



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:56 AM UTC

PDB ID : 5JRW / pdb_00005jrw
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

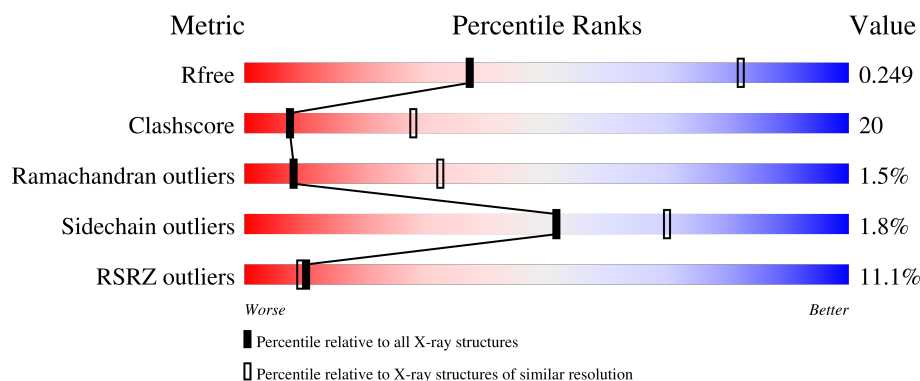
1 Overall quality at a glance

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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 $\leq 5\%$. 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	9% 57% 31% 11%
1	B	373	9% 58% 29% 11%
1	C	373	8% 55% 31% 10%
1	D	373	13% 54% 34% 9%
1	E	373	10% 59% 29% 9%

2 Entry composition

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 (CCD ID: 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

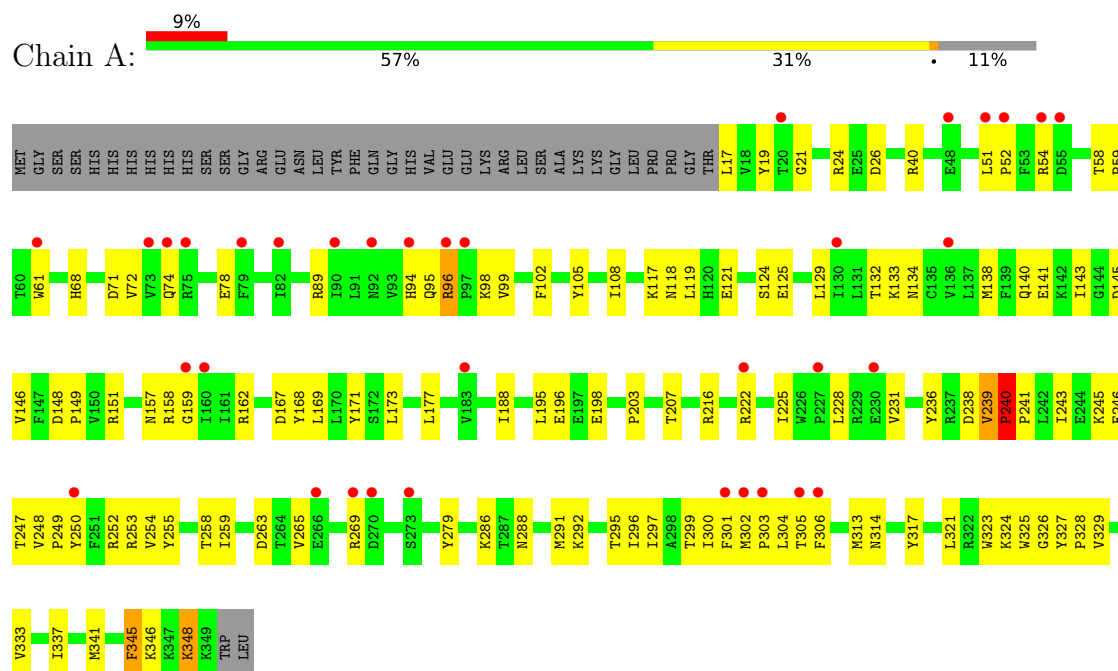
- Molecule 3 is water.

