



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 3, 2018 – 01:04 PM EST

PDB ID : 5V6Y
Title : Crystal structure of the human CLR:RAMP1 extracellular domain heterodimer with bound high-affinity and altered selectivity adrenomedullin variant
Authors : Pioszak, A.; Booe, J.
Deposited on : 2017-03-17
Resolution : 2.80 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

<http://wwpdb.org/validation/2016/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
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

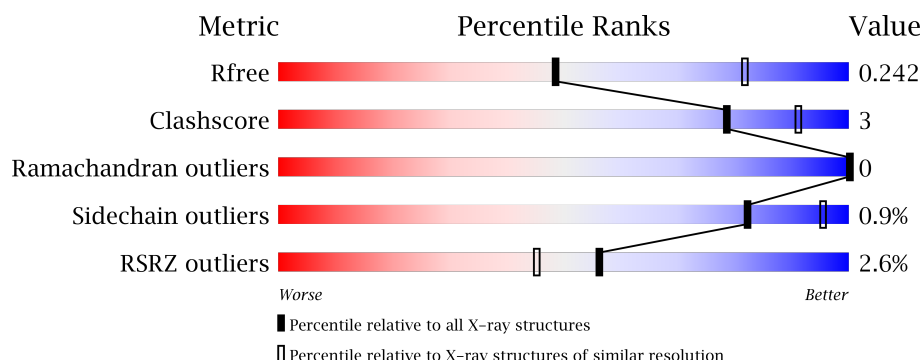
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	593	<div> <div>0.2%</div> <div>87%</div> <div>6%</div> <div>7%</div> </div>
1	B	593	<div> <div>2%</div> <div>83%</div> <div>9%</div> <div>7%</div> </div>
1	C	593	<div> <div>2%</div> <div>83%</div> <div>9%</div> <div>7%</div> </div>
1	D	593	<div> <div>5%</div> <div>84%</div> <div>9%</div> <div>8%</div> </div>
2	E	16	<div> <div>75%</div> <div>19%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	16	
2	G	16	
2	H	16	

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
4	NH2	E	101	-	-	-	X
4	NH2	F	101	-	-	-	X
4	NH2	H	101	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17855 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 Maltose-binding periplasmic protein, Receptor activity-modifying protein 1, Calcitonin gene-related peptide type 1 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	0	0	0
			4341	2773	720	825	23			
1	B	551	Total	C	N	O	S	0	0	0
			4349	2779	721	826	23			
1	C	549	Total	C	N	O	S	0	0	0
			4335	2770	718	824	23			
1	D	547	Total	C	N	O	S	0	0	0
			4278	2727	710	818	23			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P0AEY0
A	369	ASN	-	linker	UNP P0AEY0
A	370	ALA	-	linker	UNP P0AEY0
A	371	ALA	-	linker	UNP P0AEY0
A	372	ALA	-	linker	UNP P0AEY0
A	373	GLU	-	linker	UNP P0AEY0
A	374	PHE	-	linker	UNP P0AEY0
A	2020	GLY	-	linker	UNP O60894
A	2021	SER	-	linker	UNP O60894
A	2022	ALA	-	linker	UNP O60894
A	2023	GLY	-	linker	UNP O60894
A	2024	SER	-	linker	UNP O60894
A	2025	ALA	-	linker	UNP O60894
A	2026	GLY	-	linker	UNP O60894
A	2027	SER	-	linker	UNP O60894
A	2028	ALA	-	linker	UNP O60894
A	2145	HIS	-	expression tag	UNP Q16602
A	2146	HIS	-	expression tag	UNP Q16602
A	2147	HIS	-	expression tag	UNP Q16602
A	2148	HIS	-	expression tag	UNP Q16602

