



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 03:16 AM GMT

PDB ID : 1HV5
Title : CRYSTAL STRUCTURE OF THE STROMELYSIN-3 (MMP-11) CATALYTIC DOMAIN COMPLEXED WITH A PHOSPHINIC INHIBITOR
Authors : Gall, A.L.; Ruff, M.; Kannan, R.; Cuniasse, P.; Yiotakis, A.; Dive, V.; Rio, M.C.; Basset, P.; Moras, D.
Deposited on : 2001-01-08
Resolution : 2.60 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

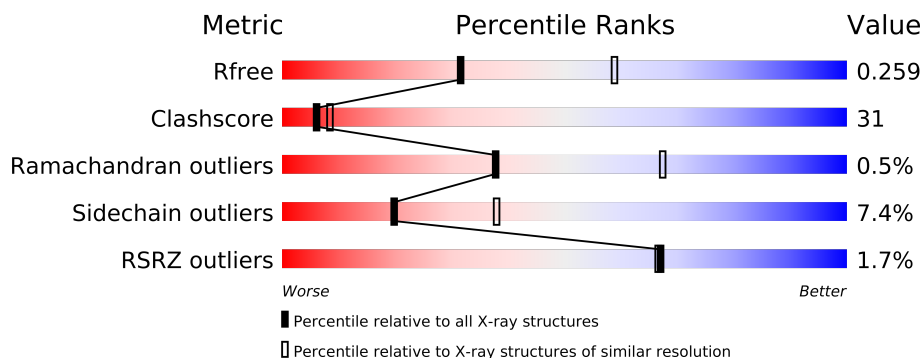
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.60 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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	165	
1	B	165	
1	C	165	
1	D	165	
1	E	165	
1	F	165	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	CPS	B	5002	-	X
4	CPS	E	5005	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	CPS	F	5091	-	X
5	RXP	A	6001	-	X
5	RXP	B	6002	-	X
5	RXP	C	6003	-	X
5	RXP	D	6004	-	X
5	RXP	E	6005	-	X
5	RXP	F	6006	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10772 atoms, of which 0 are hydrogen and 0 are deuterium.

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 STROMELYSIN 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1324	852	231	238	3			
1	B	164	Total	C	N	O	S	0	0	0
			1342	863	236	240	3			
1	C	162	Total	C	N	O	S	0	0	0
			1324	852	231	238	3			
1	D	162	Total	C	N	O	S	0	0	0
			1324	852	231	238	3			
1	E	165	Total	C	N	O	S	0	0	0
			1352	868	238	243	3			
1	F	162	Total	C	N	O	S	0	0	0
			1324	852	231	238	3			

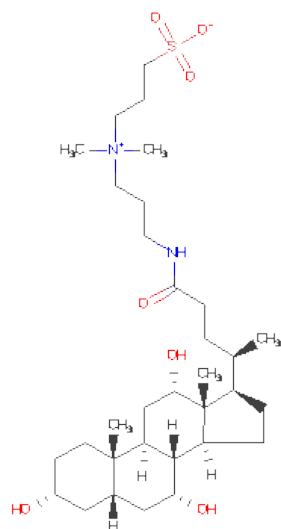
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Zn	0	0
			2	2		
2	E	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		
2	F	2	Total	Zn	0	0
			2	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0

- Molecule 4 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFONATE (three-letter code: CPS) (formula: $C_{32}H_{58}N_2O_7S$).



