



wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 10:18 pm BST

PDB ID : 2IUB
Title : Crystal structure of a divalent metal ion transporter CorA at 2.9 Å resolution.
Authors : Eshaghi, S.; Niegowski, D.; Kohl, A.; Martinez Molina, D.; Lesley, S.A.; Nordlund, P.
Deposited on : 2006-06-01
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 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 : 2.11
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) : 2.11

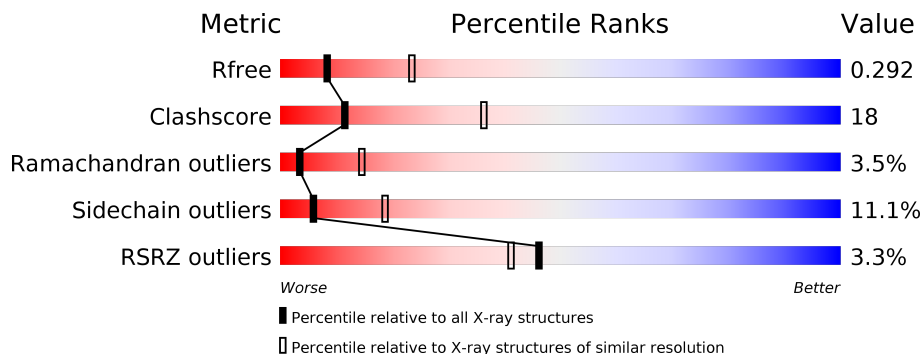
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.



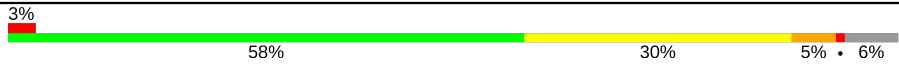

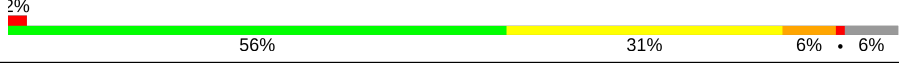

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	363	
1	B	363	
1	C	363	
1	D	363	
1	E	363	
1	F	363	

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Mol	Chain	Length	Quality of chain
1	G	363	
1	H	363	
1	I	363	
1	J	363	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 27580 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 DIVALENT CATION TRANSPORT-RELATED PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	331	Total 2736	C 1780	N 447	O 501	S 8	0	0	0
1	B	331	Total 2728	C 1775	N 444	O 501	S 8	0	0	0
1	C	331	Total 2726	C 1773	N 444	O 501	S 8	0	0	0
1	D	331	Total 2730	C 1777	N 444	O 501	S 8	0	0	0
1	E	331	Total 2730	C 1777	N 444	O 501	S 8	0	0	0
1	F	342	Total 2793	C 1814	N 458	O 512	S 9	0	0	0
1	G	342	Total 2790	C 1812	N 458	O 512	S 8	0	0	0
1	H	338	Total 2767	C 1799	N 451	O 508	S 9	0	0	0
1	I	340	Total 2776	C 1804	N 453	O 510	S 9	0	0	0
1	J	336	Total 2763	C 1796	N 452	O 506	S 9	0	0	0

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total 2	Cl 2	0	0
2	B	1	Total 1	Cl 1	0	0
2	A	1	Total 1	Cl 1	0	0
2	D	2	Total 2	Cl 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total Cl 1 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	3	Total Mg 3 3	0	0
3	J	3	Total Mg 3 3	0	0
3	D	5	Total Mg 5 5	0	0
3	E	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	2	Total Mg 2 2	0	0
3	A	2	Total Mg 2 2	0	0
3	F	3	Total Mg 3 3	0	0