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

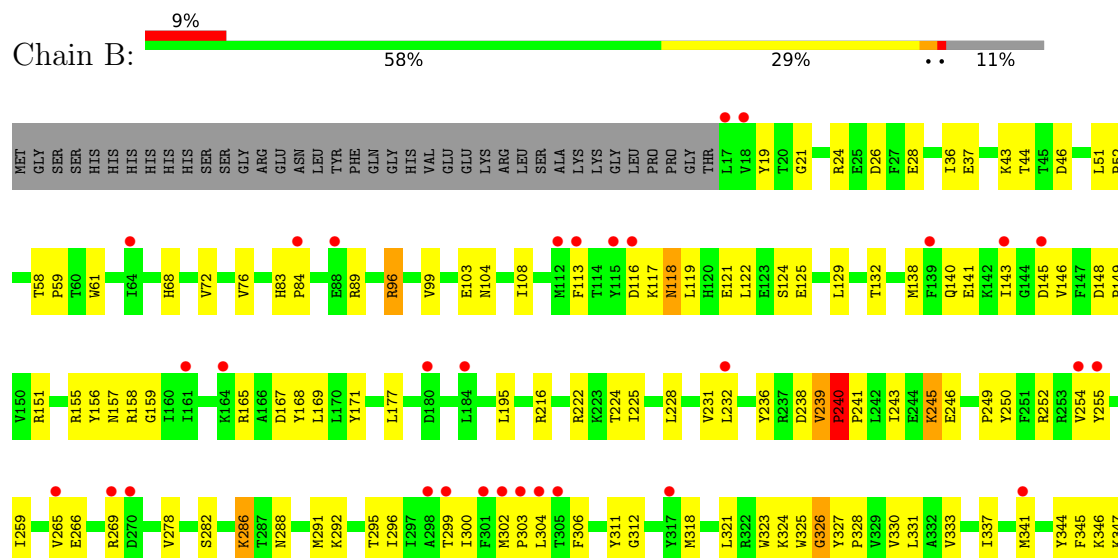
3 Residue-property plots [i](#)

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



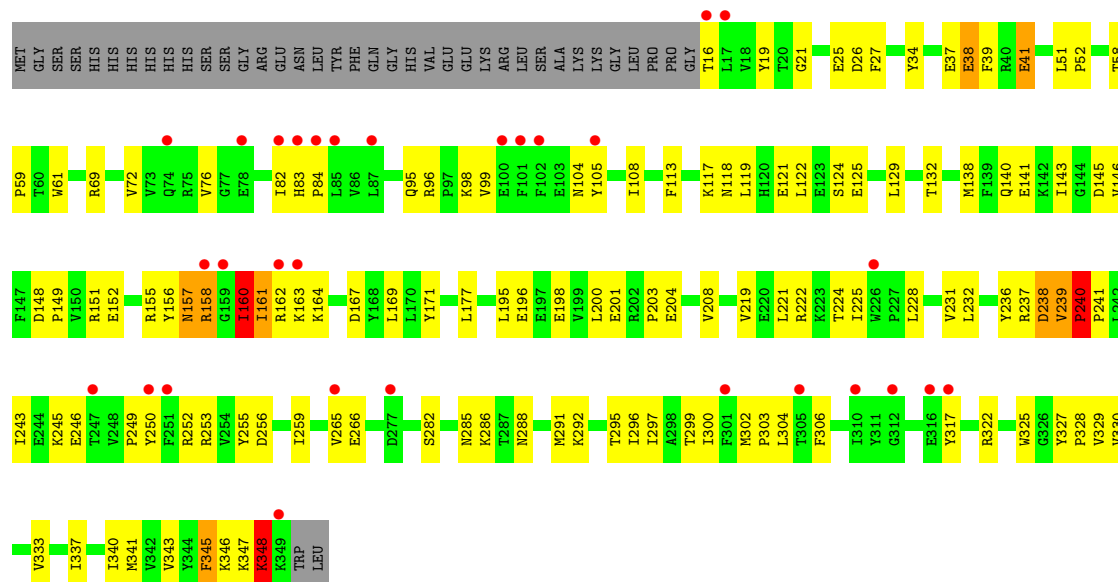
• Molecule 1: Cobalt/magnesium transport protein CorA