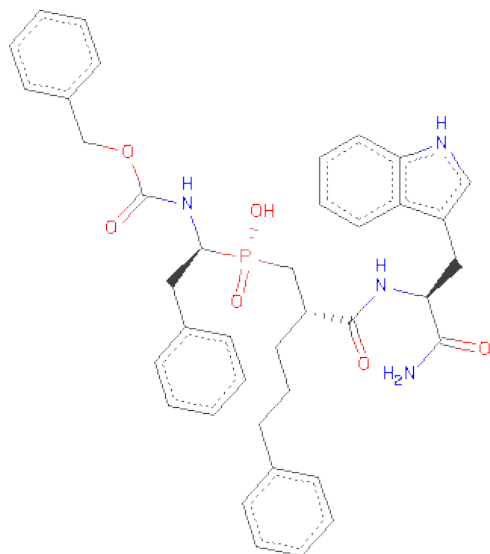
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 26 23 3	4	0
4	B	1	Total C O 26 23 3	4	0
4	C	1	Total C O 26 23 3	4	0
4	D	1	Total C O 26 23 3	4	0
4	E	1	Total C O 26 23 3	4	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	O			4	0
			26	23	3				
4	B	1	Total	C	O			4	0
			26	23	3				
4	C	1	Total	C	O			4	0
			26	23	3				
4	D	1	Total	C	O			4	0
			26	23	3				
4	E	1	Total	C	O			4	0
			26	23	3				
4	F	1	Total	C	O			4	0
			26	23	3				
4	F	1	Total	C	N	O	S	0	0
			42	32	2	7	1		

- Molecule 5 is 1-BENZYLOXYCARBONYLAMINO-2-PHENYL-ETHYL)-{2-[1-CARBAMOYL-2-(1H-INDOL-3-YL)-ETHYLCARBAMOYL]-5-PHENYL-PENTYL}-PHOSPHINIC ACID (three-letter code: RXP) (formula: C₃₉H₄₃N₄O₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			50	39	4	6	1		
5	B	1	Total	C	N	O	P	0	0
			50	39	4	6	1		
5	C	1	Total	C	N	O	P	0	0
			50	39	4	6	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	P	0	0
			50	39	4	6	1		
5	E	1	Total	C	N	O	P	0	0
			50	39	4	6	1		
5	F	1	Total	C	N	O	P	0	0
			50	39	4	6	1		

- Molecule 6 is water.

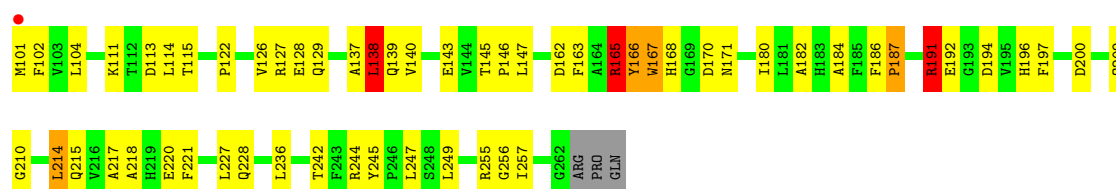
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	376	Total	O	0	0
			376	376		
6	B	318	Total	O	0	0
			318	318		
6	C	367	Total	O	0	0
			367	367		
6	D	341	Total	O	0	0
			341	341		
6	E	353	Total	O	0	0
			353	353		
6	F	381	Total	O	0	0
			381	381		

3 Residue-property plots

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

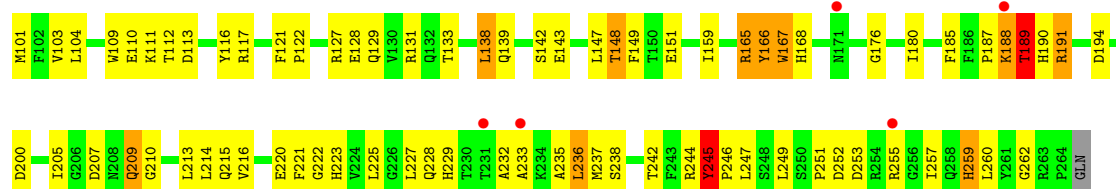
• Molecule 1: STROMELYSIN 3

Chain A: 



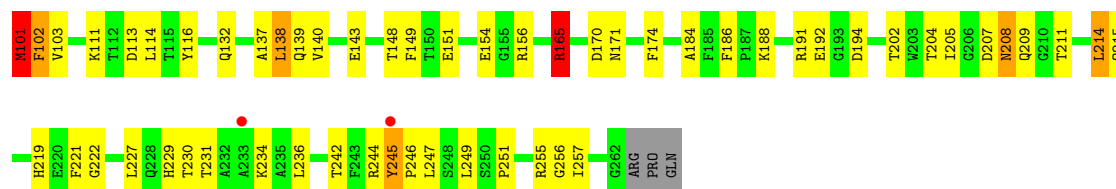
• Molecule 1: STROMELYSIN 3

Chain B: 



