Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2023 – 11:51 PM EDT

PDB ID	:	5JRW
Title	:	Crystal structure of Thermotoga maritima mutant D89R/D253R
Authors	:	Kowatz, T.; Maguire, M.
Deposited on	:	2016-05-06
Resolution	:	3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

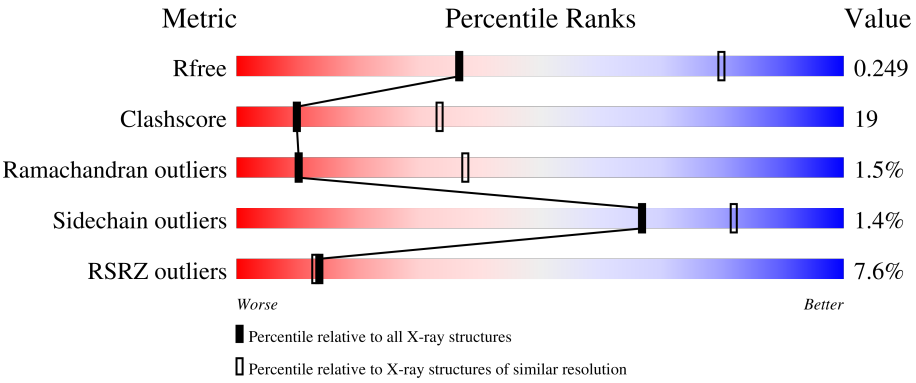
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	373	5% 59% 29% · 11%
1	B	373	4% 60% 28% · 11%
1	C	373	5% 57% 30% •• 10%
1	D	373	15% 56% 33% · 9%
1	E	373	5% 61% 27% · 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	B	402	-	-	-	X
2	MG	B	403	-	-	-	X
2	MG	D	401	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14026 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 Cobalt/magnesium transport protein CorA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2789	1819	457	503	10			
1	B	333	Total	C	N	O	S	0	0	0
			2789	1819	457	503	10			
1	C	334	Total	C	N	O	S	0	0	0
			2796	1823	458	505	10			
1	D	338	Total	C	N	O	S	0	0	0
			2822	1841	462	509	10			
1	E	338	Total	C	N	O	S	0	0	0
			2822	1841	462	509	10			

There are 125 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP Q9WZ31
A	-20	GLY	-	expression tag	UNP Q9WZ31
A	-19	SER	-	expression tag	UNP Q9WZ31
A	-18	SER	-	expression tag	UNP Q9WZ31
A	-17	HIS	-	expression tag	UNP Q9WZ31
A	-16	HIS	-	expression tag	UNP Q9WZ31
A	-15	HIS	-	expression tag	UNP Q9WZ31
A	-14	HIS	-	expression tag	UNP Q9WZ31
A	-13	HIS	-	expression tag	UNP Q9WZ31
A	-12	HIS	-	expression tag	UNP Q9WZ31
A	-11	SER	-	expression tag	UNP Q9WZ31
A	-10	SER	-	expression tag	UNP Q9WZ31
A	-9	GLY	-	expression tag	UNP Q9WZ31
A	-8	ARG	-	expression tag	UNP Q9WZ31
A	-7	GLU	-	expression tag	UNP Q9WZ31
A	-6	ASN	-	expression tag	UNP Q9WZ31
A	-5	LEU	-	expression tag	UNP Q9WZ31
A	-4	TYR	-	expression tag	UNP Q9WZ31
A	-3	PHE	-	expression tag	UNP Q9WZ31

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLN	-	expression tag	UNP Q9WZ31
A	-1	GLY	-	expression tag	UNP Q9WZ31
A	0	HIS	-	expression tag	UNP Q9WZ31
A	1	VAL	-	expression tag	UNP Q9WZ31
A	89	ARG	ASP	engineered mutation	UNP Q9WZ31
A	253	ARG	ASP	engineered mutation	UNP Q9WZ31
B	-21	MET	-	expression tag	UNP Q9WZ31
B	-20	GLY	-	expression tag	UNP Q9WZ31
B	-19	SER	-	expression tag	UNP Q9WZ31
B	-18	SER	-	expression tag	UNP Q9WZ31
B	-17	HIS	-	expression tag	UNP Q9WZ31
B	-16	HIS	-	expression tag	UNP Q9WZ31
B	-15	HIS	-	expression tag	UNP Q9WZ31
B	-14	HIS	-	expression tag	UNP Q9WZ31
B	-13	HIS	-	expression tag	UNP Q9WZ31
B	-12	HIS	-	expression tag	UNP Q9WZ31
B	-11	SER	-	expression tag	UNP Q9WZ31
B	-10	SER	-	expression tag	UNP Q9WZ31
B	-9	GLY	-	expression tag	UNP Q9WZ31
B	-8	ARG	-	expression tag	UNP Q9WZ31
B	-7	GLU	-	expression tag	UNP Q9WZ31
B	-6	ASN	-	expression tag	UNP Q9WZ31
B	-5	LEU	-	expression tag	UNP Q9WZ31
B	-4	TYR	-	expression tag	UNP Q9WZ31
B	-3	PHE	-	expression tag	UNP Q9WZ31
B	-2	GLN	-	expression tag	UNP Q9WZ31
B	-1	GLY	-	expression tag	UNP Q9WZ31
B	0	HIS	-	expression tag	UNP Q9WZ31
B	1	VAL	-	expression tag	UNP Q9WZ31
B	89	ARG	ASP	engineered mutation	UNP Q9WZ31
B	253	ARG	ASP	engineered mutation	UNP Q9WZ31
C	-21	MET	-	expression tag	UNP Q9WZ31
C	-20	GLY	-	expression tag	UNP Q9WZ31
C	-19	SER	-	expression tag	UNP Q9WZ31
C	-18	SER	-	expression tag	UNP Q9WZ31
C	-17	HIS	-	expression tag	UNP Q9WZ31
C	-16	HIS	-	expression tag	UNP Q9WZ31
C	-15	HIS	-	expression tag	UNP Q9WZ31
C	-14	HIS	-	expression tag	UNP Q9WZ31
C	-13	HIS	-	expression tag	UNP Q9WZ31
C	-12	HIS	-	expression tag	UNP Q9WZ31
C	-11	SER	-	expression tag	UNP Q9WZ31

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	SER	-	expression tag	UNP Q9WZ31
C	-9	GLY	-	expression tag	UNP Q9WZ31
C	-8	ARG	-	expression tag	UNP Q9WZ31
C	-7	GLU	-	expression tag	UNP Q9WZ31
C	-6	ASN	-	expression tag	UNP Q9WZ31
C	-5	LEU	-	expression tag	UNP Q9WZ31
C	-4	TYR	-	expression tag	UNP Q9WZ31
C	-3	PHE	-	expression tag	UNP Q9WZ31
C	-2	GLN	-	expression tag	UNP Q9WZ31
C	-1	GLY	-	expression tag	UNP Q9WZ31
C	0	HIS	-	expression tag	UNP Q9WZ31
C	1	VAL	-	expression tag	UNP Q9WZ31
C	89	ARG	ASP	engineered mutation	UNP Q9WZ31
C	253	ARG	ASP	engineered mutation	UNP Q9WZ31
D	-21	MET	-	expression tag	UNP Q9WZ31
D	-20	GLY	-	expression tag	UNP Q9WZ31
D	-19	SER	-	expression tag	UNP Q9WZ31
D	-18	SER	-	expression tag	UNP Q9WZ31
D	-17	HIS	-	expression tag	UNP Q9WZ31
D	-16	HIS	-	expression tag	UNP Q9WZ31
D	-15	HIS	-	expression tag	UNP Q9WZ31
D	-14	HIS	-	expression tag	UNP Q9WZ31
D	-13	HIS	-	expression tag	UNP Q9WZ31
D	-12	HIS	-	expression tag	UNP Q9WZ31
D	-11	SER	-	expression tag	UNP Q9WZ31
D	-10	SER	-	expression tag	UNP Q9WZ31
D	-9	GLY	-	expression tag	UNP Q9WZ31
D	-8	ARG	-	expression tag	UNP Q9WZ31
D	-7	GLU	-	expression tag	UNP Q9WZ31
D	-6	ASN	-	expression tag	UNP Q9WZ31
D	-5	LEU	-	expression tag	UNP Q9WZ31
D	-4	TYR	-	expression tag	UNP Q9WZ31
D	-3	PHE	-	expression tag	UNP Q9WZ31
D	-2	GLN	-	expression tag	UNP Q9WZ31
D	-1	GLY	-	expression tag	UNP Q9WZ31
D	0	HIS	-	expression tag	UNP Q9WZ31
D	1	VAL	-	expression tag	UNP Q9WZ31
D	89	ARG	ASP	engineered mutation	UNP Q9WZ31
D	253	ARG	ASP	engineered mutation	UNP Q9WZ31
E	-21	MET	-	expression tag	UNP Q9WZ31
E	-20	GLY	-	expression tag	UNP Q9WZ31
E	-19	SER	-	expression tag	UNP Q9WZ31

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-18	SER	-	expression tag	UNP Q9WZ31
E	-17	HIS	-	expression tag	UNP Q9WZ31
E	-16	HIS	-	expression tag	UNP Q9WZ31
E	-15	HIS	-	expression tag	UNP Q9WZ31
E	-14	HIS	-	expression tag	UNP Q9WZ31
E	-13	HIS	-	expression tag	UNP Q9WZ31
E	-12	HIS	-	expression tag	UNP Q9WZ31
E	-11	SER	-	expression tag	UNP Q9WZ31
E	-10	SER	-	expression tag	UNP Q9WZ31
E	-9	GLY	-	expression tag	UNP Q9WZ31
E	-8	ARG	-	expression tag	UNP Q9WZ31
E	-7	GLU	-	expression tag	UNP Q9WZ31
E	-6	ASN	-	expression tag	UNP Q9WZ31
E	-5	LEU	-	expression tag	UNP Q9WZ31
E	-4	TYR	-	expression tag	UNP Q9WZ31
E	-3	PHE	-	expression tag	UNP Q9WZ31
E	-2	GLN	-	expression tag	UNP Q9WZ31
E	-1	GLY	-	expression tag	UNP Q9WZ31
E	0	HIS	-	expression tag	UNP Q9WZ31
E	1	VAL	-	expression tag	UNP Q9WZ31
E	89	ARG	ASP	engineered mutation	UNP Q9WZ31
E	253	ARG	ASP	engineered mutation	UNP Q9WZ31

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	3	Total Mg 3 3	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0

- Molecule 3 is water.