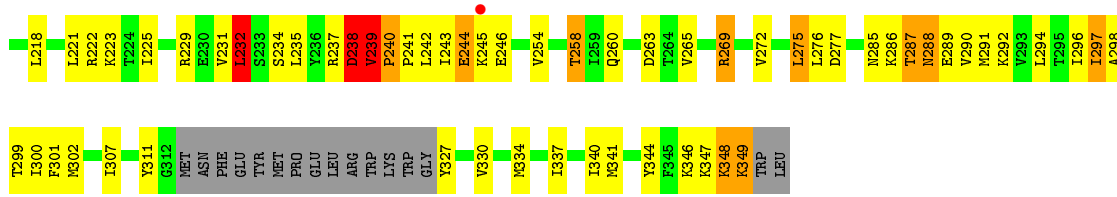
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total O 2 2	0	0
4	B	3	Total O 3 3	0	0
4	C	1	Total O 1 1	0	0
4	E	1	Total O 1 1	0	0
4	F	1	Total O 1 1	0	0
4	G	1	Total O 1 1	0	0
4	H	2	Total O 2 2	0	0

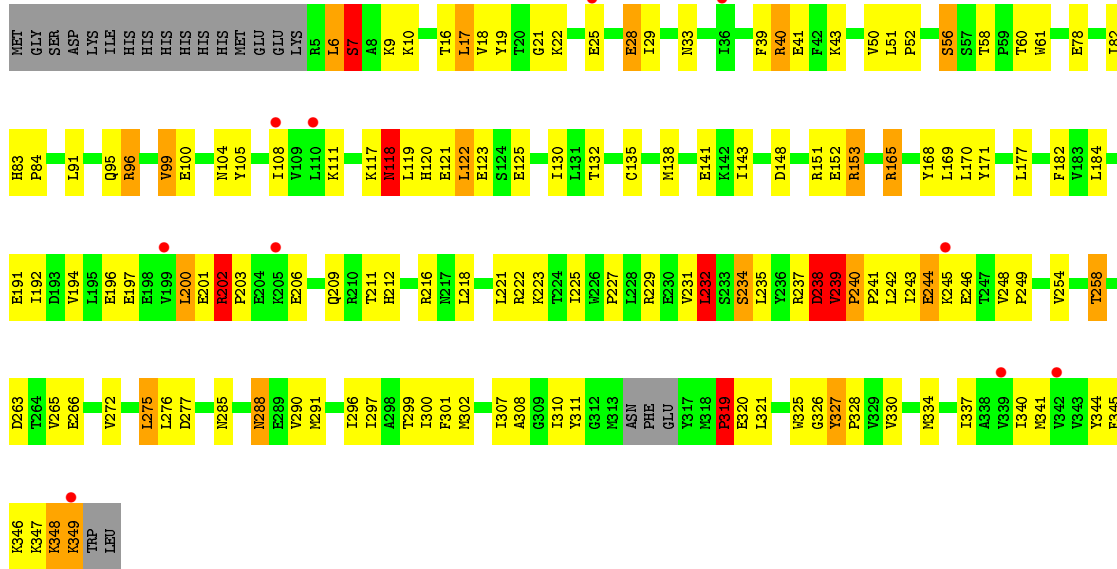
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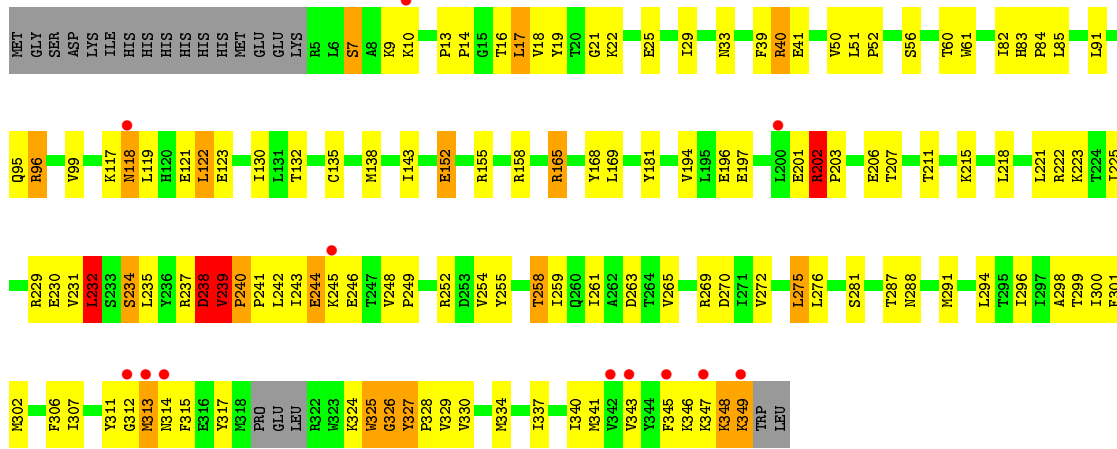
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	2	Total	O	0	0
			2	2		