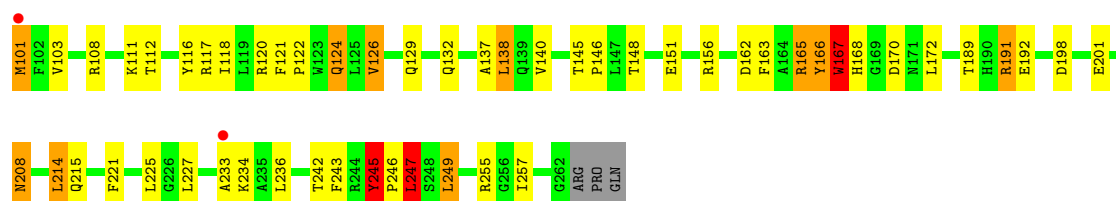
• Molecule 1: STROMELYSIN 3

Chain C: 



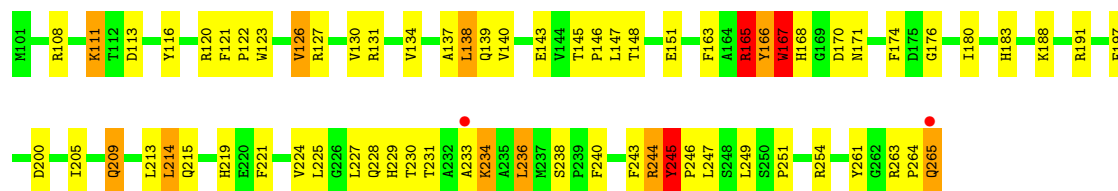
• Molecule 1: STROMELYSIN 3

Chain D: 



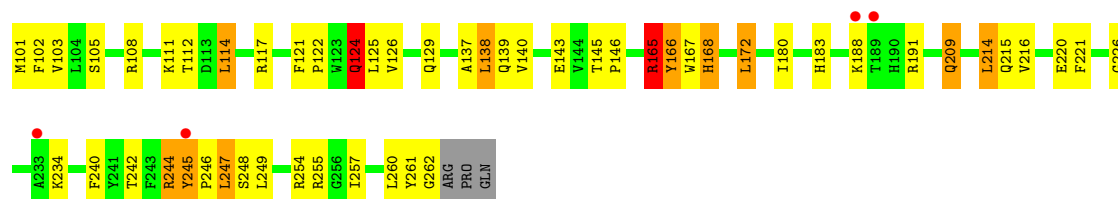
- Molecule 1: STROMELYSIN 3

Chain E:



- Molecule 1: STROMELYSIN 3

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	140.10Å 148.50Å 91.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.89 – 2.60 19.89 – 2.59	Depositor EDS
% Data completeness (in resolution range)	96.9 (19.89-2.60) 96.8 (19.89-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.50 (at 2.59Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.218 , 0.262 0.213 , 0.259	Depositor DCC
R_{free} test set	5828 reflections (10.16%)	DCC
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 59596 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10772	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RXP, ZN, CPS, CA

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	0.70	1/1367 (0.1%)	0.87	5/1861 (0.3%)
1	B	0.70	3/1386 (0.2%)	0.99	11/1887 (0.6%)
1	C	0.63	0/1367	0.94	9/1861 (0.5%)
1	D	0.79	3/1367 (0.2%)	0.97	11/1861 (0.6%)
1	E	0.66	1/1396 (0.1%)	0.88	5/1899 (0.3%)
1	F	0.75	3/1367 (0.2%)	0.94	7/1861 (0.4%)
All	All	0.70	11/8250 (0.1%)	0.93	48/11230 (0.4%)

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	1
1	D	0	3
1	E	0	1
1	F	0	1
All	All	0	6

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	166	TYR	C-N	-15.08	0.99	1.34
1	E	167	TRP	N-CA	11.29	1.69	1.46
1	A	167	TRP	N-CA	9.55	1.65	1.46
1	F	165	ARG	C-N	-9.54	1.12	1.34
1	F	168	HIS	C-N	-7.49	1.19	1.33

