ASN	C-N-CA	5.16	133.14	122.30
1	I	341	TYR	C-N-CA	5.04	134.31	121.70
1	E	108	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	206	LYS	Peptide
1	A	308	ASN	Peptide
1	A	335	LYS	Peptide
1	A	340	ASP	Peptide
3	B	11	GLY	Peptide
3	B	50	ALA	Peptide
3	B	51	GLY	Peptide
1	E	206	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	E	335	LYS	Peptide
1	E	340	ASP	Peptide
3	F	11	GLY	Peptide
3	F	50	ALA	Peptide
3	F	51	GLY	Peptide
4	G	228	ALA	Peptide
1	I	206	LYS	Peptide
1	I	335	LYS	Peptide
1	I	340	ASP	Peptide
1	I	341	TYR	Peptide
3	J	50	ALA	Peptide
3	J	51	GLY	Peptide
4	K	224	PHE	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	3012	0	3009	94	0
1	E	3012	0	3009	95	0
1	I	3012	0	3009	136	0
2	D	94	0	97	2	0
2	H	79	0	79	2	0
3	B	1964	0	1924	55	0
3	F	1964	0	1924	62	0
3	J	1964	0	1924	55	0
4	C	1695	0	1692	36	0
4	G	1706	0	1701	36	0
4	K	1706	0	1701	36	0
5	A	2	0	0	0	0
6	A	1	0	0	0	0
6	C	2	0	0	0	0
6	E	1	0	0	0	0
6	G	2	0	0	0	0
6	I	1	0	0	0	0
6	K	2	0	0	0	0
7	E	1	0	0	0	0
7	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	1	0	0	0	0
8	G	1	0	0	0	0
8	K	1	0	0	0	0
All	All	20224	0	20069	533	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 13.

All (533) 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)
3:J:116:TRP:O	4:K:47:TRP:HH2	1.31	1.13
1:I:275:GLY:HA3	1:I:276:THR:HG22	1.29	1.11
3:F:11:GLY:HA3	3:F:13:PHE:H	1.02	1.10
1:A:340:ASP:HB3	1:A:341:TYR:HB3	1.33	1.09
3:B:51:GLY:HA3	3:B:52:ASP:HB2	1.28	1.08
1:A:275:GLY:HA3	1:A:276:THR:HG22	1.28	1.08
1:A:274:GLU:H	1:A:275:GLY:CA	1.66	1.08
1:E:340:ASP:HB3	1:E:341:TYR:HB3	1.28	1.07
3:J:116:TRP:O	4:K:47:TRP:CH2	2.08	1.07
3:J:51:GLY:HA3	3:J:52:ASP:HB2	1.36	1.06
1:E:274:GLU:H	1:E:275:GLY:CA	1.67	1.06
3:B:116:TRP:O	4:C:47:TRP:HH2	1.38	1.06
4:K:245:LEU:O	4:K:246:ILE:HG13	1.54	1.05
3:F:51:GLY:HA3	3:F:52:ASP:HB2	1.36	1.05
3:B:116:TRP:O	4:C:47:TRP:CH2	2.12	1.02
1:A:348:LEU:HB2	1:A:349:SER:HB3	1.44	1.00
1:I:274:GLU:H	1:I:275:GLY:CA	1.74	0.99
1:A:274:GLU:H	1:A:275:GLY:HA3	1.30	0.97
4:C:245:LEU:O	4:C:246:ILE:HG13	1.64	0.97
4:K:121:GLY:HA2	4:K:153:SER:OG	1.63	0.97
1:I:340:ASP:HB3	1:I:341:TYR:HB3	1.46	0.96
4:G:245:LEU:O	4:G:246:ILE:HG13	1.65	0.95
1:A:275:GLY:HA3	1:A:276:THR:CG2	1.95	0.94
1:I:96:ARG:HH21	1:I:99:GLN:HE22	1.02	0.93
1:I:58:ASN:HD21	1:I:163:THR:H	1.16	0.92
4:G:245:LEU:C	4:G:246:ILE:HG13	1.90	0.92
1:I:275:GLY:HA3	1:I:276:THR:CG2	2.00	0.91
1:I:274:GLU:H	1:I:275:GLY:HA3	1.34	0.91
3:F:116:TRP:O	4:G:47:TRP:HH2	1.54	0.89
2:D:3:ALA:HA	2:D:6:ALA:HB3	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:11:GLY:HA3	3:F:13:PHE:N	1.87	0.88
4:K:245:LEU:C	4:K:246:ILE:HG13	1.89	0.88
3:F:116:TRP:O	4:G:47:TRP:CH2	2.27	0.88
4:C:121:GLY:HA2	4:C:153:SER:OG	1.73	0.88
1:E:340:ASP:HB3	1:E:341:TYR:CB	2.02	0.88
1:I:164:ASP:CB	1:I:165:PRO:HA	2.02	0.87
3:F:11:GLY:CA	3:F:13:PHE:H	1.88	0.87
1:I:137:GLN:HE21	1:I:139:ASN:HD21	1.23	0.86
1:A:340:ASP:HB3	1:A:341:TYR:CB	2.07	0.85
1:I:205:ARG:O	1:I:206:LYS:HB2	1.77	0.84
4:C:245:LEU:C	4:C:246:ILE:HG13	1.95	0.83
1:E:274:GLU:H	1:E:275:GLY:HA3	1.42	0.83
1:I:348:LEU:HB2	1:I:349:SER:HB3	1.61	0.81
4:K:245:LEU:O	4:K:246:ILE:CG1	2.30	0.80
3:B:51:GLY:CA	3:B:52:ASP:HB2	2.12	0.80
1:A:164:ASP:CB	1:A:165:PRO:HA	2.12	0.80
3:J:143:SER:O	3:J:145:SER:N	2.14	0.80
3:J:214:GLY:HA2	3:J:215:LYS:HB2	1.62	0.79
1:E:68:HIS:HE1	1:E:404:GLU:OE1	1.66	0.79
1:A:58:ASN:HD21	1:A:163:THR:H	1.30	0.79
1:I:96:ARG:HH21	1:I:99:GLN:NE2	1.80	0.79
4:G:148:ILE:HG23	4:G:152:MET:HE1	1.66	0.78
4:C:148:ILE:HG23	4:C:152:MET:HE1	1.64	0.78
3:F:214:GLY:HA2	3:F:215:LYS:HB2	1.65	0.78
1:E:58:ASN:HD21	1:E:163:THR:H	1.30	0.78
3:B:200:GLU:O	3:B:201:TYR:HB3	1.83	0.77
4:K:148:ILE:HG23	4:K:152:MET:HE1	1.64	0.77
4:G:245:LEU:O	4:G:246:ILE:CG1	2.32	0.77
4:G:53:SER:OG	4:G:139:ASP:HB2	1.84	0.77
1:I:68:HIS:HE1	1:I:404:GLU:OE1	1.67	0.76
1:I:164:ASP:HB2	1:I:165:PRO:HA	1.67	0.76
1:A:164:ASP:HB2	1:A:165:PRO:HA	1.68	0.76
1:E:274:GLU:N	1:E:275:GLY:CA	2.47	0.76
1:I:225:GLY:HA2	1:I:229:ARG:NH2	2.00	0.76
1:E:164:ASP:CB	1:E:165:PRO:HA	2.16	0.75
3:B:98:VAL:HG21	3:B:133:ALA:HB2	1.66	0.75
1:E:274:GLU:H	1:E:275:GLY:HA2	1.48	0.75
1:I:220:PRO:O	1:I:222:ASP:N	2.16	0.75
1:A:98:ALA:HB3	1:A:123:ASN:HD22	1.52	0.75
1:E:340:ASP:CB	1:E:341:TYR:HB3	2.15	0.75
3:J:106:TRP:HE1	1:I:188:HIS:CD2	2.04	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:98:VAL:HG21	3:J:133:ALA:HB2	1.67	0.74