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2149	HIS	-	expression tag	UNP Q16602
A	2150	HIS	-	expression tag	UNP Q16602
B	1	MET	-	initiating methionine	UNP P0AEY0
B	369	ASN	-	linker	UNP P0AEY0
B	370	ALA	-	linker	UNP P0AEY0
B	371	ALA	-	linker	UNP P0AEY0
B	372	ALA	-	linker	UNP P0AEY0
B	373	GLU	-	linker	UNP P0AEY0
B	374	PHE	-	linker	UNP P0AEY0
B	2020	GLY	-	linker	UNP O60894
B	2021	SER	-	linker	UNP O60894
B	2022	ALA	-	linker	UNP O60894
B	2023	GLY	-	linker	UNP O60894
B	2024	SER	-	linker	UNP O60894
B	2025	ALA	-	linker	UNP O60894
B	2026	GLY	-	linker	UNP O60894
B	2027	SER	-	linker	UNP O60894
B	2028	ALA	-	linker	UNP O60894
B	2145	HIS	-	expression tag	UNP Q16602
B	2146	HIS	-	expression tag	UNP Q16602
B	2147	HIS	-	expression tag	UNP Q16602
B	2148	HIS	-	expression tag	UNP Q16602
B	2149	HIS	-	expression tag	UNP Q16602
B	2150	HIS	-	expression tag	UNP Q16602
C	1	MET	-	initiating methionine	UNP P0AEY0
C	369	ASN	-	linker	UNP P0AEY0
C	370	ALA	-	linker	UNP P0AEY0
C	371	ALA	-	linker	UNP P0AEY0
C	372	ALA	-	linker	UNP P0AEY0
C	373	GLU	-	linker	UNP P0AEY0
C	374	PHE	-	linker	UNP P0AEY0
C	2020	GLY	-	linker	UNP O60894
C	2021	SER	-	linker	UNP O60894
C	2022	ALA	-	linker	UNP O60894
C	2023	GLY	-	linker	UNP O60894
C	2024	SER	-	linker	UNP O60894
C	2025	ALA	-	linker	UNP O60894
C	2026	GLY	-	linker	UNP O60894
C	2027	SER	-	linker	UNP O60894
C	2028	ALA	-	linker	UNP O60894
C	2145	HIS	-	expression tag	UNP Q16602
C	2146	HIS	-	expression tag	UNP Q16602

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2147	HIS	-	expression tag	UNP Q16602
C	2148	HIS	-	expression tag	UNP Q16602
C	2149	HIS	-	expression tag	UNP Q16602
C	2150	HIS	-	expression tag	UNP Q16602
D	1	MET	-	initiating methionine	UNP P0AEY0
D	369	ASN	-	linker	UNP P0AEY0
D	370	ALA	-	linker	UNP P0AEY0
D	371	ALA	-	linker	UNP P0AEY0
D	372	ALA	-	linker	UNP P0AEY0
D	373	GLU	-	linker	UNP P0AEY0
D	374	PHE	-	linker	UNP P0AEY0
D	2020	GLY	-	linker	UNP O60894
D	2021	SER	-	linker	UNP O60894
D	2022	ALA	-	linker	UNP O60894
D	2023	GLY	-	linker	UNP O60894
D	2024	SER	-	linker	UNP O60894
D	2025	ALA	-	linker	UNP O60894
D	2026	GLY	-	linker	UNP O60894
D	2027	SER	-	linker	UNP O60894
D	2028	ALA	-	linker	UNP O60894
D	2145	HIS	-	expression tag	UNP Q16602
D	2146	HIS	-	expression tag	UNP Q16602
D	2147	HIS	-	expression tag	UNP Q16602
D	2148	HIS	-	expression tag	UNP Q16602
D	2149	HIS	-	expression tag	UNP Q16602
D	2150	HIS	-	expression tag	UNP Q16602

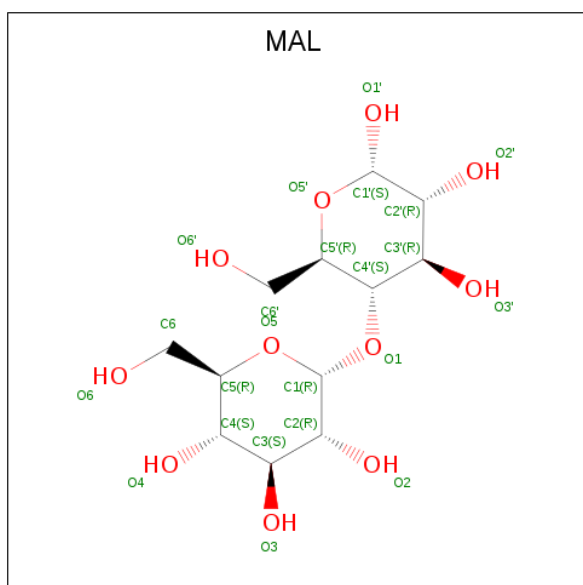
- Molecule 2 is a protein called ADM.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	15	Total	C	N	O	0	0	0
			117	80	18	19			
2	F	15	Total	C	N	O	0	1	0
			137	94	23	20			
2	G	13	Total	C	N	O	0	0	0
			110	76	19	15			
2	H	13	Total	C	N	O	0	0	0
			89	61	14	14			

There are 16 discrepancies between the modelled and reference sequences:

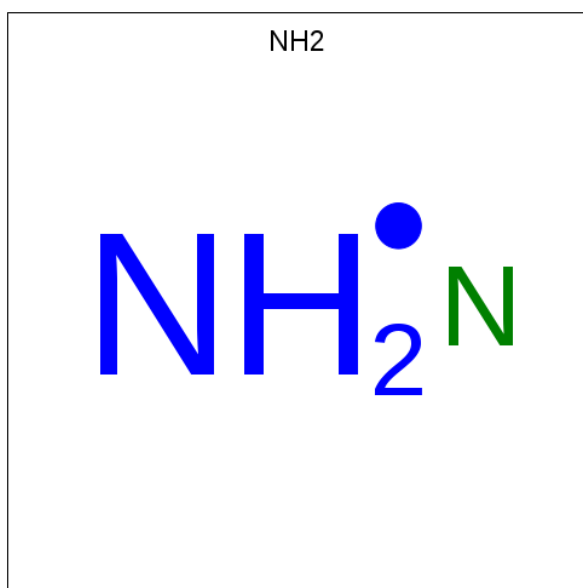
Chain	Residue	Modelled	Actual	Comment	Reference
E	45	TRP	SER	engineered mutation	UNP P35318
E	46	LEU	LYS	engineered mutation	UNP P35318
E	50	TRP	GLN	engineered mutation	UNP P35318
E	52	PHE	TYR	engineered mutation	UNP P35318
F	45	TRP	SER	engineered mutation	UNP P35318
F	46	LEU	LYS	engineered mutation	UNP P35318
F	50	TRP	GLN	engineered mutation	UNP P35318
F	52	PHE	TYR	engineered mutation	UNP P35318
G	45	TRP	SER	engineered mutation	UNP P35318
G	46	LEU	LYS	engineered mutation	UNP P35318
G	50	TRP	GLN	engineered mutation	UNP P35318
G	52	PHE	TYR	engineered mutation	UNP P35318
H	45	TRP	SER	engineered mutation	UNP P35318
H	46	LEU	LYS	engineered mutation	UNP P35318
H	50	TRP	GLN	engineered mutation	UNP P35318
H	52	PHE	TYR	engineered mutation	UNP P35318

- Molecule 3 is MALTOSE (three-letter code: MAL) (formula: C₁₂H₂₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			23	12	11		
3	B	1	Total	C	O	0	0
			23	12	11		
3	C	1	Total	C	O	0	0
			23	12	11		
3	D	1	Total	C	O	0	0
			23	12	11		

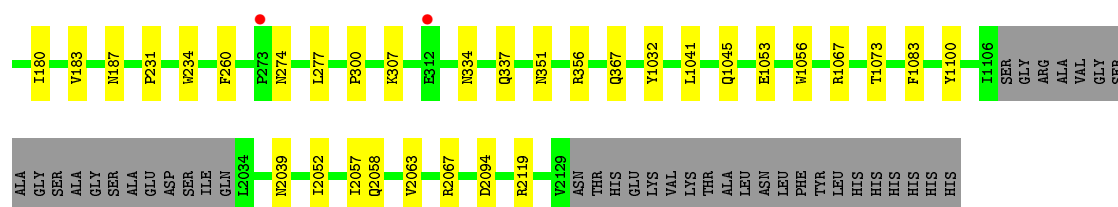
- Molecule 4 is AMINO GROUP (three-letter code: NH2) (formula: H_2N).



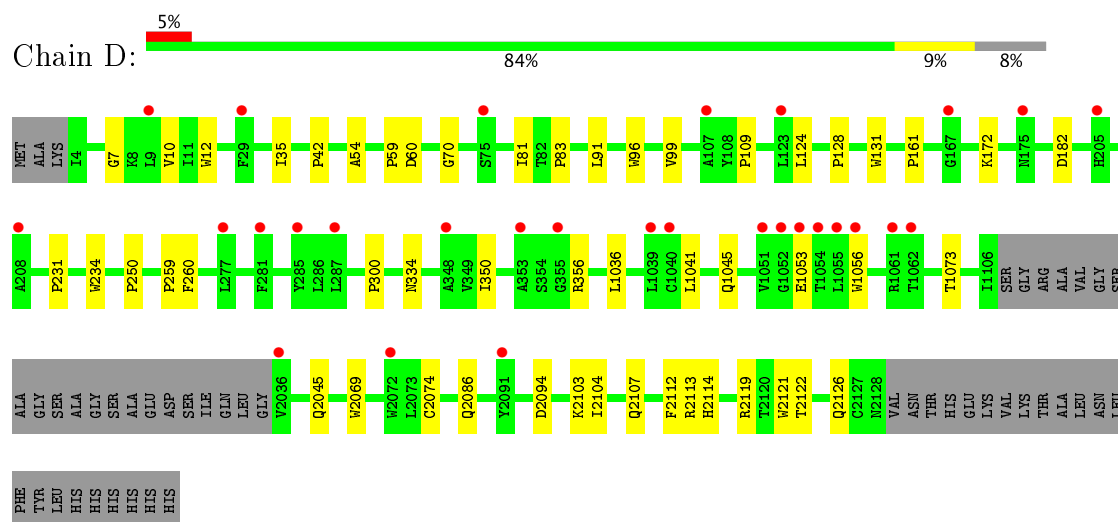
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total N 1 1	0	0
4	F	1	Total N 1 1	0	0
4	G	1	Total N 1 1	0	0
4	H	1	Total N 1 1	0	0