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	LYS	CB-CA-C	12.47	135.34	110.40
1	F	245	TYR	C-N-CD	10.84	151.17	128.40
1	C	245	TYR	C-N-CD	10.81	151.10	128.40
1	D	101	MET	N-CA-C	8.98	135.24	111.00
1	C	102	PHE	O-C-N	-8.87	108.51	122.70

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	TYR	Peptide
1	D	166	TYR	Mainchain,Peptide
1	D	245	TYR	Sidechain
1	E	166	TYR	Peptide
1	F	165	ARG	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1324	0	1253	70	0
1	B	1342	0	1272	77	0
1	C	1324	0	1253	77	0
1	D	1324	0	1252	58	0
1	E	1352	0	1281	85	0
1	F	1324	0	1252	68	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	52	0	70	16	0
4	B	52	0	70	15	0
4	C	52	0	70	15	0
4	D	52	0	70	9	0
4	E	52	0	70	16	0
4	F	68	0	91	30	0
5	A	50	0	42	5	0
5	B	50	0	42	4	0
5	C	50	0	42	1	0
5	D	50	0	42	1	0
5	E	50	0	42	9	0
5	F	50	0	42	2	0
6	A	376	0	0	35	0
6	B	318	0	0	30	0
6	C	367	0	0	31	0
6	D	341	0	0	28	0
6	E	353	0	0	31	1
6	F	381	0	0	34	0
All	All	10772	0	8256	517	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 31.

The worst 5 of 517 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:5004:CPS:C10	4:D:5004:CPS:C5	1.75	1.65
4:B:5007:CPS:C10	4:B:5007:CPS:C5	1.74	1.64
4:A:5006:CPS:C10	4:A:5006:CPS:C5	1.75	1.63
4:F:5091:CPS:C19	4:F:5091:CPS:C18	1.75	1.63
4:F:5011:CPS:C5	4:F:5011:CPS:C10	1.76	1.61

All (1) 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	Distance(Å)	Clash(Å)
1:F:101:MET:CE	6:E:6062:HOH:O[2_665]	1.33	0.87

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	160/165 (97%)	155 (97%)	5 (3%)	0	100	100
1	B	162/165 (98%)	148 (91%)	12 (7%)	2 (1%)	19	39
1	C	160/165 (97%)	151 (94%)	9 (6%)	0	100	100
1	D	160/165 (97%)	151 (94%)	7 (4%)	2 (1%)	18	35
1	E	163/165 (99%)	152 (93%)	10 (6%)	1 (1%)	33	63
1	F	160/165 (97%)	153 (96%)	7 (4%)	0	100	100
All	All	965/990 (98%)	910 (94%)	50 (5%)	5 (0%)	38	67

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	188	LYS
1	B	189	THR
1	D	167	TRP
1	E	167	TRP
1	D	245	TYR

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	137/140 (98%)	132 (96%)	5 (4%)	47	76
1	B	139/140 (99%)	126 (91%)	13 (9%)	13	23
1	C	137/140 (98%)	131 (96%)	6 (4%)	39	68
1	D	137/140 (98%)	125 (91%)	12 (9%)	14	27
1	E	140/140 (100%)	127 (91%)	13 (9%)	13	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	137/140 (98%)	125 (91%)	12 (9%)	14	27
All	All	827/840 (98%)	766 (93%)	61 (7%)	20	38