● Molecule 1: DIVALENT CATION TRANSPORT-RELATED PROTEIN

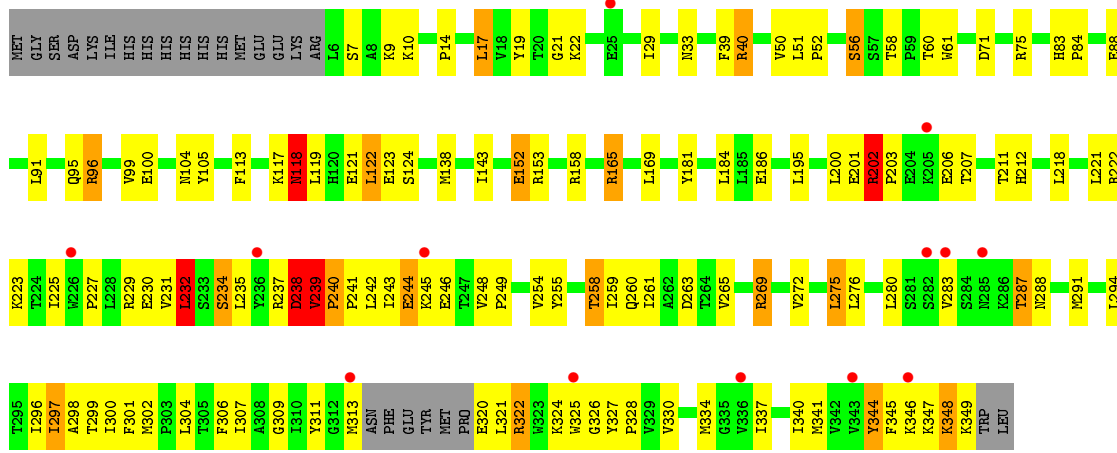


● Molecule 1: DIVALENT CATION TRANSPORT-RELATED PROTEIN

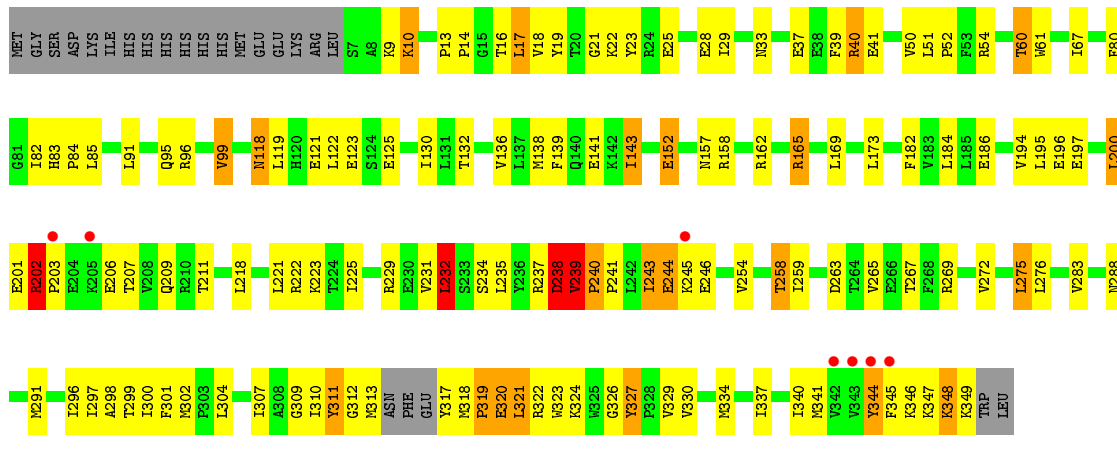


● Molecule 1: DIVALENT CATION TRANSPORT-RELATED PROTEIN

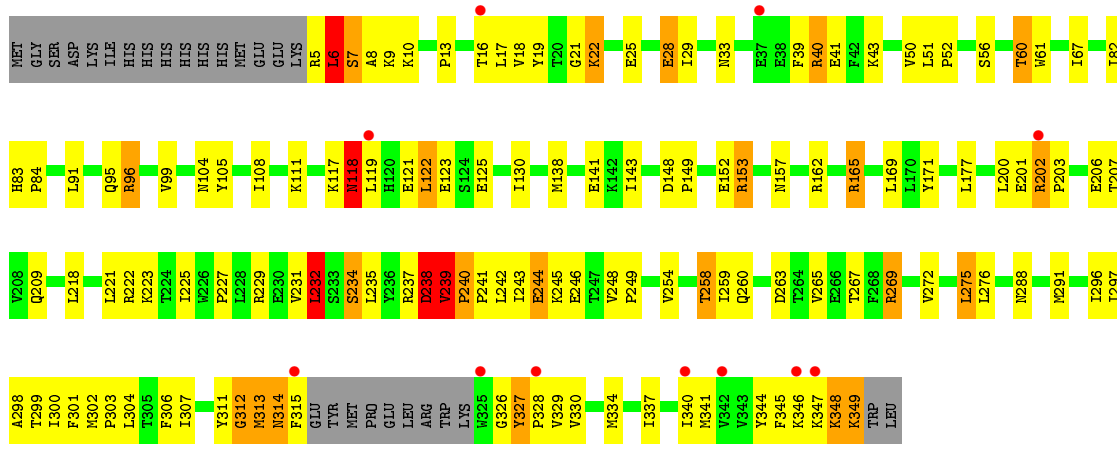




• Molecule 1: DIVALENT CATION TRANSPORT-RELATED PROTEIN



• Molecule 1: DIVALENT CATION TRANSPORT-RELATED PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	116.23Å 151.46Å 143.32Å 90.00° 98.88° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 29.82 – 2.90	Depositor EDS
% Data completeness (in resolution range)	90.3 (30.00-2.90) 90.3 (29.82-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.90Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.260 , 0.291 0.261 , 0.292	Depositor DCC
R_{free} test set	4921 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	70.7	Xtrriage
