Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:05 PM GMT

PDB ID	:	4H49
Title	:	Crystal structure of the catalytic domain of MMP-12 in complex with a twin inhibitor.
Authors	:	Antoni, C.; Stura, E.A.; Vera, L.; Nuti, E.; Carafa, L.; Cassar-Lajeunesse, E.; Dive, V.; Rossello, A.
Deposited on	:	2012-09-17
Resolution	:	2.16 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

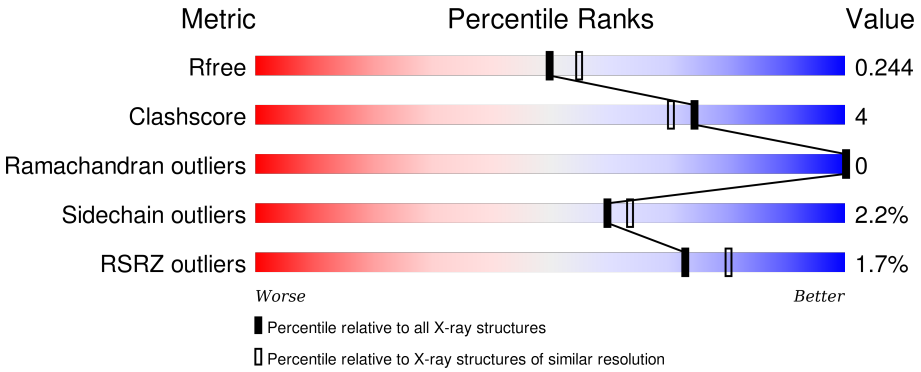
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.16 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}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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 <=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	159	2% 87% 13%
1	B	159	2% 91% 7%
1	C	159	2% 91% 6%
1	D	159	2% 97%

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	PGO	A	309	-	-	-	X
6	PEG	A	308	-	-	-	X
6	PEG	B	607	-	-	-	X
6	PEG	C	307	-	-	-	X
6	PEG	D	306	-	-	-	X
8	GOL	B	608	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5509 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 Macrophage metalloelastase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	0	1	0
			1257	800	221	232	4			
1	B	159	Total	C	N	O	S	0	0	0
			1246	794	217	231	4			
1	C	156	Total	C	N	O	S	0	4	0
			1263	804	222	234	3			
1	D	159	Total	C	N	O	S	0	3	0
			1273	809	223	237	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	MET	-	EXPRESSION TAG	UNP P39900
A	171	ASP	PHE	ENGINEERED MUTATION	UNP P39900
B	105	MET	-	EXPRESSION TAG	UNP P39900
B	171	ASP	PHE	ENGINEERED MUTATION	UNP P39900
C	105	MET	-	EXPRESSION TAG	UNP P39900
C	171	ASP	PHE	ENGINEERED MUTATION	UNP P39900
D	105	MET	-	EXPRESSION TAG	UNP P39900
D	171	ASP	PHE	ENGINEERED MUTATION	UNP P39900

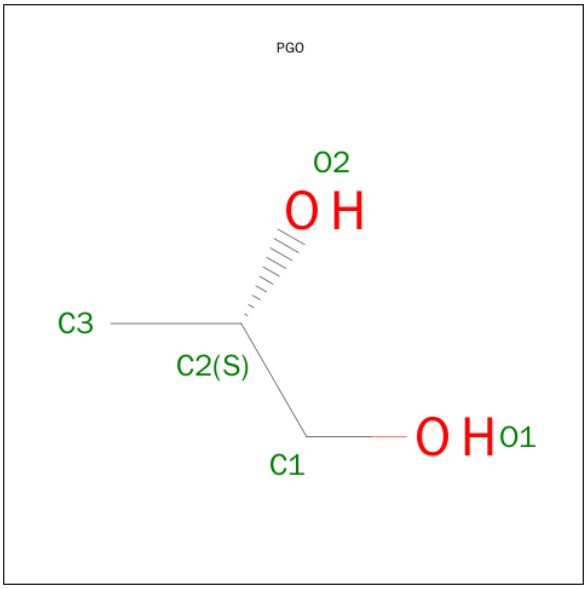
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