2:H:8:ALA:HB1	4:G:68:THR:HG21	1.68	0.74
4:C:53:SER:OG	4:C:139:ASP:HB2	1.85	0.74
1:E:275:GLY:HA3	1:E:276:THR:HG22	1.68	0.74
1:A:348:LEU:CB	1:A:349:SER:HB3	2.18	0.73
1:E:334:GLN:HA	1:E:335:LYS:HB2	1.71	0.73
3:J:177:GLU:HG3	1:E:410:ILE:HG12	1.69	0.73
3:B:214:GLY:HA2	3:B:215:LYS:HB2	1.70	0.73
1:A:220:PRO:O	1:A:222:ASP:N	2.15	0.73
1:I:70:PHE:HE1	1:I:72:ALA:HB3	1.53	0.72
3:B:143:SER:O	3:B:145:SER:N	2.21	0.72
1:E:348:LEU:HB2	1:E:349:SER:HB3	1.72	0.72
3:B:60:LYS:HD2	3:B:169:ILE:HD11	1.70	0.72
4:K:52:ASP:HB2	1:I:29:HIS:HD2	1.55	0.72
4:C:245:LEU:O	4:C:246:ILE:CG1	2.39	0.71
1:I:334:GLN:HA	1:I:335:LYS:HB2	1.71	0.71
1:E:220:PRO:O	1:E:222:ASP:N	2.20	0.71
3:J:203:ARG:O	3:J:204:MET:HB2	1.89	0.71
1:A:188:HIS:CD2	3:B:106:TRP:HE1	2.08	0.70
3:J:184:THR:HG22	1:I:258:ILE:HG13	1.74	0.70
1:I:68:HIS:HD2	1:I:117:ASP:OD1	1.75	0.69
3:F:200:GLU:O	3:F:201:TYR:HB3	1.92	0.69
1:E:164:ASP:HB2	1:E:165:PRO:HA	1.73	0.69
3:J:51:GLY:CA	3:J:52:ASP:HB2	2.19	0.69
1:I:164:ASP:CB	1:I:165:PRO:CA	2.71	0.68
1:E:40:MET:HE2	1:E:388:GLY:H	1.58	0.68
1:E:50:TRP:O	1:E:52:LYS:N	2.26	0.68
1:E:98:ALA:HB3	1:E:123:ASN:HD22	1.59	0.68
1:E:275:GLY:HA3	1:E:276:THR:CG2	2.23	0.68
3:F:60:LYS:HD2	3:F:169:ILE:HD11	1.76	0.67
1:A:334:GLN:HA	1:A:335:LYS:HB2	1.76	0.67
3:B:203:ARG:O	3:B:204:MET:HB2	1.94	0.67
1:I:68:HIS:CD2	1:I:117:ASP:OD1	2.48	0.67
4:K:45:PHE:O	4:K:49:ALA:HB3	1.94	0.67
4:G:121:GLY:HA2	4:G:153:SER:OG	1.95	0.67
1:I:276:THR:HG23	1:I:279:VAL:HB	1.77	0.66
1:I:96:ARG:NH2	1:I:99:GLN:HE22	1.86	0.66
1:I:70:PHE:CE1	1:I:72:ALA:HB3	2.30	0.66
1:I:225:GLY:HA2	1:I:229:ARG:HH21	1.58	0.66
1:A:68:HIS:HD2	1:A:117:ASP:OD1	1.79	0.66
1:A:340:ASP:CB	1:A:341:TYR:HB3	2.18	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:53:SER:OG	4:K:139:ASP:HB2	1.96	0.65
1:A:274:GLU:N	1:A:275:GLY:CA	2.48	0.65
1:A:274:GLU:H	1:A:275:GLY:HA2	1.60	0.65
3:J:214:GLY:CA	3:J:215:LYS:HB2	2.27	0.65
1:A:29:HIS:HD2	4:C:52:ASP:HB2	1.62	0.64
1:A:96:ARG:HH21	1:A:99:GLN:HE22	1.45	0.64
4:K:52:ASP:HB2	1:I:29:HIS:CD2	2.31	0.64
1:A:68:HIS:HE1	1:A:404:GLU:OE1	1.81	0.64
3:B:213:PHE:HA	1:I:33:SER:O	1.98	0.64
4:C:246:ILE:HB	4:C:249:GLU:HG2	1.78	0.64
3:J:59:TRP:CZ3	3:J:203:ARG:O	2.51	0.63
4:G:45:PHE:O	4:G:49:ALA:HB3	1.98	0.63
1:A:275:GLY:HA3	1:A:276:THR:CB	2.28	0.63
3:B:143:SER:C	3:B:145:SER:H	2.01	0.63
3:F:214:GLY:CA	3:F:215:LYS:HB2	2.29	0.63
1:I:164:ASP:OD2	1:I:176:LEU:HB2	1.99	0.63
1:I:250:THR:O	1:I:253:THR:O	2.17	0.63
4:G:246:ILE:HB	4:G:249:GLU:HG2	1.79	0.62
1:A:410:ILE:HG12	3:F:177:GLU:HG3	1.79	0.62
1:A:274:GLU:N	1:A:275:GLY:HA3	2.11	0.62
1:A:276:THR:HG23	1:A:279:VAL:HB	1.80	0.62
3:F:98:VAL:HG21	3:F:133:ALA:HB2	1.81	0.62
1:I:110:VAL:HB	1:I:268:LEU:HD11	1.81	0.62
1:E:274:GLU:N	1:E:275:GLY:HA3	2.13	0.62
4:K:246:ILE:HB	4:K:249:GLU:HG2	1.81	0.62
3:J:138:VAL:HG21	1:I:236:LEU:HB2	1.80	0.62
1:E:275:GLY:HA3	1:E:276:THR:CB	2.30	0.62
1:E:225:GLY:HA2	1:E:229:ARG:NH2	2.15	0.61
3:F:106:TRP:HE1	1:E:188:HIS:CD2	2.18	0.61
3:F:51:GLY:CA	3:F:52:ASP:HB2	2.22	0.61
3:B:214:GLY:CA	3:B:215:LYS:HB2	2.31	0.61
3:F:46:PHE:HZ	3:F:69:LEU:HD11	1.65	0.61
3:F:138:VAL:HG21	1:E:236:LEU:HB2	1.82	0.61
1:A:236:LEU:HB2	3:B:138:VAL:HG21	1.83	0.61
1:A:220:PRO:C	1:A:222:ASP:H	2.02	0.61
1:A:283:GLN:O	1:A:309:GLY:HA3	2.00	0.61
1:A:225:GLY:HA2	1:A:229:ARG:NH2	2.15	0.61
4:C:150:PHE:CZ	4:C:195:PRO:HG3	2.36	0.61
3:F:69:LEU:HB3	3:F:70:PRO:HD3	1.81	0.61
1:I:386:GLN:HG3	1:I:407:GLY:C	2.21	0.61
4:G:150:PHE:CZ	4:G:195:PRO:HG3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:348:LEU:CA	1:I:349:SER:HB3	2.31	0.60
1:A:348:LEU:CA	1:A:349:SER:HB3	2.30	0.60
1:E:205:ARG:O	1:E:206:LYS:HB2	2.01	0.60
3:B:69:LEU:HB3	3:B:70:PRO:HD3	1.82	0.60
1:I:164:ASP:HB3	1:I:165:PRO:HA	1.81	0.60
1:I:48:VAL:HG21	1:I:149:PRO:HG2	1.83	0.60
1:I:50:TRP:O	1:I:52:LYS:N	2.35	0.60
1:I:164:ASP:HB3	1:I:165:PRO:CA	2.31	0.60
1:E:214:ARG:NH1	1:E:222:ASP:O	2.34	0.60
4:K:20:ASP:O	4:K:21:LEU:HB2	2.02	0.60
1:E:348:LEU:HB2	1:E:349:SER:CB	2.30	0.60
3:B:207:ARG:HD3	1:I:75:GLN:NE2	2.15	0.60
1:I:320:THR:HG22	1:I:324:LEU:O	2.01	0.60
4:G:138:ARG:NH1	4:G:141:ASP:HA	2.17	0.60
1:I:348:LEU:CB	1:I:349:SER:HB3	2.31	0.60
3:J:203:ARG:O	3:J:204:MET:CB	2.50	0.60
3:J:143:SER:C	3:J:145:SER:H	2.05	0.59
1:A:275:GLY:CA	1:A:276:THR:HG22	2.20	0.59
4:K:69:GLU:OE1	4:K:152:MET:HB2	2.02	0.59