- Molecule 5 is water.

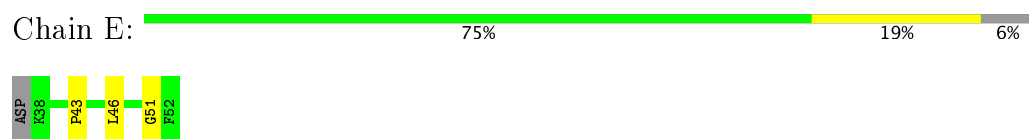
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total O 2 2	0	0
5	B	1	Total O 1 1	0	0



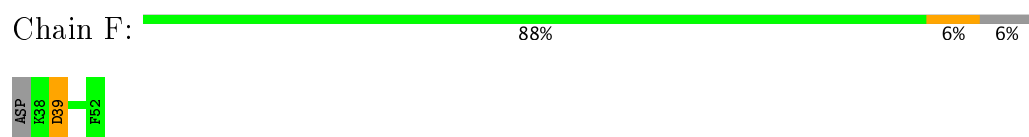
- Molecule 1: Maltose-binding periplasmic protein, Receptor activity-modifying protein 1, Calcitonin gene-related peptide type 1 receptor



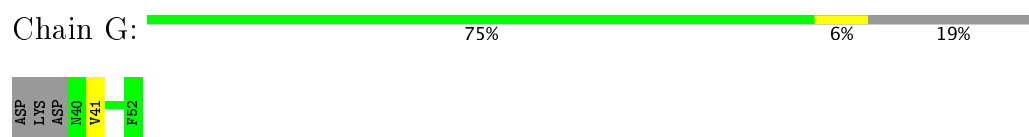
- Molecule 2: ADM



- Molecule 2: ADM



- Molecule 2: ADM



- Molecule 2: ADM



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	195.50Å 69.44Å 200.00Å 90.00° 99.43° 90.00°	Depositor
Resolution (Å)	45.11 – 2.80 45.11 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.1 (45.11-2.80) 87.7 (45.11-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.10.1 _2155	Depositor
R, R_{free}	0.212 , 0.244 0.208 , 0.242	Depositor DCC
R_{free} test set	1856 reflections (3.22%)	DCC
Wilson B-factor (Å ²)	80.6	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 55.6	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	0.94	EDS
Total number of atoms	17855	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.94% 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: MAL, NH2

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	0.24	0/4453	0.39	0/6050
1	B	0.24	0/4461	0.39	0/6061
1	C	0.24	0/4447	0.39	0/6043
1	D	0.24	0/4385	0.40	0/5961
2	E	0.22	0/123	0.32	0/171
2	F	0.21	0/145	0.31	0/201
2	G	0.25	0/116	0.36	0/160
2	H	0.26	0/93	0.36	0/129
All	All	0.24	0/18223	0.39	0/24776

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4341	0	4178	21	1
1	B	4349	0	4186	31	1
1	C	4335	0	4171	31	1
1	D	4278	0	4095	29	0
2	E	117	0	100	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	137	0	120	1	0
2	G	110	0	105	1	0
2	H	89	0	73	2	0
3	A	23	0	22	0	0
3	B	23	0	22	0	0
3	C	23	0	22	0	0
3	D	23	0	22	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	1	0	0	0	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
All	All	17855	0	17116	116	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 3.