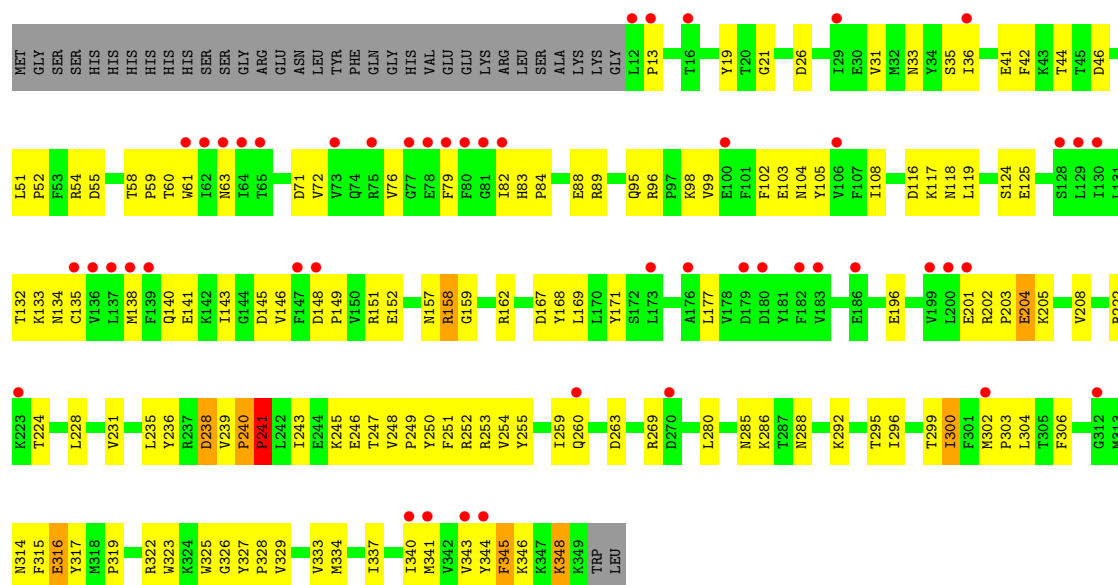
• Molecule 1: Cobalt/magnesium transport protein CorA

Chain C: 8% 55% 31% 10%



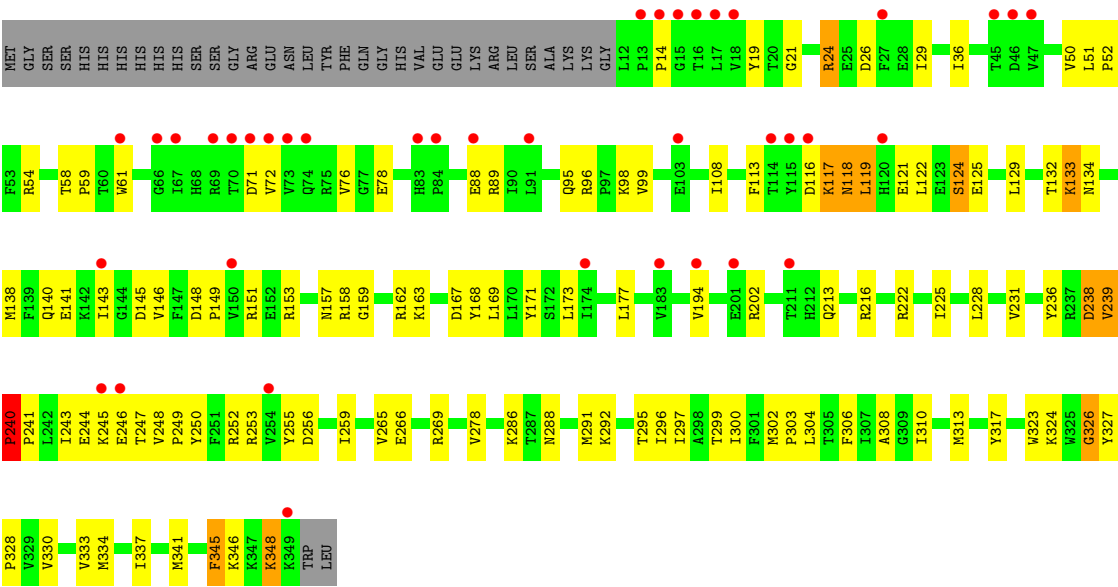
• Molecule 1: Cobalt/magnesium transport protein CorA