1:A:205:ARG:O	1:A:206:LYS:HB2	2.01	0.59
1:I:340:ASP:HB3	1:I:341:TYR:CB	2.27	0.59
4:C:45:PHE:O	4:C:49:ALA:HB3	2.02	0.59
1:I:207:GLY:O	1:I:211:SER:HB2	2.03	0.59
1:A:164:ASP:CB	1:A:165:PRO:CA	2.80	0.59
3:B:59:TRP:CZ3	3:B:203:ARG:O	2.55	0.59
3:J:172:PHE:CE2	1:I:184:ILE:HD11	2.37	0.59
4:K:150:PHE:CZ	4:K:195:PRO:HG3	2.38	0.59
1:I:214:ARG:NH1	1:I:222:ASP:O	2.36	0.59
3:F:191:LEU:HD13	1:E:107:PRO:HA	1.85	0.59
3:J:176:THR:HG21	3:J:188:LEU:HD22	1.84	0.59
1:E:275:GLY:CA	1:E:276:THR:HB	2.31	0.59
1:E:275:GLY:HA3	1:E:276:THR:HB	1.84	0.59
1:I:349:SER:OG	1:I:350:ASN:N	2.36	0.59
4:G:52:ASP:HB2	1:E:29:HIS:HD2	1.67	0.58
1:A:352:ASP:O	1:A:353:VAL:C	2.41	0.58
3:B:215:LYS:HA	1:I:381:TYR:CZ	2.39	0.58
1:I:102:GLY:HA3	1:I:268:LEU:HD22	1.85	0.58
3:J:200:GLU:O	3:J:201:TYR:HB3	2.03	0.58
4:K:137:ILE:HD13	1:I:147:ILE:CD1	2.34	0.58
1:E:320:THR:HG22	1:E:324:LEU:O	2.04	0.57
1:I:219:ARG:HB3	1:I:221:ASP:OD1	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:96:ARG:CD	1:I:99:GLN:NE2	2.68	0.57
4:C:138:ARG:NH1	4:C:141:ASP:HA	2.19	0.57
3:F:203:ARG:O	3:F:204:MET:HB2	2.04	0.57
4:G:176:ALA:O	4:G:177:HIS:CD2	2.58	0.57
1:E:352:ASP:O	1:E:353:VAL:C	2.43	0.56
1:E:68:HIS:HD2	1:E:117:ASP:OD1	1.88	0.56
1:I:220:PRO:C	1:I:222:ASP:H	2.03	0.56
3:F:167:PRO:HA	1:E:250:THR:HG21	1.85	0.56
1:I:68:HIS:CE1	1:I:404:GLU:OE1	2.54	0.56
1:A:214:ARG:NH1	1:A:222:ASP:O	2.39	0.56
1:E:395:THR:OG1	1:E:396:PRO:HD2	2.05	0.56
1:A:68:HIS:CD2	1:A:117:ASP:OD1	2.57	0.56
4:K:176:ALA:O	4:K:177:HIS:CD2	2.59	0.56
1:I:170:ASP:C	1:I:170:ASP:OD1	2.44	0.56
3:B:208:GLY:O	1:I:76:ALA:HB1	2.06	0.56
1:I:51:SER:HB3	1:I:62:ILE:O	2.05	0.55
3:J:98:VAL:HG12	3:J:99:LEU:N	2.20	0.55
3:B:203:ARG:O	3:B:204:MET:CB	2.53	0.55
1:I:203:PHE:O	1:I:207:GLY:HA2	2.07	0.55
1:A:349:SER:OG	1:A:350:ASN:N	2.39	0.54
3:F:143:SER:C	3:F:145:SER:H	2.09	0.54
1:A:220:PRO:HB3	3:B:89:ARG:HG3	1.89	0.54
3:F:46:PHE:CZ	3:F:69:LEU:HD11	2.41	0.54
3:F:96:PHE:HA	1:E:199:ILE:HD11	1.88	0.54
1:I:274:GLU:N	1:I:275:GLY:CA	2.55	0.54
1:E:164:ASP:CB	1:E:165:PRO:CA	2.84	0.54
3:F:89:ARG:HG3	1:E:220:PRO:HB3	1.89	0.54
1:I:275:GLY:HA3	1:I:276:THR:CB	2.38	0.54
1:I:58:ASN:HD22	1:I:125:ARG:HH21	1.56	0.54
4:K:24:MET:HB2	4:K:109:GLN:HG2	1.90	0.54
1:I:367:GLN:O	1:I:368:ASP:HB2	2.07	0.54
3:J:57:VAL:HG12	3:J:123:LEU:HD12	1.90	0.54
1:I:358:GLU:HG2	1:I:359:SER:N	2.23	0.54
1:A:70:PHE:HE1	1:A:72:ALA:HB3	1.73	0.53
3:F:57:VAL:HG12	3:F:123:LEU:HD12	1.90	0.53
3:B:200:GLU:O	3:B:201:TYR:CB	2.55	0.53
1:I:334:GLN:HA	1:I:335:LYS:CB	2.37	0.53
1:A:102:GLY:HA3	1:A:268:LEU:HD22	1.89	0.53
3:F:200:GLU:HG2	3:F:203:ARG:HH11	1.73	0.53
1:A:395:THR:OG1	1:A:396:PRO:HD2	2.09	0.53
1:E:110:VAL:HB	1:E:268:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:320:THR:CG2	1:E:325:ARG:HG2	2.39	0.53
3:B:57:VAL:HG12	3:B:123:LEU:HD12	1.91	0.53
3:F:135:TRP:NE1	3:F:156:GLY:HA3	2.24	0.53
3:J:92:PHE:O	3:J:96:PHE:HB2	2.09	0.52
1:I:352:ASP:O	1:I:353:VAL:C	2.46	0.52
1:I:82:VAL:HG11	1:I:141:GLU:OE1	2.08	0.52
1:A:40:MET:HE2	1:A:388:GLY:H	1.73	0.52
1:I:286:THR:HG21	1:I:391:LEU:HD12	1.91	0.52
4:K:180:SER:HB3	4:K:183:PHE:HB2	1.92	0.52
1:I:358:GLU:HG2	1:I:359:SER:H	1.73	0.52
1:A:275:GLY:CA	1:A:276:THR:CB	2.87	0.52
1:I:273:THR:HB	1:I:274:GLU:HB2	1.91	0.52
3:B:132:PRO:HB2	3:B:157:TRP:CE3	2.45	0.52
1:E:340:ASP:HB3	1:E:341:TYR:CA	2.38	0.52
1:I:348:LEU:HA	1:I:349:SER:HB3	1.92	0.52
1:E:386:GLN:HG3	1:E:407:GLY:C	2.29	0.52
1:I:395:THR:HG22	1:I:399:LYS:O	2.10	0.52
1:E:318:GLU:HB3	1:E:392:PHE:HB2	1.91	0.52
2:D:2:ALA:O	2:D:6:ALA:HB2	2.11	0.51
1:A:50:TRP:O	1:A:52:LYS:N	2.43	0.51
1:E:276:THR:HG23	1:E:279:VAL:HB	1.92	0.51
3:F:204:MET:H	3:F:207:ARG:HH12	1.59	0.51
3:J:69:LEU:HB3	3:J:70:PRO:HD3	1.92	0.51
1:A:250:THR:HG21	3:B:167:PRO:HA	1.93	0.51
4:G:246:ILE:HG21	4:G:249:GLU:OE2	2.11	0.51
3:F:77:CYS:SG	3:F:98:VAL:HG23	2.50	0.51
3:J:89:ARG:HG3	1:I:220:PRO:HB3	1.91	0.51
4:C:246:ILE:HG21	4:C:249:GLU:OE2	2.11	0.51
1:A:203:PHE:O	1:A:207:GLY:HA2	2.10	0.51
3:F:59:TRP:CZ3	3:F:203:ARG:O	2.64	0.51
3:F:176:THR:HG21	3:F:188:LEU:HD22	1.93	0.51
4:C:173:PRO:O	4:C:174:TYR:CB	2.59	0.51
1:E:102:GLY:HA3	1:E:268:LEU:HD22	1.92	0.51
4:G:102:ARG:O	4:G:106:VAL:HG23	2.10	0.51
4:K:121:GLY:HA2	4:K:153:SER:HG	1.71	0.51
1:E:37:PHE:O	1:E:41:ARG:HG3	2.12	0.50
1:A:341:TYR:H	1:A:342:LEU:CA	2.24	0.50
1:I:96:ARG:HD3	1:I:99:GLN:NE2	2.26	0.50