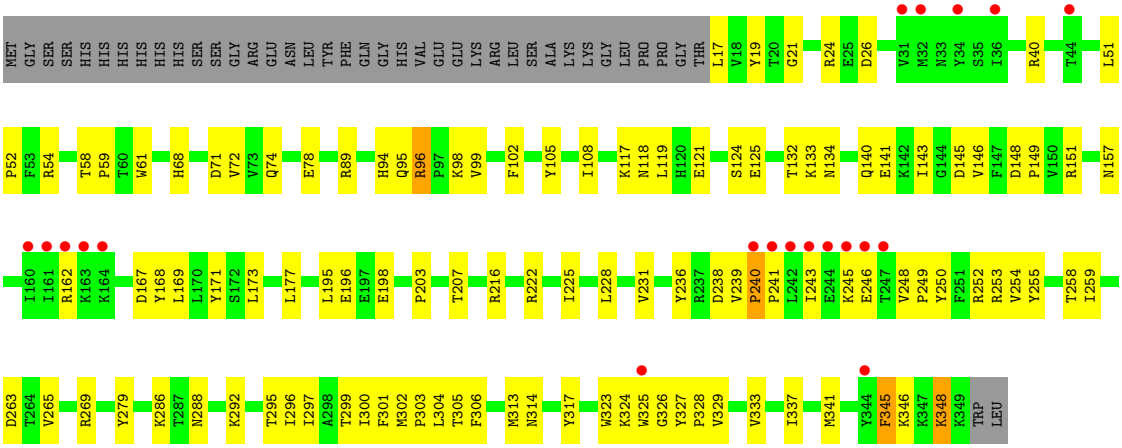
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total O 1 1	0	0
3	E	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

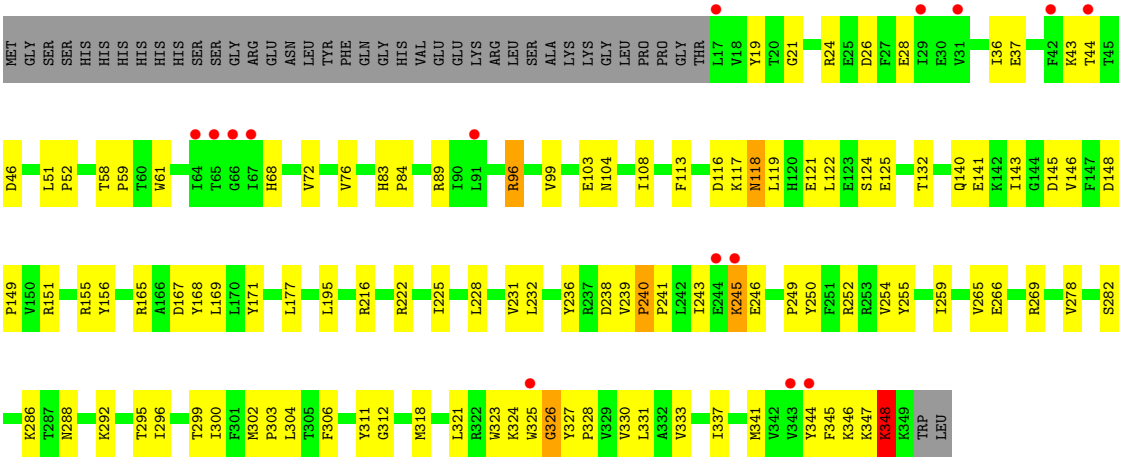
• Molecule 1: Cobalt/magnesium transport protein CorA

Chain A:



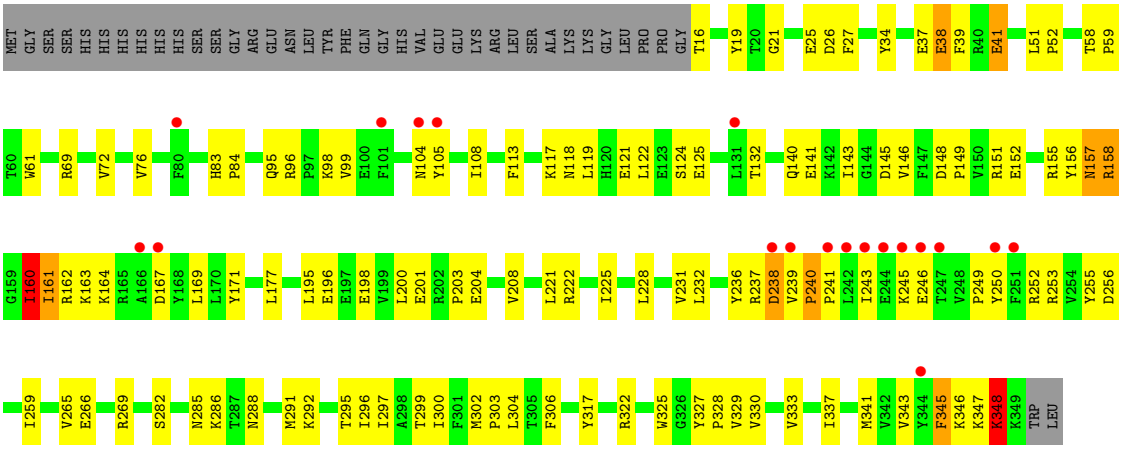
• Molecule 1: Cobalt/magnesium transport protein CorA

Chain B:



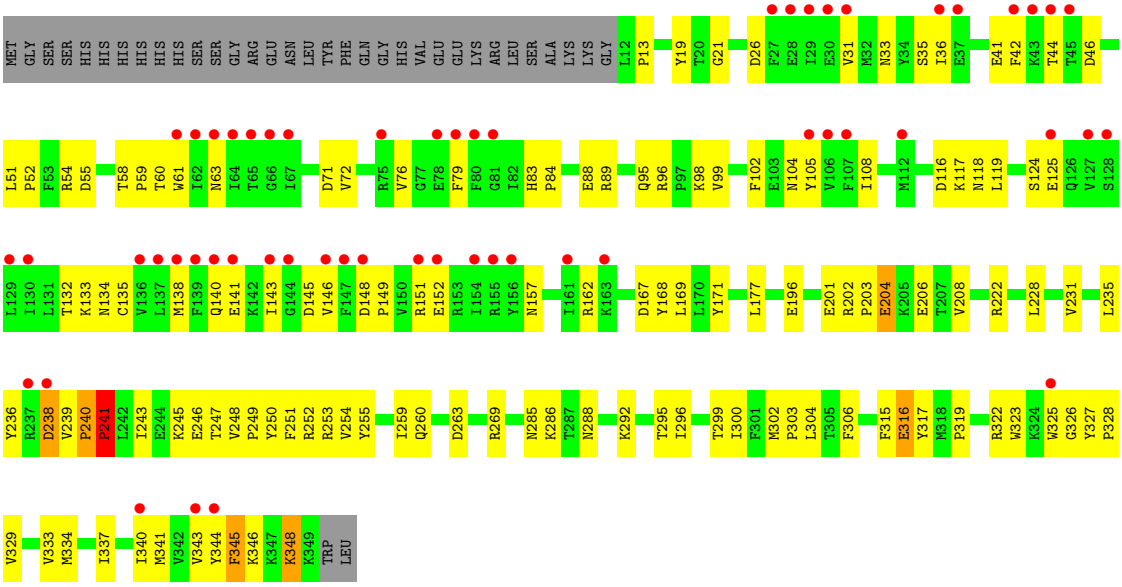
• Molecule 1: Cobalt/magnesium transport protein CorA

Chain C:



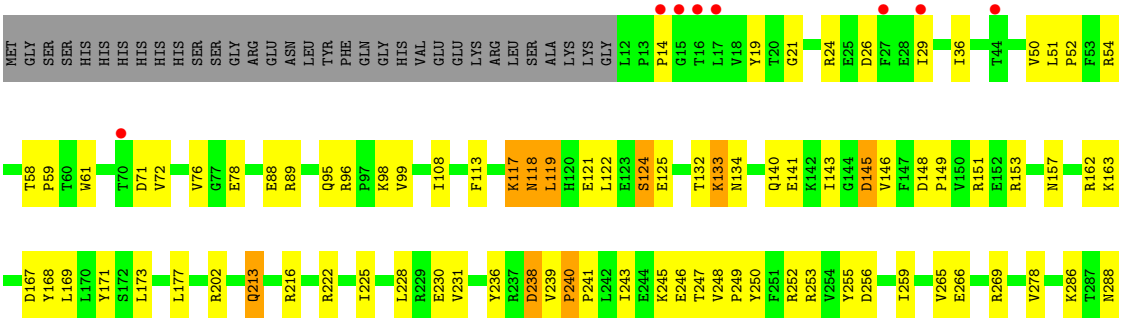
• Molecule 1: Cobalt/magnesium transport protein CorA