Chain D: 13% 54% 34% 9%



• Molecule 1: Cobalt/magnesium transport protein CorA

Chain E: 10% 59% 29% 9%



4 Data and refinement statistics

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 49.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.7 (49.00-3.30) 96.2 (49.00-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.28 , 93.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.60	1/2851 (0.0%)	0.88	3/3863 (0.1%)
1	B	0.65	1/2851 (0.0%)	0.90	3/3863 (0.1%)
1	C	0.66	0/2858	0.92	5/3873 (0.1%)
1	D	0.56	0/2886	0.84	1/3913 (0.0%)
1	E	0.63	0/2886	0.90	5/3913 (0.1%)
All	All	0.62	2/14332 (0.0%)	0.89	17/19425 (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	2
1	B	0	2
1	C	0	4
1	D	0	5
1	E	0	6
All	All	0	19

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	240	PRO	CA-C	7.55	1.59	1.52
1	B	240	PRO	CA-C	5.03	1.56	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	PRO	N-CA-C	9.13	121.84	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	239	VAL	CA-C-N	8.74	129.39	120.38
1	C	239	VAL	C-N-CA	8.74	129.39	120.38
1	A	239	VAL	CA-C-N	8.47	129.11	120.38
1	A	239	VAL	C-N-CA	8.47	129.11	120.38
1	E	239	VAL	CA-C-N	8.24	128.87	120.38
1	E	239	VAL	C-N-CA	8.24	128.87	120.38
1	B	239	VAL	CA-C-N	8.11	128.74	120.38
1	B	239	VAL	C-N-CA	8.11	128.74	120.38
1	C	240	PRO	N-CA-C	7.63	120.00	110.70
1	B	240	PRO	N-CA-C	7.25	119.55	110.70
1	E	240	PRO	N-CA-C	6.63	118.80	110.70
1	C	160	ILE	CB-CA-C	-5.98	101.48	111.29
1	C	219	VAL	N-CA-C	-5.79	105.08	110.53
1	E	24	ARG	N-CA-C	-5.68	104.12	108.78
1	E	194	VAL	CB-CA-C	-5.28	105.21	111.97
1	D	300	ILE	CB-CA-C	-5.00	105.36	111.92

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 ⓘ

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	126	1
1	B	2789	0	2839	111	0
1	C	2796	0	2846	148	1
1	D	2822	0	2874	138	0
1	E	2822	0	2874	107	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	573	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 20.