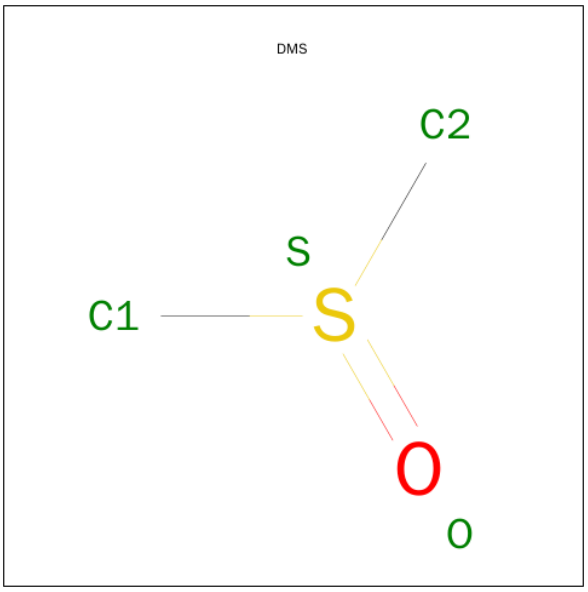
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	3	Total Ca 3 3	0	0
3	A	3	Total Ca 3 3	0	0
3	D	3	Total Ca 3 3	0	0
3	C	3	Total Ca 3 3	0	0

- Molecule 4 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: $C_3H_8O_2$).



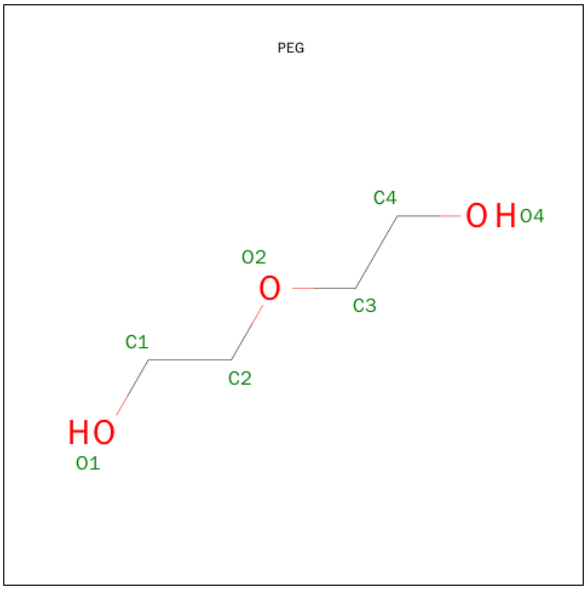
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 5 3 2	0	0
4	A	1	Total C O 5 3 2	0	0

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O S 4 2 1 1	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0

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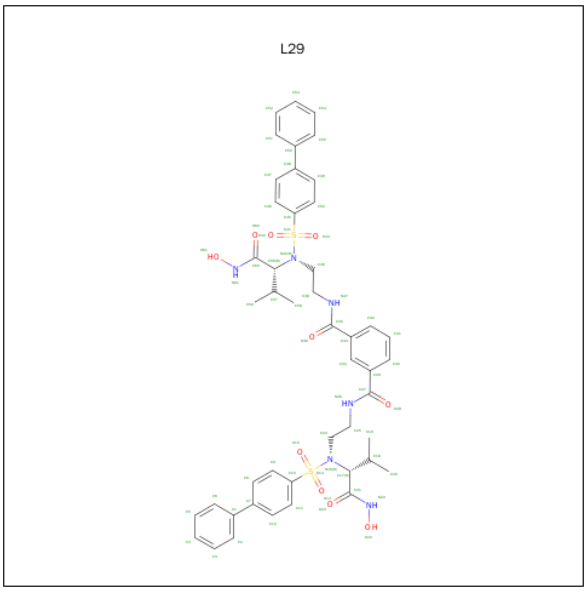
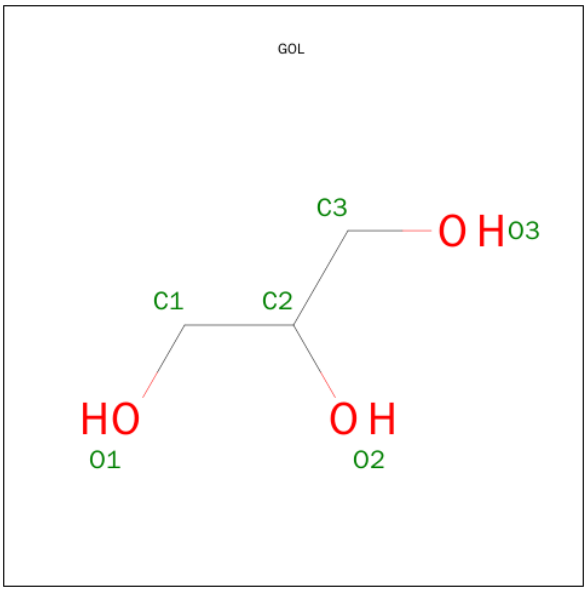
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is N,N'-BIS(2-{(BIPHENYL-4-YLSULFONYL)[(2R)-1-(HYDROXYAMINO)-3-METHYL-1-OXOBUTAN-2-YL]AMINO}ETHYL)BENZENE-1,3-DICARBOXAMIDE (NON-PREFERRED NAME) (three-letter code: L29) (formula: $C_{46}H_{52}N_6O_{10}S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			64	46	6	10	2		
7	C	1	Total	C	N	O	S	0	0
			64	46	6	10	2		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 6 3 3	0	0