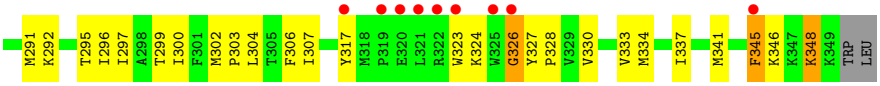
Chain D:



• Molecule 1: Cobalt/magnesium transport protein CorA

Chain E:




M291
K292
T295
I296
I297
A298
T299
I300
F301
M302
P303
L304
T305
F306
I307
Y317
M318
P319
E320
L321
R322
W323
K324
W325
G326
Y327
P328
V329
V330
V333
M334
I337
M341
F345
K346
K347
K348
K349
TRP
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	123.67Å 134.81Å 177.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 3.30 49.23 – 3.29	Depositor EDS
% Data completeness (in resolution range)	95.7 (49.00-3.30) 95.7 (49.23-3.29)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.237 , 0.274 0.212 , 0.249	Depositor DCC
R_{free} test set	1979 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å^2)	127.8	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 101.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	14026	wwPDB-VP
Average B, all atoms (Å^2)	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.43	0/2851	0.60	0/3863
1	B	0.48	0/2851	0.63	0/3863
1	C	0.49	0/2858	0.63	1/3873 (0.0%)
1	D	0.40	0/2886	0.59	0/3913
1	E	0.48	0/2886	0.63	1/3913 (0.0%)
All	All	0.46	0/14332	0.62	2/19425 (0.0%)

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	2
1	B	0	2
1	C	0	4
1	D	0	5
1	E	0	6
All	All	0	19

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	145	ASP	CB-CG-OD1	6.26	123.93	118.30
1	C	160	ILE	CB-CA-C	-5.06	101.48	111.60

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	345	PHE	Peptide
1	A	346	LYS	Peptide
1	B	312	GLY	Peptide
1	B	324	LYS	Peptide
1	C	16	THR	Peptide
1	C	160	ILE	Peptide
1	C	238	ASP	Peptide
1	C	345	PHE	Peptide
1	D	238	ASP	Peptide
1	D	241	PRO	Peptide
1	D	316	GLU	Peptide
1	D	345	PHE	Peptide
1	D	346	LYS	Peptide
1	E	238	ASP	Peptide
1	E	24	ARG	Peptide
1	E	323	TRP	Peptide
1	E	324	LYS	Peptide
1	E	345	PHE	Peptide
1	E	346	LYS	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	2789	0	2839	117	1
1	B	2789	0	2839	102	0
1	C	2796	0	2846	144	1
1	D	2822	0	2874	128	0
1	E	2822	0	2874	101	1
2	A	1	0	0	0	0
2	B	3	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
All	All	14026	0	14272	539	2

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 19.