All (573) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:MET:HE2	1:E:291:MET:SD	1.78	1.23
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:157:ASN:CG	1:C:162:ARG:HD3	1.87	1.00
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:A:117:LYS:O	1:A:118:ASN:OD1	1.85	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:117:LYS:O	1:C:118:ASN:CG	2.14	0.91
1:A:171:TYR:CZ	1:A:250:TYR:HB3	2.06	0.90
1:A:117:LYS:O	1:A:118:ASN:CG	2.16	0.89
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: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:119:LEU:HD13	1:A:121:GLU:CD	2.02	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ILE:HG13	1:D:299:THR:OG1	1.82	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:A:253:ARG:NH1	1:B:89:ARG:HG2	2.01	0.75
1:B:103:GLU:OE1	1:B:104:ASN:CG	2.29	0.75
1:D:171:TYR:CE1	1:D:250:TYR:C	2.65	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:C:157:ASN:O	1:C:158:ARG:C	2.29	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
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:E:171:TYR:CE1	1:E:250:TYR:C	2.69	0.70
1:A:240:PRO:HB2	1:A:241:PRO:HD3	1.71	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:A:171:TYR:CE1	1:A:250:TYR:C	2.70	0.69
1:C:171:TYR:CE1	1:C:250:TYR:C	2.70	0.69
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:A:71:ASP:OD1	1:A:72:VAL:N	2.24	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:341:MET:HE2	1:C:341:MET:HA	1.74	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:B:171:TYR:CE1	1:B:250:TYR:C	2.71	0.67
1:C:238:ASP:C	1:C:239:VAL:HG22	2.19	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: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
1:D:63:ASN:CG	1:D:138:MET:HE2	2.21	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:D:238:ASP:C	1:D:239:VAL:HG22	2.23	0.64
1:E:228:LEU:O	1:E:231:VAL:HG22	1.96	0.64
1:D:152:GLU:CD	1:D:152:GLU:O	2.41	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:E:238:ASP:C	1:E:239:VAL:HG22	2.24	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:ASP:OD2	1:D:143:ILE:HG22	1.99	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: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:D:315:PHE:C	1:D:316:GLU:HG2	2.25	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: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: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
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: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:61:TRP:HB2	1:D:169:LEU:HD21	1.84	0.59
1:A:238:ASP:C	1:A:239:VAL:HG22	2.28	0.59
1:D:299:THR:HG21	1:D:345:PHE:HZ	1.68	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:D:157:ASN:CG	1:D:162:ARG:HG3	2.27	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:157:ASN:CG	1:A:162:ARG:HG3	2.29	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: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:C:237:ARG:HD2	1:C:237:ARG:C	2.29	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:D:63:ASN:OD1	1:D:138:MET:CE	2.53	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: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
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:D:315:PHE:O	1:D:316:GLU:CD	2.48	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:B:238:ASP:C	1:B:239:VAL:HG22	2.30	0.56
1:B:318:MET:HE3	1:C:327:TYR:CE1	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:63:ASN:OD1	1:D:138:MET:HE2	2.06	0.55
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:A:286:LYS:HE3	1:D:292:LYS:HZ1	1.72	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:245:LYS:CB	1:B:246:GLU:CD	2.82	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:129:LEU:HD21	1:E:138:MET:HE2	1.89	0.53
1:E:317:TYR:O	1:E:317:TYR:CD2	2.61	0.53
1:E:171:TYR:HE1	1:E:250:TYR:C	2.17	0.53
1:C:118:ASN:OD1	1:C:119:LEU:N	2.41	0.52
1:C:292:LYS:HZ1	1:E:286:LYS:HE2	1.73	0.52
1:D:148:ASP:OD1	1:D:151:ARG:NH1	2.41	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:E:132:THR:C	1:E:133:LYS:HG2	2.35	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:C:238:ASP:C	1:C:239:VAL:CG2	2.82	0.52
1:B:148:ASP:OD1	1:B:151:ARG:NH1	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:VAL:CG2	1:D:231:VAL:HB	2.40	0.52
1:E:171:TYR:CE1	1:E:250:TYR:O	2.60	0.52
1:C:129:LEU:HD21	1:C:138:MET:HE2	1.90	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:C:171:TYR:HE1	1:C:250:TYR:C	2.19	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: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:171:TYR:HE1	1:A:250:TYR:C	2.16	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:129:LEU:HD21	1:B:138:MET:HE2	1.93	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:C:291:MET:HE2	1:E:291:MET:CE	2.41	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:D:245:LYS:HB2	1:D:246:GLU:CD	2.37	0.50