4:G:53:SER:OG	4:G:139:ASP:CB	2.59	0.50
3:J:56:TRP:CH2	4:K:134:MET:HG3	2.46	0.50
3:B:204:MET:H	3:B:207:ARG:HH12	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:13:ALA:O	2:H:17:ALA:HB3	2.11	0.50
3:B:176:THR:HG21	3:B:188:LEU:HD22	1.93	0.50
1:I:273:THR:CA	1:I:274:GLU:HB2	2.40	0.50
1:E:57:VAL:O	1:E:58:ASN:HB2	2.12	0.50
1:E:149:PRO:HB3	1:E:342:LEU:HD21	1.93	0.50
1:A:184:ILE:HD11	3:B:172:PHE:CE2	2.47	0.50
1:I:274:GLU:H	1:I:275:GLY:HA2	1.70	0.50
4:C:231:VAL:O	4:C:235:VAL:HG13	2.11	0.50
1:A:47:ASP:OD2	1:A:66:LYS:NZ	2.36	0.50
1:A:275:GLY:CA	1:A:276:THR:HB	2.41	0.50
3:J:201:TYR:CD1	3:J:201:TYR:C	2.85	0.50
1:E:341:TYR:H	1:E:342:LEU:CA	2.25	0.50
1:E:349:SER:OG	1:E:350:ASN:N	2.45	0.49
4:K:137:ILE:HD13	1:I:147:ILE:HD11	1.93	0.49
4:G:168:ALA:O	4:G:175:PHE:HB2	2.12	0.49
1:A:386:GLN:HG3	1:A:407:GLY:C	2.32	0.49
1:I:58:ASN:ND2	1:I:163:THR:H	1.97	0.49
1:I:205:ARG:O	1:I:206:LYS:CB	2.52	0.49
1:A:96:ARG:HH21	1:A:99:GLN:NE2	2.09	0.49
1:A:33:SER:O	3:F:213:PHE:HA	2.12	0.49
1:I:96:ARG:HD2	1:I:99:GLN:NE2	2.27	0.49
3:J:184:THR:CG2	1:I:258:ILE:HG13	2.42	0.49
1:E:348:LEU:HA	1:E:349:SER:HB2	1.94	0.49
1:I:56:ASN:HA	1:I:156:LYS:O	2.12	0.49
3:F:246:THR:HG22	4:G:237:GLN:HG3	1.93	0.49
1:I:101:ILE:HG13	1:I:120:PHE:HB3	1.95	0.49
1:I:79:ASN:C	1:I:81:ARG:H	2.14	0.49
1:A:70:PHE:CE1	1:A:72:ALA:HB3	2.48	0.49
3:F:135:TRP:CD1	3:F:153:GLY:O	2.66	0.49
3:J:191:LEU:HD13	1:I:107:PRO:HA	1.95	0.49
1:E:334:GLN:HG2	1:E:335:LYS:HB2	1.95	0.49
3:F:138:VAL:CG2	1:E:236:LEU:HD22	2.43	0.49
4:G:20:ASP:O	4:G:21:LEU:HB2	2.13	0.49
1:I:338:PHE:HB3	1:I:343:LEU:HD22	1.95	0.49
1:A:340:ASP:HB3	1:A:341:TYR:CA	2.42	0.48
1:A:334:GLN:HA	1:A:335:LYS:CB	2.42	0.48
1:E:203:PHE:O	1:E:207:GLY:HA2	2.13	0.48
1:I:320:THR:CG2	1:I:325:ARG:HG2	2.43	0.48
1:E:107:PRO:HD2	1:E:265:GLN:HE22	1.79	0.48
3:J:102:MET:HG3	3:J:130:ILE:CD1	2.43	0.48
4:K:39:ARG:NH2	4:K:43:GLN:HB2	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:334:GLN:HG2	1:I:335:LYS:HB2	1.96	0.48
4:C:176:ALA:O	4:C:177:HIS:CD2	2.67	0.48
1:E:220:PRO:C	1:E:222:ASP:H	2.13	0.48
1:A:108:ARG:NH2	1:I:384:ASP:OD1	2.46	0.48
1:A:320:THR:CG2	1:A:325:ARG:HG2	2.44	0.48
3:F:172:PHE:CZ	1:E:184:ILE:HD11	2.48	0.48
1:I:410:ILE:HG23	1:I:411:PRO:HD2	1.95	0.48
3:B:201:TYR:C	3:B:201:TYR:CD1	2.86	0.48
3:F:99:LEU:HG	3:F:103:ILE:HD12	1.95	0.48
4:C:129:ASP:O	4:C:133:HIS:HD2	1.96	0.48
1:I:58:ASN:HD21	1:I:163:THR:N	1.98	0.48
1:A:188:HIS:HD2	3:B:106:TRP:HE1	1.60	0.48
3:J:53:TRP:CE3	3:J:68:VAL:HG21	2.49	0.48
3:F:203:ARG:O	3:F:204:MET:CB	2.62	0.48
1:I:80:PRO:HA	1:I:140:VAL:HG13	1.96	0.48
3:F:185:LEU:O	3:F:189:ILE:HG13	2.13	0.47
1:A:384:ASP:OD1	1:E:108:ARG:NH2	2.46	0.47
3:J:215:LYS:HA	1:E:381:TYR:CZ	2.49	0.47
3:J:39:LEU:HD11	3:J:104:GLY:HA3	1.97	0.47
1:I:105:PHE:CE2	1:I:107:PRO:HG3	2.50	0.47
1:E:275:GLY:CA	1:E:276:THR:CB	2.92	0.47
1:A:110:VAL:HB	1:A:268:LEU:HD11	1.97	0.47
3:F:192:HIS:HD2	1:E:164:ASP:OD2	1.98	0.47
3:B:199:PRO:HB2	3:B:201:TYR:CE2	2.49	0.47
4:K:20:ASP:O	4:K:21:LEU:CB	2.62	0.47
1:A:258:ILE:HG13	3:B:184:THR:HG22	1.97	0.47
3:F:42:TYR:OH	3:F:73:GLY:O	2.25	0.47
3:F:200:GLU:HG2	3:F:203:ARG:NH1	2.30	0.47
3:F:192:HIS:CD2	1:E:164:ASP:OD2	2.68	0.46
3:F:199:PRO:HB2	3:F:201:TYR:CE2	2.50	0.46
3:F:59:TRP:CZ2	3:F:203:ARG:HA	2.51	0.46
3:F:167:PRO:HG2	1:E:187:TRP:CZ2	2.50	0.46
1:I:55:VAL:O	1:I:155:ILE:HA	2.15	0.46
4:G:173:PRO:O	4:G:174:TYR:CB	2.63	0.46
3:J:151:VAL:HG12	3:J:152:VAL:N	2.29	0.46
1:A:132:TRP:CD1	1:A:155:ILE:HD12	2.50	0.46
1:I:58:ASN:ND2	1:I:125:ARG:HH21	2.13	0.46
3:B:177:GLU:HG3	1:I:410:ILE:HG12	1.97	0.46
1:A:273:THR:HB	1:A:274:GLU:HB2	1.97	0.46
3:B:98:VAL:HG12	3:B:99:LEU:N	2.29	0.46
1:E:79:ASN:OD1	1:E:81:ARG:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:LEU:HA	1:A:349:SER:CB	2.45	0.46
4:C:173:PRO:O	4:C:174:TYR:HB2	2.15	0.46
4:K:138:ARG:NH1	4:K:141:ASP:HA	2.31	0.46
1:E:339:PRO:O	1:E:340:ASP:C	2.54	0.46
3:F:98:VAL:HG12	3:F:99:LEU:N	2.30	0.46
1:I:40:MET:HE2	1:I:388:GLY:H	1.81	0.46
1:A:137:GLN:HE21	1:A:139:ASN:HD21	1.64	0.46
3:B:135:TRP:CD1	3:B:153:GLY:O	2.69	0.46
4:G:69:GLU:OE1	4:G:152:MET:HB2	2.15	0.46
1:E:334:GLN:HA	1:E:335:LYS:CB	2.38	0.46
1:I:275:GLY:CA	1:I:276:THR:CB	2.94	0.45
4:C:24:MET:HB2	4:C:109:GLN:HG2	1.98	0.45
4:C:53:SER:OG	4:C:139:ASP:CB	2.60	0.45
1:E:385:SER:H	1:I:261:GLN:HE22	1.63	0.45
4:C:20:ASP:O	4:C:21:LEU:HB2	2.15	0.45