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	165	ARG
1	D	249	LEU
1	F	209	GLN
1	D	170	ASP
1	D	208	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	124	GLN
1	D	208	ASN
1	E	259	HIS
1	D	129	GLN
1	D	132	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 36 ligands modelled in this entry, 18 are monoatomic - leaving 18 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
4	CPS	A	5001	-	29,29,45	6.97	18 (62%)	46,47,70	4.19	27 (58%)
4	CPS	A	5006	-	29,29,45	7.05	17 (58%)	46,47,70	4.13	24 (52%)
5	RXP	A	6001	2	54,54,54	4.94	39 (72%)	73,73,73	2.85	30 (41%)
4	CPS	B	5002	-	29,29,45	7.28	17 (58%)	46,47,70	4.06	27 (58%)
4	CPS	B	5007	-	29,29,45	6.81	18 (62%)	46,47,70	4.06	27 (58%)
5	RXP	B	6002	2	54,54,54	5.63	40 (74%)	73,73,73	2.88	25 (34%)
4	CPS	C	5003	-	29,29,45	6.91	15 (51%)	46,47,70	4.19	29 (63%)
4	CPS	C	5008	-	29,29,45	6.85	18 (62%)	46,47,70	4.07	24 (52%)
5	RXP	C	6003	2	54,54,54	4.90	38 (70%)	73,73,73	3.11	30 (41%)
4	CPS	D	5004	-	29,29,45	7.29	17 (58%)	46,47,70	4.08	28 (60%)
4	CPS	D	5009	-	29,29,45	6.92	17 (58%)	46,47,70	4.02	27 (58%)
5	RXP	D	6004	2	54,54,54	5.09	35 (64%)	73,73,73	2.78	31 (42%)
4	CPS	E	5005	-	29,29,45	6.85	16 (55%)	46,47,70	4.26	27 (58%)
4	CPS	E	5010	-	29,29,45	6.84	17 (58%)	46,47,70	4.08	26 (56%)
5	RXP	E	6005	2	54,54,54	4.70	37 (68%)	73,73,73	2.76	31 (42%)
4	CPS	F	5011	-	29,29,45	6.92	18 (62%)	46,47,70	3.98	26 (56%)
4	CPS	F	5091	-	45,45,45	4.59	25 (55%)	70,70,70	3.20	33 (47%)
5	RXP	F	6006	2	54,54,54	4.70	37 (68%)	73,73,73	2.76	31 (42%)

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
4	CPS	A	5001	-	-	0/6/71/90	0/0/4/4
4	CPS	A	5006	-	-	0/6/71/90	0/0/4/4
5	RXP	A	6001	2	-	1/46/46/46	0/3/5/5
4	CPS	B	5002	-	-	0/6/71/90	0/0/4/4
4	CPS	B	5007	-	-	0/6/71/90	0/0/4/4
5	RXP	B	6002	2	-	1/46/46/46	0/3/5/5
4	CPS	C	5003	-	-	0/6/71/90	0/0/4/4
4	CPS	C	5008	-	-	0/6/71/90	0/0/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	RXP	C	6003	2	-	1/46/46/46	0/3/5/5
4	CPS	D	5004	-	-	0/6/71/90	0/0/4/4
4	CPS	D	5009	-	-	0/6/71/90	0/0/4/4
5	RXP	D	6004	2	-	0/46/46/46	0/3/5/5
4	CPS	E	5005	-	-	0/6/71/90	0/0/4/4
4	CPS	E	5010	-	-	0/6/71/90	0/0/4/4
5	RXP	E	6005	2	-	1/46/46/46	0/3/5/5
4	CPS	F	5011	-	-	0/6/71/90	0/0/4/4
4	CPS	F	5091	-	-	0/25/90/90	0/0/4/4
5	RXP	F	6006	2	-	1/46/46/46	0/3/5/5

The worst 5 of 439 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5004	CPS	C23-C22	-30.11	1.43	1.55
4	B	5002	CPS	C23-C22	-30.03	1.43	1.55
4	A	5006	CPS	C23-C22	-28.78	1.43	1.55
4	C	5003	CPS	C23-C22	-27.58	1.44	1.55
4	A	5001	CPS	C23-C22	-27.28	1.44	1.55

The worst 5 of 503 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	5005	CPS	C6-C18-C17	12.17	126.85	111.81
4	C	5008	CPS	C6-C18-C17	11.95	126.58	111.81
4	B	5007	CPS	C6-C18-C17	11.91	126.53	111.81
4	E	5010	CPS	C6-C18-C17	11.82	126.41	111.81
4	A	5001	CPS	C6-C18-C17	11.67	126.23	111.81