1:A:129:LEU:HD21	1:A:138:MET:HE2	1.93	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
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:A:292:LYS:HZ1	1:B:286:LYS:HE2	1.77	0.49
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:ASP:C	1:D:239:VAL:CG2	2.85	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:A:245:LYS:HB2	1:A:246:GLU:CD	2.38	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:E:238:ASP:C	1:E:239:VAL:CG2	2.86	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:B:344:TYR:C	1:B:346:LYS:H	2.21	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:E:157:ASN:CG	1:E:162:ARG:HG3	2.38	0.47
1:C:148:ASP:O	1:C:152:GLU:HG2	2.14	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
1:D:322:ARG:O	1:D:323:TRP:C	2.57	0.47
1:E:36:ILE:HG12	1:E:163:LYS:HA	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:171:TYR:HE1	1:D:250:TYR:C	2.14	0.47
1:E:225:ILE:HD13	1:E:265:VAL:HG21	1.97	0.47
1:A:314:ASN:C	1:B:321:LEU:HD22	2.40	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:D:302:MET:HG3	1:E:302:MET:HE2	1.97	0.47
1:A:148:ASP:N	1:A:149:PRO:CD	2.77	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: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:A:302:MET:HE2	1:B:302:MET:HG3	1.97	0.46
1:B:302:MET:N	1:B:303:PRO:HD2	2.30	0.46
1:E:245:LYS:HB2	1:E:246:GLU:CD	2.41	0.46
1:C:203:PRO:C	1:C:204:GLU:HG2	2.41	0.45
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:132:THR:C	1:A:133:LYS:HG2	2.41	0.45
1:E:167:ASP:CG	1:E:247:THR:HG21	2.42	0.45
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:D:167:ASP:CG	1:D:247:THR:HG21	2.42	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:118:ASN:CG	1:A:119:LEU:H	2.20	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: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: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: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:158:ARG:O	1:E:159:GLY:C	2.61	0.44
1:A:321:LEU:HD22	1:D:314:ASN:C	2.42	0.44
1:B:318:MET:HG2	1:C:327:TYR:CD1	2.52	0.44
1:A:238:ASP:C	1:A:239:VAL:CG2	2.91	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:C:340:ILE:HG13	1:C:341:MET:HE3	1.99	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:196:GLU:OE1	1:B:216:ARG:NH1	2.51	0.43
1:C:37:GLU:O	1:C:37:GLU:CG	2.61	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:TRP:CD1	1:D:326:GLY:N	2.86	0.43
1:B:156:TYR:O	1:B:157:ASN:C	2.62	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:E:308:ALA:HB2	1:E:334:MET:HE1	1.99	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
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: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:D:63:ASN:OD1	1:D:138:MET:HE3	2.18	0.43
1:A:96:ARG:NH1	1:D:263:ASP:OD2	2.52	0.43
1:A:158:ARG:O	1:A:159:GLY:C	2.62	0.43
1:C:148:ASP:N	1:C:149:PRO:CD	2.81	0.43
1:E:116:ASP:C	1:E:117:LYS:O	2.61	0.43
1:A:132:THR:O	1:A:132:THR:HG23	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:C:82:ILE:O	1:C:83:HIS:C	2.63	0.42
1:D:82:ILE:O	1:D:83:HIS:C	2.62	0.42
1:D:238:ASP:O	1:D:239:VAL:C	2.62	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:E:330:VAL:CG1	1:E:334:MET:HE3	2.49	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:238:ASP:OD1	1:C:238:ASP:C	2.56	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: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:D:238:ASP:OD1	1:D:238:ASP:C	2.58	0.41
1:B:158:ARG:O	1:B:159:GLY:C	2.62	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:D:54:ARG:HG3	1:D:55:ASP:CG	2.45	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:E:310:ILE:HA	1:E:313:MET:HE2	2.03	0.41
1:E:244:GLU:O	1:E:245:LYS:C	2.63	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:D:343:VAL:HG23	1:D:344:TYR:N	2.35	0.41
1:A:195:LEU:HD12	1:A:195:LEU:HA	1.90	0.41
1:A:292:LYS:NZ	1:B:286:LYS:HE2	2.35	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:B:171:TYR:HE1	1:B:250:TYR:C	2.20	0.41
1:B:238:ASP:C	1:B:239:VAL:CG2	2.94	0.41
1:C:140:GLN:HE22	1:C:145:ASP:HB3	1.85	0.41
1:C:253:ARG:HA	1:C:253:ARG:HD2	1.94	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:245:LYS:HB3	1:B:246:GLU:CD	2.45	0.41
1:C:198:GLU:O	1:C:203:PRO:HA	2.21	0.41
1:D:315:PHE:C	1:D:316:GLU:CG	2.89	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:291:MET:HE2	1:B:291:MET:HG2	2.03	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:A:167:ASP:CG	1:A:247:THR:HG21	2.46	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
1:C:282:SER:O	1:C:285:ASN:HB2	2.20	0.40
1:D:158:ARG:O	1:D:159:GLY:C	2.62	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