1:E:96:ARG:HH21	1:E:99:GLN:HE22	1.63	0.45
3:B:59:TRP:CZ2	3:B:203:ARG:HA	2.51	0.45
3:J:39:LEU:HD22	3:J:100:GLY:HA2	1.97	0.45
4:G:53:SER:HA	4:G:58:PHE:CG	2.52	0.45
3:J:98:VAL:HG22	3:J:129:MET:CE	2.47	0.45
1:E:94:LEU:HB3	1:E:124:LEU:HB3	1.98	0.45
1:I:302:ILE:HG13	1:I:364:VAL:HB	1.98	0.45
1:E:68:HIS:CE1	1:E:404:GLU:OE1	2.57	0.45
1:E:220:PRO:HB2	1:E:221:ASP:H	1.51	0.45
3:J:39:LEU:HD22	3:J:100:GLY:CA	2.47	0.45
3:J:123:LEU:HD13	3:J:189:ILE:HG22	1.99	0.45
1:I:274:GLU:N	1:I:275:GLY:HA3	2.17	0.45
1:A:341:TYR:CG	1:A:342:LEU:HB2	2.51	0.45
1:E:341:TYR:CG	1:E:342:LEU:HB2	2.52	0.45
3:F:172:PHE:CE2	1:E:184:ILE:HD11	2.51	0.45
3:J:67:THR:HG22	3:J:68:VAL:N	2.31	0.45
1:A:308:ASN:O	1:A:357:GLY:N	2.50	0.45
4:K:184:LEU:HA	4:K:184:LEU:HD23	1.88	0.45
4:C:18:VAL:HG11	4:C:101:MET:HG3	1.98	0.45
1:A:348:LEU:CA	1:A:349:SER:CB	2.95	0.45
1:E:348:LEU:CA	1:E:349:SER:CB	2.95	0.45
1:A:358:GLU:HG2	1:A:359:SER:N	2.33	0.44
4:K:137:ILE:HG22	4:K:137:ILE:O	2.17	0.44
1:I:94:LEU:HG	1:I:155:ILE:HD11	1.99	0.44
1:A:199:ILE:HD11	3:B:96:PHE:HA	2.00	0.44
1:A:61:MET:O	1:A:61:MET:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ASN:OD1	1:A:81:ARG:HB2	2.17	0.44
4:G:154:TYR:HB2	4:G:155:PRO:HD3	2.00	0.44
3:J:105:GLU:O	3:J:109:ARG:HG2	2.17	0.44
1:E:297:GLY:O	1:E:372:ASP:HB2	2.18	0.44
1:I:293:TYR:CZ	1:I:411:PRO:HB3	2.53	0.44
1:E:289:ASN:ND2	1:E:305:LYS:HE2	2.33	0.44
1:A:225:GLY:HA2	1:A:229:ARG:HH21	1.80	0.44
3:J:132:PRO:HD3	3:J:164:ASN:ND2	2.33	0.44
1:A:184:ILE:HD11	3:B:172:PHE:CZ	2.52	0.44
1:A:79:ASN:C	1:A:81:ARG:H	2.20	0.44
1:I:93:VAL:HG11	1:I:132:TRP:CE2	2.52	0.44
4:K:38:VAL:O	4:K:42:GLU:HG2	2.17	0.44
1:A:164:ASP:HB3	1:A:165:PRO:CA	2.48	0.44
1:I:318:GLU:HB3	1:I:392:PHE:HB2	1.99	0.44
4:G:231:VAL:O	4:G:235:VAL:HG13	2.18	0.44
3:J:172:PHE:HE2	1:I:184:ILE:HD11	1.79	0.44
1:A:37:PHE:O	1:A:41:ARG:HG3	2.17	0.44
3:J:135:TRP:NE1	3:J:156:GLY:HA3	2.33	0.44
3:B:77:CYS:SG	3:B:98:VAL:HG23	2.58	0.43
3:B:81:GLN:HE21	3:B:137:ASP:HA	1.84	0.43
1:A:96:ARG:HD2	1:A:99:GLN:NE2	2.33	0.43
3:J:178:GLN:HG3	3:J:188:LEU:HD11	2.00	0.43
3:B:188:LEU:HA	3:B:188:LEU:HD12	1.86	0.43
1:A:320:THR:HG22	1:A:324:LEU:O	2.18	0.43
4:G:137:ILE:HD13	1:E:147:ILE:CD1	2.49	0.43
1:I:61:MET:HG3	1:I:61:MET:O	2.17	0.43
3:F:192:HIS:HA	1:E:96:ARG:O	2.18	0.43
1:E:273:THR:O	1:E:273:THR:OG1	2.36	0.43
3:F:185:LEU:HD22	1:E:176:LEU:HD21	2.01	0.43
1:I:167:THR:HG22	1:I:168:LEU:O	2.18	0.43
1:A:295:VAL:HA	1:A:296:PRO:HA	1.92	0.43
3:J:204:MET:H	3:J:207:ARG:HH12	1.65	0.43
1:E:295:VAL:HA	1:E:296:PRO:HA	1.90	0.43
4:C:184:LEU:HD23	4:C:184:LEU:HA	1.76	0.43
1:I:306:VAL:HG12	1:I:360:LYS:O	2.19	0.43
1:I:341:TYR:CG	1:I:342:LEU:HB2	2.53	0.43
3:B:143:SER:C	3:B:145:SER:N	2.67	0.43
3:J:59:TRP:CH2	3:J:203:ARG:O	2.71	0.43
1:I:98:ALA:HB3	1:I:123:ASN:HD22	1.82	0.43
4:K:139:ASP:OD1	1:I:30:GLY:HA2	2.19	0.43
3:F:90:LEU:HA	3:F:91:PRO:HD3	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:276:THR:CG2	1:I:279:VAL:HB	2.48	0.42
1:I:129:ALA:HA	1:I:155:ILE:O	2.19	0.42
4:G:190:PRO:C	4:G:192:MET:H	2.20	0.42
3:J:116:TRP:CD1	4:K:47:TRP:CZ3	3.07	0.42
3:B:98:VAL:O	3:B:102:MET:HG2	2.19	0.42
1:A:334:GLN:HG2	1:A:335:LYS:HB2	2.00	0.42
3:B:112:ASN:CG	4:C:128:GLN:HE21	2.22	0.42
4:C:196:ASN:HA	4:C:197:VAL:HA	1.81	0.42
1:A:107:PRO:HA	3:B:191:LEU:HD13	2.01	0.42
1:I:58:ASN:HD22	1:I:125:ARG:NH2	2.17	0.42
1:A:57:VAL:O	1:A:58:ASN:HB2	2.19	0.42
3:F:92:PHE:O	3:F:96:PHE:HB2	2.19	0.42
1:I:149:PRO:HB3	1:I:342:LEU:HD21	2.02	0.42
1:E:225:GLY:HA2	1:E:229:ARG:HH21	1.81	0.42
3:J:178:GLN:HG3	3:J:188:LEU:CD1	2.49	0.42
4:C:39:ARG:NH2	4:C:43:GLN:HB2	2.34	0.42
4:C:64:SER:O	4:C:68:THR:HB	2.20	0.42
4:K:196:ASN:HA	4:K:197:VAL:HA	1.87	0.42
1:E:333:THR:O	1:E:334:GLN:CB	2.68	0.42
4:K:88:ARG:HB2	4:K:170:THR:HB	2.01	0.42
3:F:44:VAL:HG23	4:G:122:ALA:HB1	2.00	0.42
3:J:241:ARG:O	3:J:244:SER:HB2	2.19	0.42
3:F:182:LEU:HD21	1:E:258:ILE:HD13	2.02	0.42
1:I:201:PHE:HZ	1:I:231:ILE:HD13	1.84	0.42
1:I:273:THR:CB	1:I:274:GLU:HB2	2.49	0.42
1:I:220:PRO:C	1:I:222:ASP:N	2.68	0.42
3:F:112:ASN:CG	4:G:128:GLN:HE21	2.23	0.42
3:F:56:TRP:CZ2	4:G:134:MET:HG3	2.55	0.42
3:B:116:TRP:CD1	4:C:47:TRP:CZ3	3.07	0.42
1:I:342:LEU:H	1:I:370:ARG:HD3	1.84	0.42
1:A:286:THR:OG1	1:A:403:ALA:HB1	2.19	0.42
1:I:37:PHE:O	1:I:41:ARG:HG3	2.20	0.42
4:C:137:ILE:O	4:C:137:ILE:HG22	2.20	0.42
1:I:56:ASN:O	1:I:57:VAL:C	2.56	0.42
1:I:108:ARG:HD2	1:I:262:ALA:HA	2.02	0.42