- Molecule 9 is water.

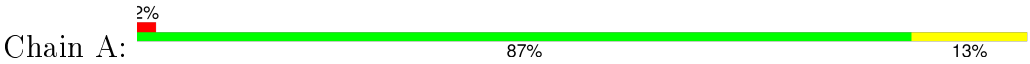
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	62	Total O 62 62	0	0
9	B	63	Total O 63 63	0	0
9	C	64	Total O 64 64	0	0
9	D	85	Total O 85 85	0	0

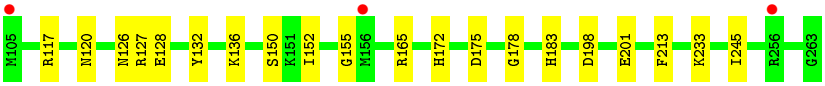
3 Residue-property plots (i)

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: Macrophage metalloelastase

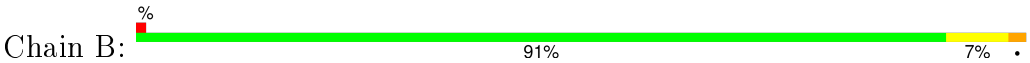
Chain A:





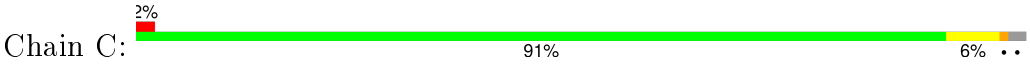
- Molecule 1: Macrophage metalloelastase

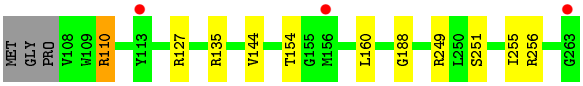
Chain B:



- Molecule 1: Macrophage metalloelastase

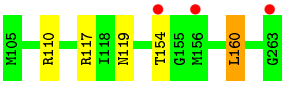
Chain C:





- Molecule 1: Macrophage metalloelastase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	47.44Å 106.49Å 65.88Å 90.00° 94.96° 90.00°	Depositor
Resolution (Å)	47.26 – 2.16 47.26 – 2.16	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.26-2.16) 99.3 (47.26-2.16)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 2.16Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.167 , 0.241 0.172 , 0.244	Depositor DCC
R_{free} test set	1741 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	30.2	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 34817 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5509	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.34% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, ZN, PGO, CA, DMS, L29, PEG

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	0.41	0/1294	0.55	0/1752
1	B	0.39	0/1283	0.52	0/1738
1	C	0.38	0/1300	0.54	0/1759
1	D	0.38	0/1310	0.52	0/1774
All	All	0.39	0/5187	0.53	0/7023

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

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	1257	0	1188	16	0
1	B	1246	0	1176	12	0
1	C	1263	0	1190	7	0
1	D	1273	0	1199	7	0
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
3	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
4	A	10	0	16	1	0
5	A	4	0	6	2	0
6	A	7	0	10	1	0
6	B	7	0	10	2	0
6	C	7	0	10	0	0
6	D	7	0	10	2	0
7	B	64	0	51	2	0
7	C	64	0	50	0	0
8	B	6	0	8	1	0
9	A	62	0	0	1	0
9	B	63	0	0	1	0
9	C	64	0	0	1	0
9	D	85	0	0	0	0
All	All	5509	0	4924	41	0

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 4.