All (539) 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:B:245:LYS:HB2	1:B:246:GLU:OE1	1.34	1.23
1:C:347:LYS:O	1:E:202:ARG:NH2	1.76	1.19
1:B:103:GLU:OE1	1:B:104:ASN:ND2	1.89	1.03
1:C:157:ASN:ND2	1:C:162:ARG:HD3	1.74	1.02
1:C:83:HIS:HD2	1:C:84:PRO:HD2	1.21	1.01
1:C:162:ARG:CZ	1:C:163:LYS:HE3	1.90	1.01
1:C:291:MET:HE2	1:E:291:MET:SD	2.01	1.01
1:D:202:ARG:HD3	1:D:204:GLU:OE1	1.62	0.99
1:B:83:HIS:HD2	1:B:84:PRO:HD2	1.24	0.99
1:C:37:GLU:O	1:C:38:GLU:HB3	1.60	0.98
1:D:54:ARG:NH1	1:D:55:ASP:OD1	1.96	0.98
1:D:315:PHE:O	1:D:316:GLU:HG2	1.63	0.95
1:B:245:LYS:CB	1:B:246:GLU:OE1	2.13	0.95
1:A:248:VAL:CG1	1:A:249:PRO:HD3	1.97	0.95
1:C:157:ASN:CG	1:C:162:ARG:HD3	1.87	0.95
1:A:117:LYS:O	1:A:118:ASN:OD1	1.85	0.94
1:C:157:ASN:O	1:C:158:ARG:O	1.86	0.93
1:D:171:TYR:CZ	1:D:250:TYR:HB3	2.04	0.93
1:C:119:LEU:HD12	1:C:119:LEU:O	1.69	0.91
1:A:248:VAL:HG13	1:A:249:PRO:HD3	1.50	0.91
1:E:171:TYR:CZ	1:E:250:TYR:HB3	2.05	0.91
1:C:117:LYS:O	1:C:118:ASN:OD1	1.87	0.91
1:C:238:ASP:OD1	1:C:239:VAL:N	2.04	0.91
1:E:238:ASP:OD1	1:E:239:VAL:N	2.02	0.91
1:A:171:TYR:CZ	1:A:250:TYR:HB3	2.06	0.90
1:C:171:TYR:CZ	1:C:250:TYR:HB3	2.06	0.89
1:C:83:HIS:HD2	1:C:84:PRO:CD	1.84	0.89
1:C:83:HIS:CD2	1:C:84:PRO:HD2	2.06	0.89
1:C:291:MET:CE	1:E:291:MET:SD	2.61	0.88
1:D:54:ARG:HD2	1:D:79:PHE:CE2	2.08	0.88
1:D:238:ASP:OD1	1:D:239:VAL:N	2.05	0.88
1:C:157:ASN:HD21	1:C:162:ARG:HD3	1.35	0.88
1:A:119:LEU:HD12	1:A:119:LEU:O	1.73	0.87
1:E:133:LYS:HG3	1:E:134:ASN:H	1.40	0.87
1:B:171:TYR:CZ	1:B:250:TYR:HB3	2.09	0.87
1:C:157:ASN:OD1	1:C:162:ARG:HD3	1.72	0.87
1:D:325:TRP:O	1:D:329:VAL:HG13	1.73	0.87
1:B:83:HIS:HD2	1:B:84:PRO:CD	1.87	0.86
1:B:83:HIS:CD2	1:B:84:PRO:HD2	2.11	0.86
1:C:117:LYS:O	1:C:118:ASN:CG	2.14	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:TYR:HB2	1:C:39:PHE:HD1	1.41	0.85
1:D:60:THR:HG23	1:D:135:CYS:SG	2.15	0.85
1:C:237:ARG:HD2	1:C:237:ARG:O	1.75	0.85
1:E:117:LYS:O	1:E:118:ASN:HB3	1.75	0.85
1:A:117:LYS:O	1:A:118:ASN:CG	2.16	0.84
1:C:157:ASN:HD21	1:C:162:ARG:CD	1.90	0.84
1:C:348:LYS:O	1:E:202:ARG:NH2	2.10	0.83
1:D:245:LYS:HB2	1:D:246:GLU:OE1	1.78	0.83
1:E:71:ASP:OD1	1:E:72:VAL:HG23	1.79	0.83
1:A:238:ASP:OD1	1:A:239:VAL:N	2.11	0.82
1:A:245:LYS:HB2	1:A:246:GLU:OE1	1.78	0.82
1:A:118:ASN:OD1	1:A:119:LEU:N	2.12	0.82
1:D:315:PHE:O	1:D:316:GLU:CG	2.26	0.81
1:C:160:ILE:HG22	1:C:161:ILE:N	1.95	0.80
1:A:71:ASP:OD1	1:A:72:VAL:HG23	1.81	0.80
1:B:117:LYS:O	1:B:118:ASN:CB	2.27	0.80
1:A:297:ILE:HG13	1:D:299:THR:OG1	1.82	0.80
1:A:119:LEU:HD13	1:A:121:GLU:CD	2.02	0.80
1:E:245:LYS:HB2	1:E:246:GLU:OE1	1.81	0.79
1:C:37:GLU:O	1:C:38:GLU:CB	2.30	0.79
1:B:36:ILE:HG23	1:B:37:GLU:HG2	1.65	0.79
1:D:240:PRO:HB2	1:D:241:PRO:CD	2.12	0.79
1:C:157:ASN:OD1	1:C:162:ARG:CD	2.32	0.78
1:D:71:ASP:OD1	1:D:72:VAL:HG23	1.82	0.78
1:A:323:TRP:O	1:A:325:TRP:N	2.18	0.77
1:B:240:PRO:HB2	1:B:241:PRO:HD3	1.68	0.76
1:C:157:ASN:ND2	1:C:162:ARG:HH11	1.82	0.76
1:E:240:PRO:HB2	1:E:241:PRO:HD3	1.66	0.76
1:C:240:PRO:HB2	1:C:241:PRO:HD3	1.68	0.75
1:D:63:ASN:OD1	1:D:138:MET:HE3	1.87	0.75
1:A:253:ARG:NH1	1:B:89:ARG:HG2	2.01	0.75
1:E:117:LYS:O	1:E:118:ASN:CB	2.35	0.75
1:C:95:GLN:HE21	1:C:98:LYS:HD3	1.52	0.74
1:B:292:LYS:CE	1:C:286:LYS:HE2	2.18	0.73
1:D:317:TYR:HD1	1:D:319:PRO:HD3	1.51	0.73
1:C:245:LYS:HB2	1:C:246:GLU:OE1	1.89	0.73
1:D:240:PRO:HB2	1:D:241:PRO:HD3	1.69	0.73
1:E:95:GLN:HE21	1:E:98:LYS:HD3	1.53	0.73
1:C:156:TYR:O	1:C:157:ASN:HB2	1.87	0.73
1:D:71:ASP:OD1	1:D:72:VAL:N	2.22	0.72
1:A:171:TYR:CE1	1:A:250:TYR:HB3	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:GLU:O	1:C:37:GLU:HG2	1.88	0.72
1:D:171:TYR:CE1	1:D:250:TYR:HB3	2.24	0.72
1:E:71:ASP:OD1	1:E:72:VAL:N	2.22	0.71
1:D:95:GLN:HE21	1:D:98:LYS:HD3	1.56	0.71
1:E:171:TYR:CE1	1:E:250:TYR:HB3	2.25	0.71
1:C:171:TYR:CE1	1:C:250:TYR:HB3	2.25	0.71
1:A:240:PRO:HB2	1:A:241:PRO:HD3	1.71	0.70
1:B:103:GLU:OE1	1:B:104:ASN:CG	2.29	0.70
1:D:171:TYR:CE1	1:D:250:TYR:C	2.65	0.70
1:C:162:ARG:HG3	1:C:163:LYS:N	2.07	0.70
1:B:83:HIS:CD2	1:B:84:PRO:CD	2.73	0.70
1:B:171:TYR:CE1	1:B:250:TYR:HB3	2.26	0.69
1:C:83:HIS:CD2	1:C:84:PRO:CD	2.70	0.69
1:C:157:ASN:O	1:C:158:ARG:C	2.29	0.69
1:A:71:ASP:OD1	1:A:72:VAL:N	2.24	0.69
1:A:74:GLN:O	1:A:78:GLU:HG2	1.91	0.69
1:E:54:ARG:O	1:E:133:LYS:HD2	1.92	0.69
1:E:240:PRO:HB2	1:E:241:PRO:CD	2.22	0.69
1:B:117:LYS:O	1:B:118:ASN:HB2	1.91	0.68
1:C:162:ARG:NE	1:C:163:LYS:HE3	2.07	0.68
1:A:301:PHE:CZ	1:D:303:PRO:HB3	2.28	0.68
1:A:313:MET:HA	1:B:311:TYR:O	1.93	0.68
1:C:240:PRO:HB2	1:C:241:PRO:CD	2.24	0.68
1:B:240:PRO:HB2	1:B:241:PRO:CD	2.22	0.68
1:A:228:LEU:O	1:A:231:VAL:HG22	1.94	0.67
1:B:346:LYS:HG3	1:B:346:LYS:O	1.94	0.67
1:C:256:ASP:OD2	1:E:89:ARG:NH1	2.25	0.67
1:D:133:LYS:HG3	1:D:134:ASN:N	2.10	0.67
1:D:317:TYR:CD1	1:D:319:PRO:HD3	2.29	0.67
1:C:157:ASN:HD21	1:C:162:ARG:HH11	1.42	0.67
1:C:343:VAL:O	1:C:346:LYS:HG3	1.94	0.67
1:A:255:TYR:O	1:A:258:THR:HG22	1.95	0.67
1:A:304:LEU:HB3	1:D:306:PHE:CE1	2.30	0.67
1:D:323:TRP:NE1	1:D:325:TRP:HB2	2.10	0.66
1:D:228:LEU:O	1:D:231:VAL:HG22	1.96	0.66
1:E:171:TYR:CE1	1:E:250:TYR:C	2.69	0.66
1:C:171:TYR:CE1	1:C:250:TYR:C	2.70	0.66
1:A:54:ARG:O	1:A:133:LYS:HD2	1.96	0.65
1:B:155:ARG:HD2	1:B:156:TYR:CE2	2.31	0.65
1:C:253:ARG:NE	1:E:88:GLU:OE2	2.29	0.65
1:B:292:LYS:HE2	1:C:286:LYS:HE2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:TYR:CE1	1:A:250:TYR:C	2.70	0.65
1:B:228:LEU:O	1:B:231:VAL:HG22	1.97	0.65
1:C:117:LYS:HG2	1:C:118:ASN:H	1.61	0.64
1:D:171:TYR:HE1	1:D:250:TYR:O	1.81	0.64
1:E:228:LEU:O	1:E:231:VAL:HG22	1.96	0.64
1:C:61:TRP:HB2	1:C:169:LEU:HD21	1.80	0.64
1:C:228:LEU:O	1:C:231:VAL:HG22	1.97	0.64
1:A:133:LYS:HG3	1:A:134:ASN:H	1.63	0.63
1:C:317:TYR:O	1:C:317:TYR:CD2	2.51	0.63
1:A:26:ASP:OD2	1:A:143:ILE:HG22	1.99	0.63
1:A:248:VAL:HG12	1:A:249:PRO:HD3	1.78	0.63
1:D:26:ASP:OD2	1:D:143:ILE:HG22	1.99	0.63
1:C:238:ASP:C	1:C:239:VAL:HG22	2.19	0.63