1:E:62:ILE:HG22	1:E:123:ASN:OD1	2.20	0.42
4:C:190:PRO:C	4:C:192:MET:H	2.23	0.42
1:I:297:GLY:O	1:I:372:ASP:HB2	2.20	0.42
3:B:53:TRP:O	3:B:60:LYS:NZ	2.53	0.41
3:F:201:TYR:C	3:F:201:TYR:CD1	2.93	0.41
1:I:201:PHE:CZ	1:I:231:ILE:HD13	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:TYR:CZ	1:A:342:LEU:HD22	2.56	0.41
1:E:276:THR:CG2	1:E:279:VAL:HB	2.50	0.41
4:K:246:ILE:HG21	4:K:249:GLU:OE2	2.19	0.41
1:I:102:GLY:HA3	1:I:268:LEU:HB3	2.02	0.41
1:I:275:GLY:CA	1:I:276:THR:HB	2.50	0.41
1:E:40:MET:HE2	1:E:387:VAL:HB	2.01	0.41
1:I:286:THR:OG1	1:I:403:ALA:HB1	2.20	0.41
4:G:129:ASP:O	4:G:133:HIS:HD2	2.02	0.41
1:A:51:SER:HB3	1:A:62:ILE:O	2.21	0.41
1:A:164:ASP:OD2	3:B:192:HIS:CD2	2.73	0.41
4:K:137:ILE:HD13	1:I:147:ILE:HD12	2.02	0.41
3:J:45:HIS:HE1	4:K:224:PHE:HA	1.85	0.41
1:I:73:TRP:HA	1:I:74:PRO:HD3	1.91	0.41
1:E:348:LEU:HA	1:E:349:SER:CB	2.50	0.41
3:B:92:PHE:O	3:B:96:PHE:HB2	2.20	0.41
1:A:129:ALA:HA	1:A:155:ILE:O	2.21	0.41
1:E:286:THR:HG21	1:E:391:LEU:HD12	2.02	0.41
4:C:154:TYR:HB2	4:C:155:PRO:HD3	2.03	0.41
1:I:295:VAL:HA	1:I:296:PRO:HA	1.92	0.41
3:B:59:TRP:CH2	3:B:203:ARG:O	2.74	0.41
1:E:294:LYS:O	1:E:297:GLY:HA2	2.21	0.41
1:I:83:SER:O	1:I:109:SER:HB2	2.21	0.41
3:B:56:TRP:CH2	4:C:134:MET:HG3	2.56	0.41
4:G:117:ALA:HB1	4:G:157:TYR:HB3	2.03	0.41
3:F:51:GLY:HA3	3:F:52:ASP:CB	2.26	0.41
3:B:98:VAL:HG11	3:B:130:ILE:HA	2.03	0.41
1:A:96:ARG:NH2	1:A:99:GLN:HE22	2.16	0.41
3:J:30:LEU:HD23	3:J:33:LEU:HD21	2.03	0.41
3:F:244:SER:O	4:G:236:LEU:HD12	2.20	0.41
3:B:60:LYS:HD3	3:B:65:TRP:CZ2	2.56	0.40
3:B:58:ASP:HB2	3:B:203:ARG:HH21	1.86	0.40
3:F:188:LEU:HA	3:F:188:LEU:HD12	1.97	0.40
4:G:190:PRO:O	4:G:193:ILE:HG13	2.21	0.40
3:J:162:TYR:O	3:J:163:PRO:C	2.56	0.40
4:C:117:ALA:HB1	4:C:157:TYR:HB3	2.02	0.40
1:E:163:THR:HG22	1:E:164:ASP:N	2.36	0.40
1:A:102:GLY:HA3	1:A:268:LEU:HB3	2.03	0.40
3:F:44:VAL:CG2	4:G:122:ALA:HB1	2.51	0.40
3:J:199:PRO:HB2	3:J:201:TYR:CE2	2.57	0.40
3:J:150:ALA:O	3:J:230:MET:HG2	2.22	0.40
1:I:48:VAL:HG21	1:I:149:PRO:CG	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:129:MET:O	3:J:132:PRO:HD2	2.21	0.40
1:E:51:SER:HB3	1:E:62:ILE:O	2.21	0.40
1:A:334:GLN:HG2	1:A:335:LYS:CB	2.52	0.40
3:J:172:PHE:CZ	1:I:184:ILE:HD11	2.57	0.40
3:F:241:ARG:O	3:F:244:SER:HB2	2.21	0.40
1:I:275:GLY:CA	1:I:276:THR:HG22	2.22	0.40
4:C:194:ILE:HA	4:C:195:PRO:HD3	2.00	0.40
4:C:39:ARG:HH22	4:C:43:GLN:HB2	1.86	0.40
4:K:102:ARG:O	4:K:106:VAL:HG23	2.22	0.40
1:A:383:THR:HG22	1:E:260:LEU:O	2.22	0.40
1:I:287:GLU:HB2	1:I:305:LYS:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	384/419 (92%)	338 (88%)	27 (7%)	19 (5%)	3 4
1	E	384/419 (92%)	340 (88%)	26 (7%)	18 (5%)	3 5
1	I	384/419 (92%)	330 (86%)	31 (8%)	23 (6%)	2 2
2	D	17/19 (90%)	13 (76%)	2 (12%)	2 (12%)	0 0
2	H	14/19 (74%)	12 (86%)	2 (14%)	0	100 100
3	B	240/252 (95%)	218 (91%)	16 (7%)	6 (2%)	7 16
3	F	240/252 (95%)	215 (90%)	22 (9%)	3 (1%)	15 35
3	J	240/252 (95%)	214 (89%)	19 (8%)	7 (3%)	6 13
4	C	206/256 (80%)	188 (91%)	10 (5%)	8 (4%)	4 7
4	G	207/256 (81%)	181 (87%)	18 (9%)	8 (4%)	4 7
4	K	207/256 (81%)	184 (89%)	16 (8%)	7 (3%)	5 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2523/2819 (90%)	2233 (88%)	189 (8%)	101 (4%)	4 7

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	GLU
1	A	164	ASP
1	A	220	PRO
1	A	221	ASP
1	A	274	GLU
1	A	276	THR
1	A	340	ASP
1	A	342	LEU
1	A	349	SER
2	D	4	ALA
3	J	52	ASP
3	J	201	TYR
3	B	201	TYR
3	F	12	PRO
3	F	52	ASP
4	C	229	LEU
4	G	49	ALA
4	G	229	LEU
4	K	229	LEU
1	E	51	SER
1	E	103	GLU
1	E	164	ASP
1	E	217	GLU
1	E	220	PRO
1	E	221	ASP
1	E	276	THR
1	E	334	GLN
1	E	340	ASP
1	E	342	LEU
1	E	349	SER
1	I	51	SER
1	I	103	GLU
1	I	164	ASP
1	I	220	PRO
1	I	221	ASP
1	I	274	GLU
1	I	276	THR

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Mol	Chain	Res	Type
1	I	335	LYS
1	I	340	ASP
1	I	342	LEU
1	I	349	SER
1	I	353	VAL
1	A	51	SER
1	A	217	GLU
1	A	353	VAL
3	J	204	MET
3	B	52	ASP
3	F	201	TYR
4	C	49	ALA
4	C	174	TYR
4	C	177	HIS
4	C	246	ILE
4	G	174	TYR
4	G	177	HIS
4	G	246	ILE
4	K	49	ALA
4	K	174	TYR
4	K	177	HIS
1	E	274	GLU
1	E	353	VAL
1	A	218	GLY
1	A	297	GLY
1	A	335	LYS
3	B	204	MET
4	G	195	PRO
4	K	179	TYR
1	E	297	GLY
1	E	335	LYS
1	I	217	GLU
1	I	218	GLY
1	I	264	LEU
1	I	334	GLN
1	I	350	ASN
1	A	334	GLN
1	A	350	ASN
4	C	179	TYR
4	C	191	PHE
4	C	195	PRO
4	G	191	PHE