All (41) 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:D:110:ARG:H	6:D:306:PEG:H42	1.52	0.75
1:D:117[B]:ARG:HH12	1:D:154:THR:HA	1.58	0.69
1:D:119:ASN:HB2	1:D:160:LEU:HD12	1.76	0.67
1:A:127:ARG:HH22	4:A:309:PGO:H12	1.62	0.65
1:C:144:VAL:HG11	1:C:255:ILE:HD12	1.85	0.59
1:A:120:ASN:HB2	6:A:308:PEG:H22	1.85	0.58
1:A:117:ARG:NH2	1:A:155:GLY:O	2.39	0.56
1:A:128:GLU:CD	1:A:128:GLU:H	2.09	0.56
1:B:128:GLU:HG3	1:C:135:ARG:HD2	1.88	0.55
1:D:110:ARG:H	6:D:306:PEG:C4	2.19	0.53
1:B:128:GLU:HB2	1:C:135:ARG:CZ	2.40	0.51
1:B:240:TYR:HD2	6:B:607:PEG:H12	1.75	0.51
1:A:165[B]:ARG:H	5:A:307:DMS:H11	1.75	0.51
1:A:165[A]:ARG:H	5:A:307:DMS:H11	1.75	0.50
1:A:132:TYR:O	1:A:136:LYS:HG2	2.11	0.50
1:C:110:ARG:HH22	1:C:188:GLY:HA2	1.76	0.50
7:B:601:L29:H28	9:B:731:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:LYS:HD3	1:B:111:LYS:H	1.79	0.48
1:B:241:LYS:H	8:B:608:GOL:H32	1.80	0.47
1:A:165[A]:ARG:NH2	9:A:449:HOH:O	2.49	0.44
1:B:244:ASP:HB3	1:B:247:THR:HG23	2.00	0.44
1:B:165:ARG:HB3	1:B:199:GLU:HB3	1.99	0.44
1:A:198:ASP:HB3	1:A:201:GLU:HG2	2.00	0.43
1:A:175:ASP:O	1:B:241:LYS:HE2	2.19	0.43
1:C:251:SER:O	1:C:255:ILE:HG12	2.19	0.43
1:A:213:PHE:HD2	1:A:245:ILE:HD12	1.83	0.43
1:D:117[A]:ARG:NH2	1:D:160:LEU:HD11	2.34	0.43
1:A:178:GLY:HA3	6:B:607:PEG:H31	2.00	0.43
1:A:126:ASN:HB3	1:A:128:GLU:OE2	2.20	0.42
1:D:117[B]:ARG:HH12	1:D:154:THR:CA	2.27	0.42
1:B:128:GLU:H	1:B:128:GLU:HG2	1.45	0.42
1:C:127:ARG:NH1	9:C:418:HOH:O	2.30	0.42
1:A:136:LYS:HD2	1:A:136:LYS:HA	1.87	0.42
1:C:160:LEU:HA	1:C:160:LEU:HD12	1.92	0.41
1:B:176:GLY:HA2	1:B:200:ASP:OD2	2.20	0.41
1:B:152:ILE:HD11	1:B:157:ALA:HB2	2.02	0.41
1:A:172:HIS:O	1:A:183:HIS:HE1	2.04	0.41
7:B:601:L29:H22	7:B:601:L29:H17	2.03	0.41
1:B:130:VAL:O	1:B:134:ILE:HG12	2.21	0.41
1:D:117[A]:ARG:HH21	1:D:160:LEU:HD21	1.86	0.40
1:A:213:PHE:CD2	1:A:245:ILE:HG23	2.56	0.40

There are no symmetry-related clashes.

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	158/159 (99%)	154 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
1	C	158/159 (99%)	151 (96%)	7 (4%)	0	100	100
1	D	160/159 (101%)	155 (97%)	5 (3%)	0	100	100
All	All	633/636 (100%)	611 (96%)	22 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	129/128 (101%)	126 (98%)	3 (2%)	58	62
1	B	128/128 (100%)	125 (98%)	3 (2%)	58	62
1	C	130/128 (102%)	126 (97%)	4 (3%)	47	47
1	D	131/128 (102%)	130 (99%)	1 (1%)	86	91
All	All	518/512 (101%)	507 (98%)	11 (2%)	60	65

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	SER
1	A	152	ILE
1	A	233	LYS
1	B	111	LYS
1	B	128	GLU
1	B	247	THR
1	C	110	ARG
1	C	154	THR
1	C	249	ARG
1	C	256	ARG
1	D	160	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no

such sidechains identified.