Anisotropy	0.019	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	27580	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.81	1/2792 (0.0%)	0.81	4/3783 (0.1%)
1	B	0.84	0/2784	0.81	4/3773 (0.1%)
1	C	0.85	1/2782 (0.0%)	0.81	5/3770 (0.1%)
1	D	0.84	1/2786 (0.0%)	0.82	4/3776 (0.1%)
1	E	0.84	1/2786 (0.0%)	0.90	6/3776 (0.2%)
1	F	0.84	4/2849 (0.1%)	0.85	5/3861 (0.1%)
1	G	0.85	1/2846 (0.0%)	0.84	6/3858 (0.2%)
1	H	0.88	2/2823 (0.1%)	0.84	4/3826 (0.1%)
1	I	0.84	0/2833	0.83	5/3841 (0.1%)
1	J	0.85	0/2819	0.95	9/3819 (0.2%)
All	All	0.84	11/28100 (0.0%)	0.85	52/38083 (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	C	0	1
1	E	0	1
1	F	0	3
1	G	0	1
1	I	0	3
All	All	0	9

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	135	CYS	CB-SG	-7.94	1.68	1.82
1	E	100	GLU	CG-CD	6.40	1.61	1.51
1	C	123	GLU	CG-CD	5.63	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	100	GLU	CG-CD	5.57	1.60	1.51
1	H	88	GLU	CG-CD	-5.53	1.43	1.51