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Mol	Chain	Res	Type
4	K	246	ILE
1	E	218	GLY
1	E	350	ASN
1	I	165	PRO
1	I	206	LYS
1	I	297	GLY
3	J	144	GLY
3	J	250	GLU
4	G	179	TYR
4	K	195	PRO
1	A	206	LYS
2	D	18	ALA
3	J	203	ARG
3	B	144	GLY
3	B	200	GLU
1	I	368	ASP
3	J	151	VAL
1	I	357	GLY
3	B	151	VAL
1	I	208	ILE
1	A	165	PRO
1	E	165	PRO

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	318/335 (95%)	305 (96%)	13 (4%)	37	66
1	E	318/335 (95%)	304 (96%)	14 (4%)	35	63
1	I	318/335 (95%)	304 (96%)	14 (4%)	35	63
3	B	201/208 (97%)	187 (93%)	14 (7%)	19	40
3	F	201/208 (97%)	186 (92%)	15 (8%)	17	36
3	J	201/208 (97%)	187 (93%)	14 (7%)	19	40
4	C	173/209 (83%)	163 (94%)	10 (6%)	25	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	G	174/209 (83%)	166 (95%)	8 (5%)	33 61
4	K	174/209 (83%)	165 (95%)	9 (5%)	29 55
All	All	2078/2256 (92%)	1967 (95%)	111 (5%)	28 54

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	97	THR
1	A	117	ASP
1	A	253	THR
1	A	266	LYS
1	A	285	THR
1	A	320	THR
1	A	340	ASP
1	A	348	LEU
1	A	349	SER
1	A	378	ASP
1	A	383	THR
1	A	414	VAL
3	J	33	LEU
3	J	39	LEU
3	J	42	TYR
3	J	48	LEU
3	J	52	ASP
3	J	67	THR
3	J	69	LEU
3	J	92	PHE
3	J	98	VAL
3	J	152	VAL
3	J	164	ASN
3	J	169	ILE
3	J	201	TYR
3	J	234	PHE
3	B	33	LEU
3	B	39	LEU
3	B	42	TYR
3	B	48	LEU
3	B	69	LEU
3	B	92	PHE
3	B	98	VAL

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Mol	Chain	Res	Type
3	B	152	VAL
3	B	164	ASN
3	B	169	ILE
3	B	192	HIS
3	B	201	TYR
3	B	220	VAL
3	B	234	PHE
3	F	33	LEU
3	F	39	LEU
3	F	42	TYR
3	F	48	LEU
3	F	69	LEU
3	F	88	PHE
3	F	92	PHE
3	F	98	VAL
3	F	138	VAL
3	F	152	VAL
3	F	164	ASN
3	F	169	ILE
3	F	201	TYR
3	F	220	VAL
3	F	234	PHE
4	C	68	THR
4	C	72	LEU
4	C	118	ILE
4	C	145	SER
4	C	147	ILE
4	C	177	HIS
4	C	183	PHE
4	C	229	LEU
4	C	235	VAL
4	C	246	ILE
4	G	36	LEU
4	G	72	LEU
4	G	118	ILE
4	G	145	SER
4	G	147	ILE
4	G	183	PHE
4	G	229	LEU
4	G	246	ILE
4	K	60	THR
4	K	68	THR

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Mol	Chain	Res	Type
4	K	72	LEU
4	K	118	ILE
4	K	145	SER
4	K	183	PHE
4	K	229	LEU
4	K	235	VAL
4	K	246	ILE
1	E	29	HIS
1	E	63	LEU
1	E	94	LEU
1	E	95	VAL
1	E	97	THR
1	E	99	GLN
1	E	253	THR
1	E	285	THR
1	E	320	THR
1	E	348	LEU
1	E	349	SER
1	E	378	ASP
1	E	383	THR
1	E	414	VAL
1	I	29	HIS
1	I	51	SER
1	I	97	THR
1	I	133	HIS
1	I	166	VAL
1	I	253	THR
1	I	266	LYS
1	I	285	THR
1	I	310	THR
1	I	320	THR
1	I	348	LEU
1	I	353	VAL
1	I	378	ASP
1	I	414	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	44	ASN
1	A	58	ASN

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Mol	Chain	Res	Type
1	A	68	HIS
1	A	99	GLN
1	A	137	GLN
1	A	188	HIS
1	A	261	GLN
3	J	45	HIS
3	B	192	HIS
3	F	45	HIS
3	F	174	GLN
3	F	192	HIS
4	C	109	GLN
4	C	128	GLN
4	C	177	HIS
4	G	109	GLN
4	G	128	GLN
4	G	177	HIS
4	K	109	GLN
4	K	128	GLN
4	K	177	HIS
1	E	44	ASN
1	E	58	ASN
1	E	68	HIS
1	E	99	GLN
1	E	104	GLN
1	E	188	HIS
1	E	261	GLN
1	E	265	GLN
1	I	58	ASN
1	I	68	HIS
1	I	99	GLN
1	I	139	ASN
1	I	188	HIS
1	I	261	GLN
1	I	386	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 11 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	CUA	A	420	1	0,1,1	0.00	-	0,0,0	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CUA	A	420	1	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

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	386/419 (92%)	0.51	38 (9%) 10 7	50, 69, 98, 114	0
1	E	386/419 (92%)	0.52	38 (9%) 10 7	48, 68, 101, 123	0
1	I	386/419 (92%)	0.45	49 (12%) 5 4	34, 50, 74, 90	0
2	D	19/19 (100%)	0.39	2 (10%) 8 6	78, 80, 83, 83	0
2	H	16/19 (84%)	1.52	5 (31%) 1 0	97, 99, 104, 104	0
3	B	242/252 (96%)	0.29	14 (5%) 26 24	43, 58, 90, 109	0
3	F	242/252 (96%)	0.44	17 (7%) 19 17	42, 57, 93, 117	0
3	J	242/252 (96%)	0.11	10 (4%) 41 39	40, 55, 89, 109	0
4	C	210/256 (82%)	0.56	21 (10%) 9 6	53, 69, 101, 114	0
4	G	211/256 (82%)	0.46	14 (6%) 22 19	53, 78, 112, 125	0
4	K	211/256 (82%)	0.50	18 (8%) 13 10	54, 72, 106, 119	0
All	All	2551/2819 (90%)	0.44	226 (8%) 12 9	34, 63, 100, 125	0

All (226) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	394	PHE	8.4
4	K	56	PRO	7.4
1	I	349	SER	7.4
1	I	365	LYS	7.0
3	B	11	GLY	6.9
3	F	248	ARG	6.7
3	J	13	PHE	6.3
4	K	48	ARG	6.3
4	K	60	THR	6.3
1	I	311	SER	6.1
3	F	251	GLN	5.6
1	A	222	ASP	5.6

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Mol	Chain	Res	Type	RSRZ
1	E	226	ASP	5.6