1:D:117:LYS:O	1:D:118:ASN:HB2	1.98	0.63
1:D:235:LEU:HD23	1:D:251:PHE:CE1	2.34	0.63
1:A:240:PRO:HB2	1:A:241:PRO:CD	2.28	0.63
1:D:304:LEU:HD21	1:D:337:ILE:HG23	1.79	0.63
1:B:171:TYR:CE1	1:B:250:TYR:C	2.71	0.63
1:D:60:THR:CG2	1:D:135:CYS:SG	2.87	0.62
1:C:157:ASN:ND2	1:C:162:ARG:NH1	2.46	0.62
1:B:330:VAL:HA	1:B:333:VAL:HG12	1.81	0.62
1:A:40:ARG:HB2	1:A:40:ARG:CZ	2.29	0.62
1:C:162:ARG:NH2	1:C:163:LYS:HE3	2.15	0.61
1:B:26:ASP:OD2	1:B:143:ILE:HG22	2.00	0.61
1:B:171:TYR:HE1	1:B:250:TYR:O	1.83	0.61
1:E:26:ASP:OD2	1:E:143:ILE:HG22	2.00	0.61
1:C:26:ASP:OD2	1:C:143:ILE:HG22	2.01	0.61
1:C:157:ASN:ND2	1:C:162:ARG:CD	2.52	0.61
1:E:119:LEU:O	1:E:121:GLU:N	2.32	0.61
1:B:61:TRP:HB2	1:B:169:LEU:HD21	1.83	0.61
1:C:291:MET:HE3	1:E:291:MET:SD	2.40	0.61
1:E:337:ILE:O	1:E:341:MET:HG2	2.01	0.61
1:A:286:LYS:NZ	1:D:348:LYS:HG2	2.16	0.61
1:A:171:TYR:HE1	1:A:250:TYR:O	1.83	0.61
1:C:341:MET:HE2	1:C:341:MET:HA	1.82	0.61
1:E:171:TYR:HE1	1:E:250:TYR:O	1.82	0.61
1:E:330:VAL:HA	1:E:333:VAL:HG12	1.82	0.61
1:A:286:LYS:HE3	1:D:292:LYS:NZ	2.16	0.60
1:A:337:ILE:O	1:A:341:MET:HG2	2.01	0.60
1:D:33:ASN:ND2	1:D:60:THR:HB	2.15	0.60
1:D:133:LYS:HG3	1:D:134:ASN:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:VAL:HA	1:C:333:VAL:HG12	1.82	0.60
1:C:337:ILE:O	1:C:341:MET:HG2	2.00	0.60
1:A:248:VAL:HG13	1:A:249:PRO:CD	2.27	0.60
1:B:299:THR:HG21	1:B:345:PHE:HZ	1.66	0.59
1:C:171:TYR:HE1	1:C:250:TYR:O	1.84	0.59
1:D:238:ASP:C	1:D:239:VAL:HG22	2.23	0.59
1:C:160:ILE:HG23	1:C:163:LYS:HB2	1.84	0.59
1:C:104:ASN:HB2	1:C:105:TYR:HD2	1.66	0.59
1:D:152:GLU:CD	1:D:152:GLU:O	2.41	0.59
1:D:61:TRP:HB2	1:D:169:LEU:HD21	1.84	0.59
1:D:299:THR:HG21	1:D:345:PHE:HZ	1.68	0.59
1:E:238:ASP:C	1:E:239:VAL:HG22	2.24	0.59
1:D:337:ILE:O	1:D:341:MET:HG2	2.03	0.58
1:A:317:TYR:O	1:A:317:TYR:CD2	2.57	0.58
1:C:325:TRP:O	1:C:329:VAL:HG23	2.02	0.58
1:B:337:ILE:O	1:B:341:MET:HG2	2.02	0.58
1:B:306:PHE:CE1	1:C:304:LEU:HB3	2.38	0.58
1:C:196:GLU:OE1	1:E:216:ARG:NH1	2.37	0.58
1:E:19:TYR:CZ	1:E:21:GLY:HA3	2.39	0.58
1:A:327:TYR:HB3	1:A:328:PRO:HD3	1.86	0.58
1:E:299:THR:HG21	1:E:345:PHE:HZ	1.69	0.58
1:A:198:GLU:OE1	1:A:207:THR:HG22	2.03	0.58
1:A:61:TRP:CD1	1:A:173:LEU:HD11	2.39	0.58
1:D:315:PHE:C	1:D:316:GLU:HG2	2.25	0.57
1:A:118:ASN:OD1	1:A:119:LEU:HG	2.04	0.57
1:A:305:THR:HG22	1:D:306:PHE:HA	1.86	0.57
1:C:162:ARG:HG3	1:C:163:LYS:H	1.69	0.57
1:C:255:TYR:CE2	1:C:259:ILE:HD11	2.39	0.57
1:B:292:LYS:NZ	1:C:286:LYS:HE2	2.20	0.57
1:C:157:ASN:OD1	1:C:162:ARG:NE	2.36	0.57
1:D:340:ILE:O	1:D:343:VAL:HG22	2.04	0.57
1:E:61:TRP:CD1	1:E:173:LEU:HD11	2.39	0.57
1:A:148:ASP:N	1:A:149:PRO:HD2	2.18	0.57
1:C:118:ASN:OD1	1:C:119:LEU:HG	2.05	0.57
1:C:291:MET:HE2	1:E:291:MET:CE	2.35	0.57
1:E:239:VAL:HG23	1:E:239:VAL:O	2.05	0.57
1:C:239:VAL:HG23	1:C:239:VAL:O	2.04	0.57
1:D:63:ASN:OD1	1:D:138:MET:CE	2.53	0.57
1:D:171:TYR:CE1	1:D:250:TYR:O	2.58	0.57
1:D:239:VAL:O	1:D:239:VAL:HG23	2.04	0.56
1:B:239:VAL:HG23	1:B:239:VAL:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:TYR:CE2	1:B:259:ILE:HD11	2.41	0.56
1:A:148:ASP:OD1	1:A:151:ARG:NH1	2.38	0.56
1:D:35:SER:O	1:D:162:ARG:NH2	2.37	0.56
1:E:255:TYR:CE2	1:E:259:ILE:HD11	2.41	0.56
1:C:162:ARG:HG3	1:C:163:LYS:HG3	1.87	0.56
1:A:299:THR:HG21	1:A:345:PHE:HZ	1.70	0.56
1:C:160:ILE:HG21	1:C:164:LYS:HG2	1.88	0.56
1:C:295:THR:O	1:C:299:THR:HG22	2.06	0.56
1:D:255:TYR:CE2	1:D:259:ILE:HD11	2.40	0.56
1:E:295:THR:O	1:E:299:THR:HG22	2.06	0.56
1:E:327:TYR:HB3	1:E:328:PRO:HD3	1.87	0.56
1:A:239:VAL:HG23	1:A:239:VAL:O	2.04	0.56
1:A:61:TRP:HB2	1:A:169:LEU:HD21	1.88	0.56
1:A:95:GLN:HE21	1:A:98:LYS:HD2	1.69	0.56
1:D:54:ARG:HG3	1:D:55:ASP:OD1	2.05	0.56
1:E:61:TRP:HB2	1:E:169:LEU:HD21	1.88	0.56
1:B:167:ASP:OD2	1:B:243:ILE:HG12	2.06	0.55
1:E:58:THR:HB	1:E:59:PRO:HD2	1.87	0.55
1:D:19:TYR:CZ	1:D:21:GLY:HA3	2.41	0.55
1:A:99:VAL:CG2	1:A:231:VAL:HB	2.37	0.55
1:A:167:ASP:OD2	1:A:243:ILE:HG12	2.07	0.55
1:C:327:TYR:HB3	1:C:328:PRO:HD3	1.87	0.55
1:D:167:ASP:OD2	1:D:243:ILE:HG12	2.06	0.55
1:E:148:ASP:OD1	1:E:151:ARG:NH1	2.40	0.55
1:A:304:LEU:HD23	1:A:337:ILE:HD11	1.89	0.55
1:C:58:THR:HB	1:C:59:PRO:HD2	1.89	0.55
1:B:327:TYR:HB3	1:B:328:PRO:HD3	1.88	0.55
1:C:19:TYR:CZ	1:C:21:GLY:HA3	2.42	0.55
1:C:200:LEU:O	1:C:201:GLU:HG3	2.07	0.55
1:D:243:ILE:HD12	1:D:246:GLU:OE1	2.06	0.55
1:E:167:ASP:OD2	1:E:243:ILE:HG12	2.06	0.55
1:D:327:TYR:HB3	1:D:328:PRO:HD3	1.88	0.55
1:E:51:LEU:N	1:E:52:PRO:CD	2.70	0.55
1:A:133:LYS:O	1:A:134:ASN:ND2	2.40	0.54
1:C:167:ASP:OD2	1:C:243:ILE:HG12	2.07	0.54
1:C:171:TYR:CE1	1:C:250:TYR:O	2.61	0.54
1:D:54:ARG:HD2	1:D:79:PHE:HE2	1.70	0.54
1:B:99:VAL:CG2	1:B:231:VAL:HB	2.38	0.54
1:B:122:LEU:HD12	1:B:122:LEU:O	2.07	0.54
1:C:299:THR:HG21	1:C:345:PHE:HZ	1.72	0.54
1:A:238:ASP:C	1:A:239:VAL:HG22	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:TYR:CZ	1:B:21:GLY:HA3	2.43	0.54
1:A:19:TYR:CZ	1:A:21:GLY:HA3	2.42	0.54
1:A:89:ARG:NH1	1:D:253:ARG:HH11	2.05	0.54
1:E:171:TYR:CE1	1:E:250:TYR:O	2.60	0.54
1:A:58:THR:HB	1:A:59:PRO:HD2	1.90	0.54
1:A:255:TYR:CE2	1:A:259:ILE:HD11	2.42	0.54
1:C:148:ASP:N	1:C:149:PRO:HD2	2.23	0.54
1:D:295:THR:O	1:D:299:THR:HG22	2.08	0.54
1:E:99:VAL:CG2	1:E:231:VAL:HB	2.38	0.54
1:E:243:ILE:HD12	1:E:246:GLU:OE1	2.08	0.54
1:D:58:THR:HB	1:D:59:PRO:HD2	1.90	0.54
1:A:243:ILE:HD12	1:A:246:GLU:OE1	2.08	0.54
1:B:243:ILE:HD12	1:B:246:GLU:OE1	2.07	0.54
1:C:160:ILE:CG2	1:C:161:ILE:N	2.67	0.54
1:D:246:GLU:O	1:D:249:PRO:HD2	2.08	0.54
1:A:295:THR:O	1:A:299:THR:HG22	2.07	0.53
1:C:243:ILE:HD12	1:C:246:GLU:OE1	2.07	0.53
1:D:157:ASN:CG	1:D:162:ARG:HG3	2.27	0.53
1:B:58:THR:HB	1:B:59:PRO:HD2	1.90	0.53
1:B:171:TYR:CE1	1:B:250:TYR:O	2.61	0.53
1:D:88:GLU:OE2	1:E:253:ARG:NE	2.42	0.53
1:D:201:GLU:OE1	1:D:202:ARG:NH1	2.41	0.53
1:A:279:TYR:OH	1:D:285:ASN:ND2	2.41	0.53
1:A:313:MET:HG2	1:B:311:TYR:O	2.08	0.53
1:B:323:TRP:CD1	1:B:325:TRP:O	2.61	0.53
1:C:51:LEU:N	1:C:52:PRO:CD	2.72	0.53