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	6003	RXP	O5-C30-N4-C22
5	F	6006	RXP	O5-C30-N4-C22
5	E	6005	RXP	O5-C30-N4-C22
5	A	6001	RXP	O5-C30-N4-C22
5	B	6002	RXP	O5-C30-N4-C22

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	162/165 (98%)	-0.55	1 (0%) 86 89	15, 26, 38, 50	0
1	B	164/165 (99%)	-0.22	5 (3%) 48 45	20, 36, 53, 60	0
1	C	162/165 (98%)	-0.45	2 (1%) 75 77	19, 30, 44, 53	0
1	D	162/165 (98%)	-0.42	2 (1%) 75 77	16, 29, 45, 55	0
1	E	165/165 (100%)	-0.41	2 (1%) 75 77	14, 31, 48, 56	0
1	F	162/165 (98%)	-0.42	4 (2%) 54 52	17, 31, 43, 56	0
All	All	977/990 (98%)	-0.41	16 (1%) 67 69	14, 30, 47, 60	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	233	ALA	6.7
1	C	245	TYR	4.3
1	E	233	ALA	4.3
1	F	233	ALA	3.9
1	F	245	TYR	3.7

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	RXP	E	6005	50/50	0.30	8.01	32,41,62,62	0
4	CPS	E	5005	26/42	0.27	5.32	46,48,49,50	4
4	CPS	F	5091	42/42	0.33	4.70	17,17,17,17	0
5	RXP	C	6003	50/50	0.21	4.02	25,34,53,54	0
5	RXP	A	6001	50/50	0.20	2.89	22,29,50,51	0
4	CPS	B	5002	26/42	0.26	2.42	50,51,52,53	4
5	RXP	B	6002	50/50	0.25	2.40	36,44,63,64	0
5	RXP	D	6004	50/50	0.18	2.20	21,27,42,43	0
5	RXP	F	6006	50/50	0.18	2.18	20,25,52,53	0
4	CPS	C	5008	26/42	0.20	1.37	48,49,50,50	4
4	CPS	D	5004	26/42	0.20	1.19	35,37,38,39	4
4	CPS	F	5011	26/42	0.22	0.95	53,54,55,55	4
4	CPS	D	5009	26/42	0.19	0.89	58,59,59,60	4
4	CPS	A	5006	26/42	0.18	0.66	49,50,51,51	4
4	CPS	C	5003	26/42	0.17	0.45	34,36,38,38	4
4	CPS	A	5001	26/42	0.15	0.33	34,36,37,39	4
3	CA	D	5512	1/1	0.11	-0.05	15,15,15,15	0
4	CPS	E	5010	26/42	0.12	-0.38	30,32,34,34	4
4	CPS	B	5007	26/42	0.12	-0.53	33,34,35,37	4
3	CA	F	5518	1/1	0.07	-1.74	18,18,18,18	0
3	CA	B	5506	1/1	0.05	-2.09	26,26,26,26	0
2	ZN	A	5501	1/1	0.07	-2.46	24,24,24,24	0
2	ZN	C	5507	1/1	0.08	-2.49	23,23,23,23	0
2	ZN	A	5502	1/1	0.07	-2.53	19,19,19,19	0
2	ZN	D	5511	1/1	0.08	-2.54	18,18,18,18	0
2	ZN	D	5510	1/1	0.08	-2.74	22,22,22,22	0
3	CA	A	5503	1/1	0.04	-2.86	18,18,18,18	0
2	ZN	E	5513	1/1	0.07	-3.39	24,24,24,24	0
3	CA	E	5515	1/1	0.06	-3.85	28,28,28,28	0
2	ZN	B	5505	1/1	0.06	-3.86	26,26,26,26	0
2	ZN	F	5517	1/1	0.08	-4.11	23,23,23,23	0
2	ZN	F	5516	1/1	0.08	-4.50	26,26,26,26	0
3	CA	C	5509	1/1	0.05	-4.55	24,24,24,24	0
2	ZN	B	5504	1/1	0.07	-5.16	25,25,25,25	0
2	ZN	C	5508	1/1	0.04	-7.81	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	E	5514	1/1	0.04	-13.73	21,21,21,21	0

6.5 Other polymers ⓘ

There are no such residues in this entry.