2	H	5	ALA	5.4
1	I	348	LEU	5.3
4	C	251	VAL	5.0
1	E	393	PHE	5.0
1	I	354	ILE	4.9
1	E	359	SER	4.9
1	I	351	ASP	4.9
1	E	396	PRO	4.8
1	A	399	LYS	4.8
2	H	6	ALA	4.7
1	I	316	LEU	4.7
1	E	275	GLY	4.7
1	I	364	VAL	4.7
1	A	398	GLY	4.6
1	I	350	ASN	4.5
3	F	11	GLY	4.4
3	F	250	GLU	4.3
4	K	197	VAL	4.2
4	C	19	VAL	4.2
4	K	59	GLN	4.1
1	I	332	PHE	4.1
3	F	249	ILE	4.0
1	E	402	ALA	3.9
1	A	397	ASP	3.9
4	C	85	TRP	3.9
4	G	48	ARG	3.8
4	C	250	GLY	3.8
1	E	353	VAL	3.8
3	B	251	GLN	3.7
3	F	252	ILE	3.6
1	I	357	GLY	3.6
4	G	67	TRP	3.6
1	E	205	ARG	3.6
3	B	231	MET	3.6
4	C	139	ASP	3.5
1	A	280	GLY	3.5
1	E	274	GLU	3.5
3	B	16	VAL	3.5
1	I	331	VAL	3.4
4	G	45	PHE	3.4
4	C	60	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	353	VAL	3.4
3	F	13	PHE	3.4
1	E	264	LEU	3.4
1	E	362	ILE	3.4
4	K	61	TYR	3.3
4	K	178	GLY	3.3
1	E	399	LYS	3.3
4	K	57	GLU	3.3
1	E	330	THR	3.3
1	E	219	ARG	3.3
1	I	273	THR	3.3
1	E	360	LYS	3.2
3	B	13	PHE	3.2
3	J	17	ALA	3.2
3	B	17	ALA	3.2
3	F	20	ALA	3.2
1	I	366	ILE	3.2
4	C	61	TYR	3.2
2	H	7	ALA	3.2
1	I	363	VAL	3.1
4	C	92	VAL	3.1
1	I	399	LYS	3.1
4	C	249	GLU	3.1
1	I	338	PHE	3.1
1	A	176	LEU	3.1
1	I	362	ILE	3.1
4	C	17	SER	3.1
3	F	17	ALA	3.1
3	F	245	THR	3.1
1	I	393	PHE	3.1
4	G	251	VAL	3.1
2	H	4	ALA	3.1
4	G	16	GLU	3.1
3	B	25	THR	3.1
3	F	22	CYS	3.1
1	I	353	VAL	3.1
1	A	312	GLN	3.1
1	E	304	VAL	3.0
1	A	363	VAL	3.0
1	E	400	ARG	3.0
1	E	252	SER	3.0
1	I	394	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
4	K	55	ALA	3.0
4	C	48	ARG	3.0
1	I	313	PRO	3.0
1	E	225	GLY	2.9
1	I	272	GLU	2.9
4	G	59	GLN	2.9
1	A	281	LYS	2.9
3	B	248	ARG	2.9
1	I	252	SER	2.9
1	I	310	THR	2.9
1	A	247	TYR	2.9
1	I	328	ASN	2.8
4	C	170	THR	2.8
1	I	314	VAL	2.8
1	E	315	ARG	2.8
4	K	62	TRP	2.8
1	E	351	ASP	2.8
4	C	252	ALA	2.8
4	K	196	ASN	2.7
3	F	247	LYS	2.7
1	A	340	ASP	2.7
1	A	354	ILE	2.7
3	B	224	PHE	2.7
1	A	359	SER	2.7
3	B	15	SER	2.7
1	I	356	PRO	2.7
4	G	64	SER	2.7
1	I	318	GLU	2.7
1	A	220	PRO	2.7
4	K	226	TRP	2.7
1	E	398	GLY	2.7
1	E	321	ALA	2.7
1	A	361	GLU	2.7
1	A	348	LEU	2.7
4	G	194	ILE	2.7
1	A	396	PRO	2.7
2	D	17	ALA	2.7
3	F	23	VAL	2.6
1	A	311	SER	2.6
1	A	283	GLN	2.6
1	I	340	ASP	2.6
1	A	179	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	279	VAL	2.6
3	B	172	PHE	2.6
2	D	5	ALA	2.6
1	E	395	THR	2.6
4	K	139	ASP	2.6
1	E	230	ARG	2.6
4	G	197	VAL	2.6
1	I	327	LEU	2.6
1	I	227	ASP	2.6
4	K	252	ALA	2.5
1	I	206	LYS	2.5
3	B	14	ASN	2.5
3	J	16	VAL	2.5
1	A	304	VAL	2.5
1	E	220	PRO	2.5
3	J	224	PHE	2.5
1	E	346	ARG	2.4
1	I	154	GLU	2.4
4	K	140	THR	2.4
3	B	20	ALA	2.4
1	E	78	ALA	2.4
1	I	330	THR	2.4
4	C	165	PHE	2.4
1	E	221	ASP	2.4
1	A	313	PRO	2.4
3	F	19	ALA	2.4
1	A	219	ARG	2.4
1	I	337	ASP	2.4
1	E	401	PHE	2.4
3	F	28	TRP	2.4
4	C	81	ALA	2.4
4	G	57	GLU	2.4
1	A	379	LEU	2.3
1	E	313	PRO	2.3
3	J	63	ARG	2.3
1	E	334	GLN	2.3
3	J	11	GLY	2.3
4	C	22	ARG	2.3
1	I	222	ASP	2.3
4	C	18	VAL	2.3
1	A	282	GLU	2.3
1	I	249	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	317	GLY	2.3
1	E	361	GLU	2.3
1	A	351	ASP	2.3
1	A	284	VAL	2.3
1	E	331	VAL	2.3
3	F	24	ALA	2.2
3	F	243	TYR	2.2
1	A	392	PHE	2.2
1	I	292	VAL	2.2
4	G	193	ILE	2.2
1	I	367	GLN	2.2
1	I	398	GLY	2.2
1	E	227	ASP	2.2
1	I	392	PHE	2.2
3	B	12	PRO	2.2
1	A	251	ASN	2.2
3	J	248	ARG	2.2
1	E	243	THR	2.2
1	E	284	VAL	2.2
4	K	194	ILE	2.1
4	G	224	PHE	2.1
1	I	326	PHE	2.1
2	H	9	ALA	2.1
1	A	332	PHE	2.1
4	C	88	ARG	2.1
4	K	192	MET	2.1
1	A	300	LEU	2.1
1	A	362	ILE	2.1
1	A	226	ASP	2.1
1	I	397	ASP	2.1
1	A	308	ASN	2.1
4	C	20	ASP	2.1
4	G	140	THR	2.1
1	A	302	ILE	2.1
1	I	205	ARG	2.1
1	I	312	GLN	2.0
4	G	230	GLY	2.0
1	I	307	LYS	2.0
3	J	211	ARG	2.0
3	J	252	ILE	2.0
1	A	164	ASP	2.0
4	C	187	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	220	PRO	2.0
4	K	85	TRP	2.0
3	J	19	ALA	2.0
4	C	94	ALA	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	ZN	I	421	1/1	0.97	0.28	0.42	70,70,70,70	0
5	CUA	A	420	2/2	0.96	0.11	-2.27	72,72,72,93	0
7	CU	E	420	1/1	0.96	0.04	-	63,63,63,63	0
7	CU	I	420	1/1	0.95	0.08	-	76,76,76,76	0
6	ZN	K	258	1/1	0.80	0.20	-	141,141,141,141	0
6	ZN	K	257	1/1	0.99	0.10	-	70,70,70,70	0
6	ZN	C	257	1/1	0.99	0.11	-	57,57,57,57	0
6	ZN	G	258	1/1	0.82	0.11	-	129,129,129,129	0
6	ZN	G	257	1/1	0.98	0.14	-	64,64,64,64	0
6	ZN	C	258	1/1	0.97	0.03	-	87,87,87,87	0
6	ZN	E	421	1/1	0.98	0.08	-	90,90,90,90	0
6	ZN	A	421	1/1	0.93	0.08	-	88,88,88,88	0

6.5 Other polymers (i)

There are no such residues in this entry.