5.3.1 Protein backbone

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%)	10	37
1	B	331/373 (89%)	306 (92%)	20 (6%)	5 (2%)	8	32
1	C	332/373 (89%)	303 (91%)	23 (7%)	6 (2%)	6	29
1	D	336/373 (90%)	312 (93%)	21 (6%)	3 (1%)	14	43
1	E	336/373 (90%)	307 (91%)	22 (6%)	7 (2%)	5	26
All	All	1666/1865 (89%)	1529 (92%)	112 (7%)	25 (2%)	8	32

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	LYS
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 ⓘ

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%)	311 (99%)	4 (1%)	61	74
1	B	315/349 (90%)	309 (98%)	6 (2%)	50	68
1	C	316/349 (90%)	310 (98%)	6 (2%)	50	68
1	D	319/349 (91%)	310 (97%)	9 (3%)	38	62
1	E	319/349 (91%)	316 (99%)	3 (1%)	70	78
All	All	1584/1745 (91%)	1556 (98%)	28 (2%)	51	70

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ARG
1	A	124	SER
1	A	188	ILE
1	A	348	LYS
1	B	96	ARG
1	B	124	SER
1	B	224	THR
1	B	282	SER
1	B	286	LYS
1	B	348	LYS
1	C	25	GLU
1	C	41	GLU
1	C	96	ARG
1	C	124	SER
1	C	224	THR
1	C	348	LYS
1	D	96	ARG
1	D	103	GLU
1	D	124	SER
1	D	158	ARG
1	D	204	GLU
1	D	205	LYS
1	D	224	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	280	LEU
1	D	348	LYS
1	E	96	ARG
1	E	124	SER
1	E	348	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	92	ASN
1	A	94	HIS
1	A	95	GLN
1	A	120	HIS
1	A	134	ASN
1	A	140	GLN
1	A	213	GLN
1	A	288	ASN
1	A	314	ASN
1	B	63	ASN
1	B	83	HIS
1	B	94	HIS
1	B	95	GLN
1	B	104	ASN
1	B	140	GLN
1	B	213	GLN
1	B	288	ASN
1	B	314	ASN
1	C	33	ASN
1	C	83	HIS
1	C	94	HIS
1	C	95	GLN
1	C	104	ASN
1	C	120	HIS
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	92	ASN
1	D	94	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	95	GLN
1	D	104	ASN
1	D	257	HIS
1	D	288	ASN
1	D	314	ASN
1	E	63	ASN
1	E	74	GLN
1	E	92	ASN
1	E	94	HIS
1	E	95	GLN
1	E	120	HIS
1	E	140	GLN
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 oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	333/373 (89%)	0.50	35 (10%) 11 9	94, 157, 207, 235	0
1	B	333/373 (89%)	0.39	33 (9%) 13 10	85, 130, 172, 208	0
1	C	334/373 (89%)	0.27	30 (8%) 15 11	94, 133, 181, 230	0
1	D	338/373 (90%)	0.64	49 (14%) 6 5	96, 161, 238, 286	0
1	E	338/373 (90%)	0.69	39 (11%) 9 8	91, 140, 197, 244	0
All	All	1676/1865 (89%)	0.50	186 (11%) 10 9	85, 142, 209, 286	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	15	GLY	12.4
1	E	17	LEU	11.9
1	E	70	THR	11.6
1	E	74	GLN	9.7
1	C	84	PRO	8.6
1	C	78	GLU	8.4
1	C	83	HIS	8.2
1	A	94	HIS	8.0
1	E	16	THR	7.3
1	E	246	GLU	7.2
1	D	344	TYR	6.9
1	B	302	MET	6.9
1	D	137	LEU	6.9
1	B	301	PHE	6.9
1	A	269	ARG	6.8
1	E	71	ASP	6.6
1	B	305	THR	6.4
1	D	78	GLU	6.3
1	E	115	TYR	6.3
1	A	48	GLU	5.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	18	VAL	5.8
1	B	303	PRO	5.8
1	A	302	MET	5.7
1	A	96	ARG	5.7
1	B	269	ARG	5.4
1	D	138	MET	5.4
1	D	62	ILE	5.4
1	A	270	ASP	5.3
1	D	182	PHE	5.1
1	E	114	THR	5.0
1	C	250	TYR	5.0
1	B	299	THR	4.9
1	A	52	PRO	4.9
1	D	183	VAL	4.8
1	E	73	VAL	4.8
1	D	130	ILE	4.8
1	D	61	TRP	4.8
1	B	180	ASP	4.8
1	D	64	ILE	4.7
1	E	69	ARG	4.7