1:C:246:GLU:O	1:C:249:PRO:HD2	2.08	0.53
1:E:113:PHE:CE1	1:E:124:SER:HB2	2.44	0.53
1:A:51:LEU:N	1:A:52:PRO:CD	2.71	0.53
1:E:246:GLU:O	1:E:249:PRO:HD2	2.09	0.53
1:A:157:ASN:CG	1:A:162:ARG:HG3	2.29	0.53
1:B:246:GLU:O	1:B:249:PRO:HD2	2.07	0.53
1:D:323:TRP:CE2	1:D:325:TRP:HB2	2.44	0.53
1:A:246:GLU:O	1:A:249:PRO:HD2	2.08	0.53
1:E:122:LEU:HD12	1:E:122:LEU:O	2.08	0.53
1:A:171:TYR:CE1	1:A:250:TYR:O	2.62	0.53
1:A:304:LEU:CD2	1:A:337:ILE:HD11	2.38	0.53
1:B:295:THR:O	1:B:299:THR:HG22	2.09	0.53
1:E:317:TYR:O	1:E:317:TYR:CD2	2.61	0.53
1:C:118:ASN:OD1	1:C:119:LEU:N	2.41	0.52
1:C:237:ARG:HD2	1:C:237:ARG:C	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:ASP:OD1	1:D:151:ARG:NH1	2.41	0.52
1:E:307:ILE:HG22	1:E:334:MET:HE3	1.91	0.52
1:E:113:PHE:CD1	1:E:122:LEU:HD13	2.44	0.52
1:B:299:THR:OG1	1:C:297:ILE:HG13	2.10	0.52
1:C:99:VAL:CG2	1:C:231:VAL:HB	2.39	0.52
1:A:17:LEU:HD23	1:A:74:GLN:HG3	1.91	0.52
1:B:44:THR:HB	1:B:46:ASP:H	1.75	0.52
1:C:125:GLU:HG3	1:C:141:GLU:HB2	1.91	0.52
1:D:31:VAL:O	1:D:41:GLU:HA	2.10	0.52
1:B:148:ASP:OD1	1:B:151:ARG:NH1	2.43	0.52
1:D:99:VAL:CG2	1:D:231:VAL:HB	2.40	0.52
1:D:116:ASP:O	1:D:119:LEU:O	2.28	0.52
1:D:171:TYR:CE2	1:D:250:TYR:HB3	2.44	0.52
1:C:148:ASP:OD1	1:C:151:ARG:NH1	2.41	0.51
1:D:171:TYR:HE1	1:D:250:TYR:C	2.14	0.51
1:C:292:LYS:NZ	1:E:286:LYS:HE2	2.25	0.51
1:E:148:ASP:N	1:E:149:PRO:HD2	2.25	0.51
1:B:238:ASP:C	1:B:239:VAL:HG22	2.30	0.51
1:D:315:PHE:O	1:D:316:GLU:CD	2.48	0.51
1:A:300:ILE:O	1:A:304:LEU:HG	2.11	0.51
1:B:326:GLY:H	1:B:328:PRO:HD2	1.76	0.51
1:C:113:PHE:CD1	1:C:122:LEU:HD13	2.46	0.51
1:C:171:TYR:CE2	1:C:250:TYR:HB3	2.46	0.51
1:D:304:LEU:HD21	1:D:337:ILE:CG2	2.40	0.51
1:A:286:LYS:HE3	1:D:292:LYS:HZ1	1.75	0.51
1:B:51:LEU:N	1:B:52:PRO:CD	2.74	0.51
1:D:89:ARG:NH1	1:E:256:ASP:OD2	2.44	0.51
1:A:288:ASN:HD21	1:A:292:LYS:NZ	2.09	0.50
1:B:119:LEU:HB3	1:B:121:GLU:HG2	1.93	0.50
1:B:278:VAL:HG13	1:C:208:VAL:CG1	2.40	0.50
1:D:44:THR:HB	1:D:46:ASP:H	1.76	0.50
1:D:300:ILE:O	1:D:304:LEU:HG	2.12	0.50
1:B:116:ASP:OD2	1:B:119:LEU:HD22	2.11	0.50
1:B:240:PRO:CB	1:B:241:PRO:CD	2.90	0.50
1:D:51:LEU:N	1:D:52:PRO:CD	2.74	0.50
1:D:148:ASP:N	1:D:149:PRO:HD2	2.26	0.50
1:D:302:MET:N	1:D:303:PRO:HD2	2.27	0.50
1:E:300:ILE:O	1:E:304:LEU:HG	2.11	0.50
1:D:35:SER:O	1:D:162:ARG:NE	2.42	0.50
1:B:125:GLU:HG3	1:B:141:GLU:HB2	1.94	0.50
1:B:148:ASP:N	1:B:149:PRO:HD2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:LYS:HG3	1:E:134:ASN:N	2.17	0.50
1:E:125:GLU:HG3	1:E:141:GLU:HB2	1.94	0.50
1:B:300:ILE:O	1:B:304:LEU:HG	2.10	0.49
1:A:306:PHE:CE1	1:B:304:LEU:HB3	2.47	0.49
1:A:301:PHE:O	1:A:305:THR:HG23	2.13	0.49
1:A:286:LYS:HZ3	1:D:348:LYS:HG2	1.77	0.49
1:A:125:GLU:HG3	1:A:141:GLU:HB2	1.94	0.49
1:D:326:GLY:O	1:D:329:VAL:HG22	2.13	0.49
1:E:302:MET:N	1:E:303:PRO:HD2	2.27	0.49
1:D:304:LEU:HB3	1:E:306:PHE:CE1	2.47	0.49
1:C:300:ILE:O	1:C:304:LEU:HG	2.12	0.49
1:C:146:VAL:HG21	1:C:177:LEU:HA	1.94	0.49
1:C:240:PRO:CB	1:C:241:PRO:CD	2.91	0.49
1:C:162:ARG:NH2	1:C:163:LYS:NZ	2.61	0.48
1:B:167:ASP:OD1	1:B:168:TYR:N	2.47	0.48
1:C:104:ASN:HB2	1:C:105:TYR:CD2	2.47	0.48
1:D:243:ILE:O	1:D:243:ILE:HG13	2.14	0.48
1:A:329:VAL:O	1:A:333:VAL:HG23	2.14	0.48
1:B:165:ARG:CZ	1:B:243:ILE:HG21	2.43	0.48
1:D:167:ASP:OD1	1:D:168:TYR:N	2.46	0.48
1:D:329:VAL:O	1:D:333:VAL:HG23	2.14	0.48
1:C:27:PHE:CD2	1:C:69:ARG:HG3	2.49	0.48
1:D:125:GLU:HG3	1:D:141:GLU:HB2	1.95	0.48
1:E:326:GLY:H	1:E:328:PRO:HD2	1.77	0.48
1:B:113:PHE:CD1	1:B:122:LEU:HD13	2.49	0.48
1:E:132:THR:O	1:E:133:LYS:HG2	2.13	0.48
1:A:243:ILE:HG13	1:A:243:ILE:O	2.14	0.48
1:E:240:PRO:CB	1:E:241:PRO:CD	2.89	0.48
1:B:222:ARG:HD2	1:B:266:GLU:OE1	2.13	0.48
1:C:162:ARG:NH2	1:C:163:LYS:CE	2.77	0.48
1:E:222:ARG:HD3	1:E:269:ARG:HD3	1.94	0.48
1:A:146:VAL:HG21	1:A:177:LEU:HA	1.95	0.47
1:D:146:VAL:HG21	1:D:177:LEU:HA	1.96	0.47
1:E:171:TYR:CE2	1:E:250:TYR:HB3	2.48	0.47
1:C:148:ASP:O	1:C:152:GLU:HG2	2.14	0.47
1:C:238:ASP:C	1:C:239:VAL:CG2	2.82	0.47
1:E:132:THR:C	1:E:133:LYS:HG2	2.35	0.47
1:D:208:VAL:CG1	1:E:278:VAL:HG13	2.44	0.47
1:B:99:VAL:HG23	1:B:231:VAL:HB	1.97	0.47
1:C:302:MET:N	1:C:303:PRO:HD2	2.30	0.47
1:D:315:PHE:O	1:D:316:GLU:OE2	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:ILE:HG12	1:E:163:LYS:HA	1.96	0.47
1:A:99:VAL:HG23	1:A:231:VAL:HB	1.95	0.47
1:A:225:ILE:HD13	1:A:265:VAL:HG21	1.97	0.47
1:E:225:ILE:HD13	1:E:265:VAL:HG21	1.97	0.47
1:B:171:TYR:CE2	1:B:250:TYR:HB3	2.49	0.47
1:D:201:GLU:HB2	1:D:202:ARG:NH1	2.28	0.47
1:E:243:ILE:O	1:E:243:ILE:HG13	2.14	0.47
1:E:99:VAL:HG23	1:E:231:VAL:HB	1.97	0.47
1:A:148:ASP:N	1:A:149:PRO:CD	2.77	0.47
1:A:292:LYS:HZ1	1:B:286:LYS:HE2	1.80	0.47
1:B:146:VAL:HG21	1:B:177:LEU:HA	1.96	0.46
1:B:347:LYS:O	1:B:348:LYS:O	2.33	0.46
1:C:243:ILE:HG13	1:C:243:ILE:O	2.15	0.46
1:E:146:VAL:HG21	1:E:177:LEU:HA	1.97	0.46
1:A:296:ILE:HG22	1:A:345:PHE:CE2	2.50	0.46
1:C:288:ASN:HD21	1:C:292:LYS:NZ	2.14	0.46
1:D:222:ARG:HD3	1:D:269:ARG:HD3	1.96	0.46
1:D:288:ASN:HD21	1:D:292:LYS:NZ	2.13	0.46
1:D:333:VAL:O	1:D:337:ILE:HG22	2.15	0.46
1:C:292:LYS:HZ1	1:E:286:LYS:HE2	1.80	0.46
1:A:94:HIS:O	1:D:260:GLN:NE2	2.48	0.46
1:C:221:LEU:HD12	1:C:221:LEU:HA	1.77	0.46
1:C:306:PHE:CE1	1:E:304:LEU:HB3	2.50	0.46
1:E:132:THR:O	1:E:133:LYS:CG	2.64	0.46
1:B:292:LYS:HZ1	1:C:286:LYS:HE2	1.81	0.46
1:C:122:LEU:HD12	1:C:122:LEU:O	2.15	0.46
1:A:99:VAL:HG22	1:A:108:ILE:HG12	1.98	0.46
1:B:28:GLU:OE2	1:B:43:LYS:HD3	2.16	0.46
1:B:99:VAL:HG22	1:B:108:ILE:HG12	1.98	0.46
1:C:121:GLU:HG2	1:C:122:LEU:N	2.31	0.46
1:D:99:VAL:HG22	1:D:108:ILE:HG12	1.97	0.46
1:E:132:THR:O	1:E:132:THR:HG23	2.16	0.46
1:B:302:MET:N	1:B:303:PRO:HD2	2.30	0.46
1:A:61:TRP:HH2	1:A:151:ARG:HH21	1.62	0.45
1:C:34:TYR:HB2	1:C:39:PHE:CD1	2.33	0.45
1:C:99:VAL:HG22	1:C:108:ILE:HG12	1.99	0.45
1:C:99:VAL:HG23	1:C:231:VAL:HB	1.98	0.45
1:C:225:ILE:HD13	1:C:265:VAL:HG21	1.98	0.45
1:E:61:TRP:HH2	1:E:151:ARG:HH21	1.63	0.45