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 30 ligands modelled in this entry, 20 are monoatomic - leaving 10 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	PGO	A	306	-	4,4,4	0.61	0	2,4,4	0.16	0
5	DMS	A	307	-	3,3,3	0.52	0	3,3,3	0.81	0
6	PEG	A	308	-	6,6,6	0.55	0	5,5,5	0.55	0
4	PGO	A	309	-	4,4,4	0.45	0	2,4,4	0.43	0
7	L29	B	601	2	66,68,68	5.35	34 (51%)	88,96,96	2.14	22 (25%)
6	PEG	B	607	-	6,6,6	0.57	0	5,5,5	0.36	0
8	GOL	B	608	-	5,5,5	0.39	0	5,5,5	0.24	0
7	L29	C	306	2	66,68,68	5.37	36 (54%)	88,96,96	2.03	18 (20%)
6	PEG	C	307	-	6,6,6	0.51	0	5,5,5	0.19	0
6	PEG	D	306	-	6,6,6	0.52	0	5,5,5	0.18	0

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	PGO	A	306	-	-	0/2/2/2	0/0/0/0
5	DMS	A	307	-	-	0/0/0/0	0/0/0/0
6	PEG	A	308	-	-	0/4/4/4	0/0/0/0
4	PGO	A	309	-	-	0/2/2/2	0/0/0/0
7	L29	B	601	2	-	0/80/80/80	0/5/5/5
6	PEG	B	607	-	-	0/4/4/4	0/0/0/0
8	GOL	B	608	-	-	0/4/4/4	0/0/0/0
7	L29	C	306	2	-	0/80/80/80	0/5/5/5
6	PEG	C	307	-	-	0/4/4/4	0/0/0/0
6	PEG	D	306	-	-	0/4/4/4	0/0/0/0

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	601	L29	S13-N16	-5.85	1.54	1.63
7	C	306	L29	S13-N16	-5.72	1.54	1.63
7	B	601	L29	C56-N40	-3.56	1.43	1.48
7	C	306	L29	C56-N40	-3.09	1.44	1.48
7	C	306	L29	O23-C21	-3.05	1.17	1.23
7	B	601	L29	O23-C21	-2.81	1.17	1.23
7	C	306	L29	O28-C27	-2.26	1.18	1.23
7	B	601	L29	O28-C27	-2.25	1.18	1.23
7	C	306	L29	C17-N16	-2.23	1.45	1.48
7	C	306	L29	O36-C35	-2.18	1.18	1.23
7	C	306	L29	O62-C60	-2.15	1.19	1.23
7	B	601	L29	O62-C60	-2.12	1.19	1.23
7	B	601	L29	C8-C9	2.04	1.42	1.38
7	B	601	L29	C50-C48	2.07	1.54	1.49
7	B	601	L29	C1-C7	2.10	1.54	1.49
7	C	306	L29	C49-C48	2.12	1.43	1.39
7	C	306	L29	C53-C52	2.14	1.43	1.38
7	C	306	L29	C1-C7	2.32	1.55	1.49
7	B	601	L29	C49-C48	2.53	1.44	1.39
7	C	306	L29	C52-C51	2.55	1.44	1.38
7	C	306	L29	C8-C9	2.56	1.43	1.38
7	B	601	L29	C49-C5A	2.80	1.43	1.38
7	C	306	L29	C49-C5A	2.97	1.44	1.38
7	B	601	L29	C52-C51	3.05	1.45	1.38
7	C	306	L29	C55-C50	3.38	1.46	1.39
7	B	601	L29	C55-C50	3.45	1.46	1.39
7	B	601	L29	C5-C6	3.54	1.46	1.38
7	C	306	L29	C9-C10	3.59	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	306	L29	C5-C6	3.60	1.46	1.38
7	C	306	L29	C34-C33	3.71	1.44	1.39
7	B	601	L29	C47-C48	3.74	1.47	1.39
7	B	601	L29	C9-C10	3.76	1.45	1.38
7	C	306	L29	C47-C48	3.92	1.47	1.39
7	C	306	L29	C45-S41	4.10	1.82	1.76
7	B	601	L29	C34-C33	4.43	1.46	1.39
7	B	601	L29	C10-S13	4.79	1.83	1.76
7	B	601	L29	C12-C11	4.80	1.47	1.38
7	B	601	L29	S41-N40	4.91	1.70	1.63
7	B	601	L29	C45-S41	4.95	1.83	1.76
7	B	601	L29	C11-C10	5.34	1.47	1.38
7	B	601	L29	C47-C46	5.35	1.48	1.38
7	C	306	L29	C47-C46	5.36	1.48	1.38
7	C	306	L29	C12-C11	5.47	1.48	1.38
7	C	306	L29	C31-C30	5.77	1.50	1.38
7	C	306	L29	C35-N37	5.85	1.46	1.33
7	C	306	L29	C10-S13	5.90	1.85	1.76
7	C	306	L29	C11-C10	5.91	1.48	1.38
7	C	306	L29	S41-N40	5.97	1.71	1.63
7	B	601	L29	C31-C30	6.04	1.51	1.38
7	B	601	L29	C8-C7	6.07	1.52	1.39
7	B	601	L29	C35-N37	6.08	1.47	1.33
7	C	306	L29	C31-C32	6.11	1.51	1.38
7	B	601	L29	C31-C32	6.19	1.51	1.38
7	B	601	L29	C27-N26	6.21	1.47	1.33
7	C	306	L29	C8-C7	6.34	1.53	1.39
7	C	306	L29	C3-C2	6.48	1.52	1.38
7	B	601	L29	C3-C2	6.50	1.52	1.38
7	C	306	L29	C27-N26	6.76	1.48	1.33
7	C	306	L29	C5A-C45	8.27	1.52	1.38
7	B	601	L29	C5A-C45	8.41	1.52	1.38
7	C	306	L29	C34-C29	10.04	1.54	1.39
7	B	601	L29	C34-C29	10.47	1.54	1.39
7	B	601	L29	O14-S13	15.66	1.63	1.43
7	C	306	L29	O14-S13	15.94	1.63	1.43
7	C	306	L29	O42-S41	16.36	1.64	1.43
7	B	601	L29	O42-S41	16.37	1.64	1.43
7	B	601	L29	O15-S13	16.94	1.65	1.43
7	C	306	L29	O43-S41	17.04	1.65	1.43
7	C	306	L29	O15-S13	17.39	1.65	1.43
7	B	601	L29	O43-S41	17.83	1.66	1.43