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	269	ARG	NE-CZ-NH2	-16.96	111.82	120.30
1	J	269	ARG	NE-CZ-NH1	16.64	128.62	120.30
1	J	269	ARG	NE-CZ-NH2	-16.34	112.13	120.30
1	E	269	ARG	NE-CZ-NH1	15.27	127.94	120.30
1	J	6	LEU	CA-CB-CG	8.43	134.70	115.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	326	GLY	Peptide
1	E	5	ARG	Peptide
1	F	319	PRO	Peptide
1	F	325	TRP	Peptide
1	F	7	SER	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2736	0	2797	108	0
1	B	2728	0	2779	117	0
1	C	2726	0	2778	110	2
1	D	2730	0	2786	93	1
1	E	2730	0	2786	102	2
1	F	2793	0	2826	119	2
1	G	2790	0	2820	106	0
1	H	2767	0	2808	114	2
1	I	2776	0	2808	128	1
1	J	2763	0	2815	116	0
2	A	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	D	2	0	0	0	0
2	F	1	0	0	0	0
2	G	2	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	5	0	0	0	0
3	E	1	0	0	0	0
3	F	3	0	0	0	0
3	G	3	0	0	0	0
3	H	1	0	0	0	0
3	J	3	0	0	0	0
4	A	2	0	0	2	0
4	B	3	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	2	0	0	0	0
4	I	2	0	0	0	0
All	All	27580	0	28003	980	5

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 18.

The worst 5 of 980 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:I:320:GLU:CB	1:I:321:LEU:HA	1.72	1.19
1:A:186:GLU:OE1	1:B:6:LEU:HG	1.45	1.16
1:E:165:ARG:HH12	1:E:243:ILE:HD13	1.01	1.16
1:H:165:ARG:HH12	1:H:243:ILE:HD13	0.99	1.13
1:A:165:ARG:HH12	1:A:243:ILE:HD13	0.98	1.11

All (5) 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:C:37:GLU:OE2	1:E:348:LYS:CA[2_555]	1.99	0.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:78:GLU:OE1	1:H:202:ARG:NH1[2_546]	2.00	0.20
1:D:38:GLU:OE1	1:H:75:ARG:CD[2_546]	2.05	0.15
1:C:37:GLU:OE2	1:E:348:LYS:N[2_555]	2.11	0.09
1:F:348:LYS:CA	1:I:37:GLU:OE2[2_556]	2.14	0.06

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	327/363 (90%)	284 (87%)	32 (10%)	11 (3%)	3	15
1	B	327/363 (90%)	291 (89%)	28 (9%)	8 (2%)	6	22
1	C	327/363 (90%)	289 (88%)	29 (9%)	9 (3%)	5	19
1	D	327/363 (90%)	289 (88%)	26 (8%)	12 (4%)	3	13
1	E	327/363 (90%)	289 (88%)	25 (8%)	13 (4%)	3	11
1	F	338/363 (93%)	293 (87%)	34 (10%)	11 (3%)	4	15
1	G	338/363 (93%)	292 (86%)	32 (10%)	14 (4%)	3	11
1	H	334/363 (92%)	291 (87%)	32 (10%)	11 (3%)	4	15
1	I	336/363 (93%)	289 (86%)	33 (10%)	14 (4%)	3	10
1	J	332/363 (92%)	291 (88%)	29 (9%)	12 (4%)	3	14
All	All	3313/3630 (91%)	2898 (88%)	300 (9%)	115 (4%)	3	14

5 of 115 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	PRO
1	A	244	GLU
1	A	245	LYS
1	A	348	LYS
1	B	7	SER

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	311/341 (91%)	278 (89%)	33 (11%)	6	20
1	B	309/341 (91%)	272 (88%)	37 (12%)	5	15
1	C	309/341 (91%)	275 (89%)	34 (11%)	6	19
1	D	310/341 (91%)	278 (90%)	32 (10%)	7	22
1	E	310/341 (91%)	275 (89%)	35 (11%)	6	18
1	F	312/341 (92%)	277 (89%)	35 (11%)	6	18
1	G	311/341 (91%)	278 (89%)	33 (11%)	6	20
1	H	311/341 (91%)	275 (88%)	36 (12%)	5	16
1	I	311/341 (91%)	279 (90%)	32 (10%)	7	22
1	J	312/341 (92%)	274 (88%)	38 (12%)	5	15
All	All	3106/3410 (91%)	2761 (89%)	345 (11%)	6	19