1:E:288:ASN:HD21	1:E:292:LYS:NZ	2.14	0.45
1:D:99:VAL:HG23	1:D:231:VAL:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:ARG:HD2	1:E:266:GLU:OE1	2.16	0.45
1:A:24:ARG:O	1:A:68:HIS:CE1	2.70	0.45
1:A:314:ASN:O	1:B:321:LEU:HD22	2.17	0.45
1:E:99:VAL:HG22	1:E:108:ILE:HG12	1.98	0.45
1:E:167:ASP:OD1	1:E:168:TYR:N	2.50	0.45
1:C:296:ILE:HG22	1:C:345:PHE:CE2	2.52	0.45
1:A:216:ARG:NH1	1:D:196:GLU:OE1	2.49	0.45
1:A:302:MET:N	1:A:303:PRO:HD2	2.32	0.45
1:D:238:ASP:C	1:D:239:VAL:CG2	2.85	0.45
1:A:296:ILE:HA	1:A:299:THR:HG22	1.99	0.45
1:B:24:ARG:O	1:B:68:HIS:CE1	2.69	0.45
1:B:132:THR:HG23	1:B:132:THR:O	2.17	0.45
1:C:341:MET:HE2	1:C:341:MET:CA	2.47	0.45
1:D:236:TYR:CE1	1:D:252:ARG:HB2	2.52	0.45
1:D:296:ILE:HA	1:D:299:THR:HG22	1.99	0.45
1:B:245:LYS:CB	1:B:246:GLU:CD	2.82	0.44
1:C:236:TYR:CE1	1:C:252:ARG:HB2	2.52	0.44
1:A:140:GLN:HE22	1:A:145:ASP:HB3	1.83	0.44
1:B:243:ILE:HG13	1:B:243:ILE:O	2.17	0.44
1:E:171:TYR:HE1	1:E:250:TYR:C	2.17	0.44
1:B:318:MET:HG2	1:C:327:TYR:CD1	2.52	0.44
1:A:297:ILE:HG21	1:D:299:THR:HA	1.99	0.44
1:B:140:GLN:HE22	1:B:145:ASP:HB3	1.83	0.44
1:C:317:TYR:O	1:C:317:TYR:CG	2.71	0.44
1:E:29:ILE:HG21	1:E:50:VAL:HG21	1.99	0.44
1:A:17:LEU:CD2	1:A:74:GLN:HG3	2.48	0.44
1:A:236:TYR:CE1	1:A:252:ARG:HB2	2.53	0.44
1:D:171:TYR:CE1	1:D:250:TYR:CB	2.99	0.44
1:C:160:ILE:HG22	1:C:161:ILE:CA	2.47	0.44
1:E:213:GLN:HA	1:E:213:GLN:OE1	2.17	0.44
1:A:171:TYR:CE2	1:A:250:TYR:HB3	2.48	0.44
1:E:140:GLN:HE22	1:E:145:ASP:HB3	1.83	0.44
1:A:245:LYS:HB2	1:A:246:GLU:CD	2.38	0.43
1:A:196:GLU:OE1	1:B:216:ARG:NH1	2.51	0.43
1:E:157:ASN:CG	1:E:162:ARG:HG3	2.38	0.43
1:C:37:GLU:O	1:C:37:GLU:CG	2.61	0.43
1:D:323:TRP:CD1	1:D:326:GLY:N	2.86	0.43
1:D:42:PHE:CD2	1:D:44:THR:HG23	2.53	0.43
1:D:140:GLN:HE22	1:D:145:ASP:HB3	1.84	0.43
1:A:239:VAL:N	1:A:240:PRO:HD3	2.33	0.43
1:A:263:ASP:OD2	1:B:96:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LYS:O	1:B:118:ASN:HB3	2.14	0.43
1:C:171:TYR:HE2	1:E:14:PRO:HG3	1.83	0.43
1:E:148:ASP:N	1:E:149:PRO:CD	2.81	0.43
1:A:167:ASP:OD1	1:A:168:TYR:N	2.52	0.43
1:A:333:VAL:O	1:A:337:ILE:HG12	2.17	0.43
1:B:225:ILE:HD13	1:B:265:VAL:HG21	1.99	0.43
1:B:344:TYR:C	1:B:346:LYS:H	2.21	0.43
1:C:231:VAL:HG23	1:C:232:LEU:N	2.33	0.43
1:A:133:LYS:HG3	1:A:134:ASN:N	2.33	0.43
1:B:288:ASN:HD21	1:B:292:LYS:NZ	2.17	0.43
1:C:132:THR:O	1:C:132:THR:HG23	2.18	0.43
1:A:96:ARG:NH1	1:D:263:ASP:OD2	2.52	0.43
1:C:148:ASP:N	1:C:149:PRO:CD	2.81	0.43
1:A:132:THR:HG23	1:A:132:THR:O	2.19	0.43
1:D:296:ILE:HG22	1:D:345:PHE:CE2	2.54	0.43
1:B:83:HIS:HA	1:B:84:PRO:HD3	1.86	0.42
1:C:157:ASN:HD21	1:C:162:ARG:HD2	1.80	0.42
1:D:132:THR:O	1:D:132:THR:HG23	2.18	0.42
1:E:296:ILE:HA	1:E:299:THR:HG22	2.00	0.42
1:A:119:LEU:HD13	1:A:121:GLU:OE2	2.17	0.42
1:A:314:ASN:C	1:B:321:LEU:HD22	2.40	0.42
1:D:322:ARG:O	1:D:323:TRP:C	2.57	0.42
1:D:286:LYS:HE2	1:E:292:LYS:CE	2.49	0.42
1:C:296:ILE:HA	1:C:299:THR:HG22	1.99	0.42
1:A:171:TYR:CE1	1:A:250:TYR:CB	2.99	0.42
1:A:198:GLU:O	1:A:203:PRO:HA	2.19	0.42
1:B:296:ILE:HA	1:B:299:THR:HG22	2.01	0.42
1:D:36:ILE:HA	1:D:162:ARG:HB3	2.01	0.42
1:A:292:LYS:NZ	1:B:286:LYS:HE2	2.35	0.42
1:D:54:ARG:CD	1:D:79:PHE:CE2	2.93	0.42
1:C:299:THR:OG1	1:E:297:ILE:HG13	2.19	0.42
1:D:42:PHE:HD2	1:D:44:THR:HG23	1.84	0.42
1:E:248:VAL:N	1:E:249:PRO:CD	2.83	0.42
1:B:231:VAL:HG23	1:B:232:LEU:N	2.34	0.42
1:C:222:ARG:HD2	1:C:266:GLU:OE1	2.20	0.42
1:E:238:ASP:C	1:E:239:VAL:CG2	2.86	0.42
1:A:99:VAL:HG23	1:A:231:VAL:CB	2.49	0.42
1:B:236:TYR:CE1	1:B:252:ARG:HB2	2.55	0.42
1:C:195:LEU:HD12	1:C:195:LEU:HA	1.86	0.42
1:D:334:MET:O	1:D:337:ILE:HG22	2.20	0.42
1:D:343:VAL:HG23	1:D:344:TYR:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:230:GLU:OE1	1:E:230:GLU:HA	2.18	0.42
1:A:96:ARG:O	1:A:98:LYS:HG3	2.20	0.41
1:A:305:THR:HG22	1:D:306:PHE:CA	2.50	0.41
1:C:41:GLU:O	1:C:41:GLU:HG2	2.20	0.41
1:D:83:HIS:HA	1:D:84:PRO:HD3	1.87	0.41
1:B:195:LEU:HD12	1:B:195:LEU:HA	1.90	0.41
1:C:162:ARG:CG	1:C:163:LYS:N	2.82	0.41
1:D:13:PRO:HB3	1:E:153:ARG:CD	2.51	0.41
1:E:99:VAL:HG23	1:E:231:VAL:CB	2.50	0.41
1:A:171:TYR:CE1	1:A:254:VAL:HG23	2.56	0.41
1:C:37:GLU:N	1:C:37:GLU:OE1	2.54	0.41
1:D:148:ASP:N	1:D:149:PRO:CD	2.83	0.41
1:E:236:TYR:CE1	1:E:252:ARG:HB2	2.56	0.41
1:B:72:VAL:O	1:B:76:VAL:HG23	2.20	0.41
1:B:222:ARG:HE	1:B:269:ARG:HD3	1.85	0.41
1:D:245:LYS:HB2	1:D:246:GLU:CD	2.37	0.41
1:E:296:ILE:HG22	1:E:345:PHE:CE2	2.55	0.41
1:B:344:TYR:CE1	1:B:345:PHE:CE1	3.08	0.41
1:C:161:ILE:HG23	1:C:162:ARG:H	1.86	0.41
1:A:195:LEU:HD12	1:A:195:LEU:HA	1.90	0.41
1:B:99:VAL:HG23	1:B:231:VAL:CB	2.51	0.41
1:B:165:ARG:NH1	1:B:243:ILE:HG21	2.35	0.41
1:B:171:TYR:CE1	1:B:250:TYR:CB	3.00	0.41
1:C:140:GLN:HE22	1:C:145:ASP:HB3	1.85	0.41
1:C:203:PRO:C	1:C:204:GLU:HG2	2.41	0.41
1:C:253:ARG:HA	1:C:253:ARG:HD2	1.94	0.41
1:D:54:ARG:HG3	1:D:55:ASP:N	2.36	0.41
1:E:36:ILE:O	1:E:36:ILE:HG22	2.20	0.41
1:A:248:VAL:N	1:A:249:PRO:CD	2.84	0.41
1:C:198:GLU:O	1:C:203:PRO:HA	2.21	0.41
1:A:102:PHE:CD2	1:A:105:TYR:CE2	3.09	0.40
1:B:344:TYR:HE1	1:B:345:PHE:HE1	1.69	0.40
1:C:72:VAL:O	1:C:76:VAL:HG23	2.21	0.40
1:D:248:VAL:N	1:D:249:PRO:CD	2.84	0.40
1:A:132:THR:C	1:A:133:LYS:HG2	2.41	0.40
1:C:171:TYR:CE1	1:C:250:TYR:CB	3.00	0.40
1:D:72:VAL:O	1:D:76:VAL:HG23	2.21	0.40
1:D:102:PHE:CD2	1:D:105:TYR:CE2	3.09	0.40
1:E:167:ASP:CG	1:E:247:THR:HG21	2.42	0.40
1:A:222:ARG:HD3	1:A:269:ARG:HD3	2.03	0.40
1:B:330:VAL:HG23	1:B:331:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:SER:O	1:C:285:ASN:HB2	2.20	0.40
1:D:167:ASP:CG	1:D:247:THR:HG21	2.42	0.40
1:B:171:TYR:CE1	1:B:254:VAL:HG23	2.56	0.40
1:B:239:VAL:N	1:B:240:PRO:HD3	2.36	0.40
1:D:104:ASN:HD22	1:D:104:ASN:N	2.19	0.40
1:E:72:VAL:O	1:E:76:VAL:HG23	2.22	0.40
1:D:171:TYR:CE1	1:D:254:VAL:HG23	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ARG:NH1	1:E:78:GLU:OE1[2_555]	2.18	0.02
1:C:155:ARG:O	1:C:322:ARG:NH2[2_454]	2.18	0.02