1	D	136	VAL	4.7
1	D	139	PHE	4.6
1	B	18	VAL	4.6
1	C	17	LEU	4.5
1	B	88	GLU	4.5
1	E	88	GLU	4.4
1	D	129	LEU	4.4
1	C	74	GLN	4.3
1	D	173	LEU	4.3
1	E	91	LEU	4.3
1	D	260	GLN	4.2
1	A	20	THR	4.2
1	A	306	PHE	4.2
1	E	84	PRO	4.2
1	B	317	TYR	4.1
1	C	82	ILE	4.1
1	B	17	LEU	4.0
1	D	81	GLY	4.0
1	A	305	THR	4.0
1	D	147	PHE	4.0
1	B	298	ALA	3.9
1	E	14	PRO	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	270	ASP	3.8
1	E	201	GLU	3.8
1	D	79	PHE	3.8
1	A	301	PHE	3.7
1	A	250	TYR	3.7
1	A	75	ARG	3.7
1	B	115	TYR	3.6
1	D	341	MET	3.6
1	D	223	LYS	3.6
1	D	77	GLY	3.6
1	E	183	VAL	3.6
1	E	194	VAL	3.6
1	B	265	VAL	3.5
1	D	340	ILE	3.5
1	A	79	PHE	3.5
1	A	97	PRO	3.5
1	C	162	ARG	3.5
1	D	63	ASN	3.5
1	B	304	LEU	3.5
1	E	116	ASP	3.5
1	D	200	LEU	3.4
1	A	90	ILE	3.4
1	C	158	ARG	3.3
1	D	180	ASP	3.3
1	D	75	ARG	3.2
1	D	12	LEU	3.2
1	B	112	MET	3.2
1	D	199	VAL	3.2
1	E	120	HIS	3.2
1	C	251	PHE	3.2
1	B	254	VAL	3.1
1	B	349	LYS	3.1
1	D	176	ALA	3.1
1	E	45	THR	3.1
1	D	106	VAL	3.1
1	C	305	THR	3.0
1	B	116	ASP	3.0
1	C	85	LEU	3.0
1	A	273	SER	2.9
1	E	27	PHE	2.9
1	C	87	LEU	2.9
1	A	61	TRP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	16	THR	2.9
1	C	301	PHE	2.9
1	B	84	PRO	2.9
1	C	100	GLU	2.9
1	E	254	VAL	2.8
1	A	159	GLY	2.8
1	D	29	ILE	2.8
1	C	105	TYR	2.8
1	D	135	CYS	2.8
1	C	163	LYS	2.8
1	E	245	LYS	2.8
1	E	67	ILE	2.8
1	B	145	ASP	2.7
1	D	312	GLY	2.7
1	A	222	ARG	2.7
1	C	159	GLY	2.7
1	E	61	TRP	2.6
1	A	303	PRO	2.6
1	D	13	PRO	2.6
1	D	186	GLU	2.6
1	A	54	ARG	2.6
1	B	232	LEU	2.5
1	A	51	LEU	2.5
1	E	174	ILE	2.5
1	C	317	TYR	2.5
1	E	349	LYS	2.5
1	A	73	VAL	2.5
1	B	164	LYS	2.5
1	D	80	PHE	2.4
1	D	148	ASP	2.4
1	E	83	HIS	2.4
1	A	160	ILE	2.4
1	D	100	GLU	2.4
1	C	349	LYS	2.4
1	C	226	TRP	2.4
1	B	341	MET	2.4
1	D	73	VAL	2.4
1	A	55	ASP	2.4
1	A	227	PRO	2.4
1	C	312	GLY	2.3
1	A	82	ILE	2.3
1	A	266	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	103	GLU	2.3
1	E	66	GLY	2.3
1	E	211	THR	2.3
1	E	46	ASP	2.3
1	C	265	VAL	2.3
1	B	64	ILE	2.3
1	D	343	VAL	2.2
1	C	316	GLU	2.2
1	B	270	ASP	2.2
1	D	179	ASP	2.2
1	A	136	VAL	2.2
1	D	82	ILE	2.2
1	B	113	PHE	2.2
1	C	102	PHE	2.2
1	C	277	ASP	2.2
1	E	47	VAL	2.1
1	B	348	LYS	2.1
1	D	201	GLU	2.1
1	D	16	THR	2.1
1	B	255	TYR	2.1
1	C	310	ILE	2.1
1	A	74	GLN	2.1
1	A	230	GLU	2.1
1	D	128	SER	2.1
1	C	101	PHE	2.1
1	E	150	VAL	2.1
1	B	143	ILE	2.1
1	D	36	ILE	2.1
1	A	92	ASN	2.1
1	D	302	MET	2.1
1	B	139	PHE	2.1
1	E	143	ILE	2.0
1	C	247	THR	2.0
1	E	13	PRO	2.0
1	B	184	LEU	2.0
1	A	130	ILE	2.0
1	D	65	THR	2.0
1	A	183	VAL	2.0
1	E	72	VAL	2.0
1	B	161	ILE	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 oligosaccharides 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, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	B	403	1/1	0.74	0.10	115,115,115,115	0
2	MG	E	401	1/1	0.77	0.24	111,111,111,111	0
2	MG	D	401	1/1	0.83	0.14	116,116,116,116	0
2	MG	B	402	1/1	0.87	0.10	104,104,104,104	0
2	MG	B	401	1/1	0.87	0.38	97,97,97,97	0
2	MG	A	401	1/1	0.93	0.08	107,107,107,107	0

6.5 Other polymers [i](#)

There are no such residues in this entry.