The worst 5 of 116 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:97:ASP:OD1	1:C:100:ARG:NH1	2.00	0.95
1:B:80:GLU:OE2	1:B:104:LYS:NZ	2.09	0.85
1:C:1067:ARG:NH1	1:C:2039:ASN:OD1	2.09	0.85
1:B:97:ASP:OD1	1:B:100:ARG:NH1	2.24	0.69
1:C:274:ASN:HB3	1:C:277:LEU:HB2	1.78	0.64

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:B:85:LYS:NZ	1:B:179:ASP:OD2[4_655]	1.80	0.40
1:A:1050:ALA:O	1:C:36:LYS:NZ[3_545]	1.97	0.23

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	546/593 (92%)	535 (98%)	11 (2%)	0	100	100
1	B	547/593 (92%)	534 (98%)	13 (2%)	0	100	100
1	C	545/593 (92%)	532 (98%)	13 (2%)	0	100	100
1	D	543/593 (92%)	529 (97%)	14 (3%)	0	100	100
2	E	13/16 (81%)	13 (100%)	0	0	100	100
2	F	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
2	G	11/16 (69%)	11 (100%)	0	0	100	100
2	H	11/16 (69%)	11 (100%)	0	0	100	100
All	All	2230/2436 (92%)	2178 (98%)	52 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	450/484 (93%)	445 (99%)	5 (1%)	78	94
1	B	451/484 (93%)	448 (99%)	3 (1%)	87	97
1	C	450/484 (93%)	444 (99%)	6 (1%)	73	93
1	D	440/484 (91%)	438 (100%)	2 (0%)	91	97
2	E	11/14 (79%)	11 (100%)	0	100	100
2	F	13/14 (93%)	12 (92%)	1 (8%)	15	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	11/14 (79%)	11 (100%)	0	100	100
2	H	7/14 (50%)	7 (100%)	0	100	100
All	All	1833/1992 (92%)	1816 (99%)	17 (1%)	82	95

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1089	VAL
1	C	10	VAL
1	C	2063	VAL
1	B	260	PHE
1	D	260	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1028	GLN
1	D	2045	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are modelled with single atom - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	MAL	A	2201	-	24,24,24	0.82	0	35,35,35	1.03	3 (8%)
3	MAL	B	2201	-	24,24,24	0.82	0	35,35,35	0.99	3 (8%)
3	MAL	C	2201	-	24,24,24	0.81	0	35,35,35	1.02	2 (5%)
3	MAL	D	2201	-	24,24,24	0.82	0	35,35,35	1.02	3 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAL	A	2201	-	-	0/8/48/48	0/2/2/2
3	MAL	B	2201	-	-	0/8/48/48	0/2/2/2
3	MAL	C	2201	-	-	0/8/48/48	0/2/2/2
3	MAL	D	2201	-	-	0/8/48/48	0/2/2/2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2201	MAL	C1-O1-C4'	-3.37	109.78	118.00
3	D	2201	MAL	C1-O1-C4'	-3.20	110.20	118.00
3	C	2201	MAL	C1-O1-C4'	-3.13	110.37	118.00
3	B	2201	MAL	C1-O1-C4'	-3.04	110.59	118.00
3	D	2201	MAL	C1'-O5'-C5'	-2.58	108.74	113.39

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	550/593 (92%)	-0.16	7 (1%) 77 71	71, 108, 156, 199	0
1	B	551/593 (92%)	-0.05	13 (2%) 59 49	58, 111, 180, 214	0
1	C	549/593 (92%)	-0.08	10 (1%) 69 60	58, 103, 161, 211	0
1	D	547/593 (92%)	0.20	29 (5%) 27 18	82, 138, 186, 246	0
2	E	15/16 (93%)	-0.15	0 100 100	97, 113, 175, 192	0
2	F	15/16 (93%)	-0.28	0 100 100	64, 81, 144, 148	0
2	G	13/16 (81%)	0.16	0 100 100	55, 67, 128, 148	0
2	H	13/16 (81%)	0.09	0 100 100	145, 177, 218, 254	0
All	All	2253/2436 (92%)	-0.02	59 (2%) 56 45	55, 115, 175, 254	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	119	TYR	5.4
1	D	175	ASN	5.1
1	B	1101	PHE	4.6
1	D	1040	CYS	4.5
1	D	1055	LEU	4.2

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
4	NH2	E	101	1/1	0.99	0.57	17.31	108,108,108,108	0
4	NH2	F	101	1/1	0.98	0.67	13.30	96,96,96,96	0
4	NH2	H	101	1/1	0.98	0.36	7.42	201,201,201,201	0
4	NH2	G	101	1/1	0.97	0.21	0.91	86,86,86,86	0
3	MAL	C	2201	23/23	0.97	0.22	0.40	61,70,85,89	0
3	MAL	B	2201	23/23	0.98	0.18	0.26	60,67,83,92	0
3	MAL	A	2201	23/23	0.98	0.17	0.02	70,75,82,86	0
3	MAL	D	2201	23/23	0.96	0.17	-0.77	90,101,109,113	0

6.5 Other polymers

There are no such residues in this entry.