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	331/373 (89%)	301 (91%)	26 (8%)	4 (1%)	13	42
1	B	331/373 (89%)	306 (92%)	20 (6%)	5 (2%)	10	38
1	C	332/373 (89%)	303 (91%)	23 (7%)	6 (2%)	8	35
1	D	336/373 (90%)	312 (93%)	21 (6%)	3 (1%)	17	48
1	E	336/373 (90%)	307 (91%)	22 (6%)	7 (2%)	7	31
All	All	1666/1865 (89%)	1529 (92%)	112 (7%)	25 (2%)	10	38

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	LYS

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Mol	Chain	Res	Type
1	A	348	LYS
1	B	240	PRO
1	B	348	LYS
1	C	158	ARG
1	C	161	ILE
1	C	240	PRO
1	C	348	LYS
1	D	240	PRO
1	E	240	PRO
1	E	348	LYS
1	A	240	PRO
1	A	326	GLY
1	B	245	LYS
1	B	326	GLY
1	C	38	GLU
1	C	157	ASN
1	E	119	LEU
1	E	326	GLY
1	B	118	ASN
1	E	117	LYS
1	E	133	LYS
1	E	118	ASN
1	D	203	PRO
1	D	241	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	315/349 (90%)	312 (99%)	3 (1%)	76	86
1	B	315/349 (90%)	311 (99%)	4 (1%)	69	82
1	C	316/349 (90%)	310 (98%)	6 (2%)	57	77
1	D	319/349 (91%)	314 (98%)	5 (2%)	62	79
1	E	319/349 (91%)	315 (99%)	4 (1%)	69	82
All	All	1584/1745 (91%)	1562 (99%)	22 (1%)	67	82

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ARG
1	A	124	SER
1	A	348	LYS
1	B	96	ARG
1	B	124	SER
1	B	282	SER
1	B	348	LYS
1	C	25	GLU
1	C	41	GLU
1	C	96	ARG
1	C	124	SER
1	C	269	ARG
1	C	348	LYS
1	D	96	ARG
1	D	124	SER
1	D	204	GLU
1	D	206	GLU
1	D	348	LYS
1	E	96	ARG
1	E	124	SER
1	E	213	GLN
1	E	348	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	95	GLN
1	A	134	ASN
1	A	140	GLN
1	A	213	GLN
1	A	288	ASN
1	B	33	ASN
1	B	83	HIS
1	B	95	GLN
1	B	104	ASN
1	B	140	GLN
1	B	213	GLN
1	B	288	ASN
1	C	83	HIS
1	C	95	GLN

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Mol	Chain	Res	Type
1	C	104	ASN
1	C	126	GLN
1	C	140	GLN
1	C	288	ASN
1	C	314	ASN
1	D	33	ASN
1	D	74	GLN
1	D	95	GLN
1	D	104	ASN
1	D	288	ASN
1	D	314	ASN
1	E	33	ASN
1	E	74	GLN
1	E	95	GLN
1	E	120	HIS
1	E	288	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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 (i)

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	333/373 (89%)	0.14	20 (6%)	21	21	94, 157, 207, 235	0
1	B	333/373 (89%)	0.16	15 (4%)	33	32	85, 130, 172, 208	0
1	C	334/373 (89%)	0.13	19 (5%)	23	23	94, 133, 181, 230	0
1	D	338/373 (90%)	0.59	56 (16%)	1	2	96, 161, 238, 286	0
1	E	338/373 (90%)	0.04	17 (5%)	28	27	91, 140, 197, 244	0
All	All	1676/1865 (89%)	0.21	127 (7%)	13	13	85, 142, 209, 286	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	138	MET	6.7
1	A	244	GLU	6.4
1	C	244	GLU	6.4
1	D	139	PHE	6.0
1	E	320	GLU	5.7
1	D	61	TRP	5.6
1	E	321	LEU	5.3
1	D	63	ASN	5.1
1	D	44	THR	5.1
1	A	34	TYR	4.8
1	D	140	GLN	4.7
1	D	137	LEU	4.5
1	D	45	THR	4.4
1	A	163	LYS	4.3
1	D	29	ILE	4.3
1	D	128	SER	4.3
1	D	28	GLU	4.3
1	B	44	THR	4.2
1	C	246	GLU	4.2
1	A	246	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	161	ILE	4.2
1	D	64	ILE	4.0
1	E	325	TRP	4.0
1	D	147	PHE	3.9
1	D	65	THR	3.7
1	B	67	ILE	3.7
1	D	127	VAL	3.6
1	D	79	PHE	3.6
1	C	247	THR	3.5
1	A	160	ILE	3.4
1	D	62	ILE	3.4
1	A	31	VAL	3.3
1	B	17	LEU	3.3
1	B	29	ILE	3.3
1	D	130	ILE	3.2
1	D	30	GLU	3.2
1	E	15	GLY	3.2
1	B	343	VAL	3.2
1	D	152	GLU	3.2
1	E	16	THR	3.1
1	D	344	TYR	3.0
1	A	164	LYS	3.0
1	D	106	VAL	3.0
1	B	42	PHE	3.0
1	D	237	ARG	3.0
1	B	245	LYS	3.0
1	D	129	LEU	3.0
1	C	131	LEU	3.0
1	D	81	GLY	3.0
1	C	242	LEU	2.9
1	D	163	LYS	2.9
1	D	151	ARG	2.9
1	A	245	LYS	2.9
1	D	146	VAL	2.9
1	D	144	GLY	2.9
1	B	64	ILE	2.9
1	D	161	ILE	2.9
1	E	345	PHE	2.9
1	B	91	LEU	2.8
1	E	317	TYR	2.8
1	A	162	ARG	2.8
1	D	143	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	44	THR	2.8
1	D	31	VAL	2.8
1	A	344	TYR	2.8
1	C	243	ILE	2.8
1	D	343	VAL	2.8
1	D	67	ILE	2.7
1	C	239	VAL	2.7
1	E	44	THR	2.7
1	D	156	TYR	2.7
1	E	319	PRO	2.7
1	D	141	GLU	2.6
1	A	243	ILE	2.6
1	D	27	PHE	2.6
1	D	325	TRP	2.6
1	D	66	GLY	2.6
1	D	154	ILE	2.6
1	D	105	TYR	2.6
1	D	75	ARG	2.6
1	A	242	LEU	2.5
1	A	32	MET	2.5
1	C	245	LYS	2.5
1	D	136	VAL	2.5
1	D	43	LYS	2.5
1	E	323	TRP	2.5
1	E	326	GLY	2.5
1	E	29	ILE	2.5
1	C	344	TYR	2.4
1	D	36	ILE	2.4
1	C	105	TYR	2.4
1	D	155	ARG	2.4
1	E	17	LEU	2.4
1	D	107	PHE	2.4
1	B	244	GLU	2.4
1	C	101	PHE	2.4
1	D	125	GLU	2.3
1	D	42	PHE	2.3
1	C	241	PRO	2.3
1	A	247	THR	2.3
1	C	104	ASN	2.3
1	B	325	TRP	2.3
1	B	65	THR	2.3
1	D	78	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	251	PHE	2.2
1	D	340	ILE	2.2
1	C	167	ASP	2.2
1	A	36	ILE	2.2
1	B	344	TYR	2.2
1	D	238	ASP	2.2
1	D	112	MET	2.2
1	D	80	PHE	2.1
1	A	325	TRP	2.1
1	E	14	PRO	2.1
1	C	238	ASP	2.1
1	C	80	PHE	2.1
1	B	66	GLY	2.1
1	C	166	ALA	2.1
1	E	27	PHE	2.1
1	D	37	GLU	2.1
1	A	241	PRO	2.1
1	B	31	VAL	2.0
1	E	70	THR	2.0
1	E	322	ARG	2.0
1	C	250	TYR	2.0
1	A	240	PRO	2.0
1	D	148	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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. 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	B	403	1/1	0.08	0.44	115,115,115,115	0
2	MG	B	402	1/1	0.69	0.55	104,104,104,104	0
2	MG	D	401	1/1	0.77	0.75	116,116,116,116	0
2	MG	A	401	1/1	0.87	0.92	107,107,107,107	0
2	MG	E	401	1/1	0.93	0.52	111,111,111,111	0
2	MG	B	401	1/1	0.96	0.61	97,97,97,97	0

6.5 Other polymers (i)

There are no such residues in this entry.