5 of 345 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	218	LEU
1	F	232	LEU
1	J	96	ARG
1	E	238	ASP
1	F	28	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	217	ASN
1	F	120	HIS
1	J	118	ASN
1	E	260	GLN
1	F	217	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 28 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	331/363 (91%)	0.07	13 (3%) 39 35	43, 68, 98, 103	0
1	B	331/363 (91%)	0.17	14 (4%) 36 32	43, 68, 98, 103	0
1	C	331/363 (91%)	0.21	15 (4%) 33 29	43, 68, 98, 103	0
1	D	331/363 (91%)	0.19	12 (3%) 42 37	43, 68, 98, 103	0
1	E	331/363 (91%)	0.13	5 (1%) 73 73	43, 68, 98, 103	0
1	F	342/363 (94%)	0.14	10 (2%) 51 47	43, 69, 98, 103	0
1	G	342/363 (94%)	0.17	12 (3%) 44 38	43, 69, 98, 103	0
1	H	338/363 (93%)	0.19	13 (3%) 40 36	43, 68, 98, 103	0
1	I	340/363 (93%)	0.09	7 (2%) 63 61	43, 69, 98, 103	0
1	J	336/363 (92%)	0.17	11 (3%) 46 41	43, 68, 98, 103	0
All	All	3353/3630 (92%)	0.15	112 (3%) 46 41	43, 68, 98, 103	0

The worst 5 of 112 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	245	LYS	6.5
1	H	282	SER	6.1
1	D	343	VAL	5.0
1	H	343	VAL	4.9
1	B	329	VAL	4.7

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(\AA^2)	Q<0.9
3	MG	D	1353	1/1	0.79	0.30	65,65,65,65	0
3	MG	F	1350	1/1	0.81	0.26	55,55,55,55	0
3	MG	F	1352	1/1	0.81	0.39	46,46,46,46	0
3	MG	D	1352	1/1	0.84	0.38	71,71,71,71	0
3	MG	C	1350	1/1	0.88	0.24	43,43,43,43	0
3	MG	D	1356	1/1	0.91	0.33	46,46,46,46	0
3	MG	G	1353	1/1	0.91	0.18	43,43,43,43	0
3	MG	J	1352	1/1	0.92	0.61	63,63,63,63	0
2	CL	B	1350	1/1	0.92	0.10	68,68,68,68	0
3	MG	J	1350	1/1	0.92	0.40	61,61,61,61	0
3	MG	J	1351	1/1	0.92	0.30	43,43,43,43	0
3	MG	D	1355	1/1	0.93	0.25	56,56,56,56	0
3	MG	F	1353	1/1	0.94	0.28	45,45,45,45	0
2	CL	F	1351	1/1	0.94	0.15	61,61,61,61	0
3	MG	C	1351	1/1	0.94	0.29	38,38,38,38	0
3	MG	B	1351	1/1	0.95	0.54	56,56,56,56	0
2	CL	D	1351	1/1	0.95	0.08	59,59,59,59	0
2	CL	G	1351	1/1	0.96	0.14	69,69,69,69	0
3	MG	A	1352	1/1	0.96	0.18	35,35,35,35	0
3	MG	G	1354	1/1	0.96	0.52	50,50,50,50	0
2	CL	G	1350	1/1	0.97	0.08	47,47,47,47	0
3	MG	G	1352	1/1	0.97	0.31	44,44,44,44	0
3	MG	H	1350	1/1	0.97	0.62	54,54,54,54	0
3	MG	A	1351	1/1	0.97	0.31	47,47,47,47	0
3	MG	D	1354	1/1	0.97	0.69	55,55,55,55	0
3	MG	E	1350	1/1	0.98	0.57	56,56,56,56	0
2	CL	A	1350	1/1	0.98	0.06	50,50,50,50	0
2	CL	D	1350	1/1	0.98	0.14	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.