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	601	L29	O14-S13-C10	-9.19	96.08	108.00
7	C	306	L29	O14-S13-C10	-9.18	96.08	108.00
7	B	601	L29	O15-S13-C10	-8.73	96.67	108.00
7	C	306	L29	O15-S13-C10	-5.89	100.36	108.00
7	C	306	L29	O22-N22-C21	-4.80	113.08	119.86
7	B	601	L29	O61-N61-C60	-4.16	113.97	119.86
7	B	601	L29	O43-S41-O42	-3.80	112.91	119.47
7	C	306	L29	C39-N40-S41	-3.46	110.42	117.81
7	B	601	L29	C39-N40-S41	-3.14	111.11	117.81
7	B	601	L29	C38-C39-N40	-2.88	107.39	112.34
7	C	306	L29	O43-S41-O42	-2.77	114.69	119.47
7	C	306	L29	C25-N26-C27	-2.69	116.13	122.15
7	C	306	L29	C33-C34-C29	-2.42	117.82	120.47
7	B	601	L29	C33-C34-C29	-2.38	117.86	120.47
7	B	601	L29	C38-N37-C35	-2.38	116.83	122.15
7	C	306	L29	C38-N37-C35	-2.33	116.94	122.15
7	C	306	L29	C6-C1-C7	-2.30	117.27	121.39
7	C	306	L29	C47-C48-C50	-2.20	117.45	121.39
7	B	601	L29	C55-C50-C48	-2.15	117.54	121.39
7	B	601	L29	O42-S41-C45	-2.09	105.28	108.00
7	C	306	L29	C51-C50-C48	-2.09	117.65	121.39
7	B	601	L29	C8-C7-C1	-2.03	117.74	121.39
7	C	306	L29	O42-S41-C45	-2.02	105.39	108.00
7	B	601	L29	C49-C48-C47	2.06	121.45	117.55
7	B	601	L29	C60-C56-N40	2.18	116.19	110.35
7	C	306	L29	C30-C29-C34	2.22	121.93	119.24
7	B	601	L29	O14-S13-O15	2.29	123.42	119.47
7	B	601	L29	C6-C1-C2	2.30	121.90	117.55
7	C	306	L29	C49-C48-C47	2.38	122.05	117.55
7	B	601	L29	C8-C7-C12	2.43	122.15	117.55
7	B	601	L29	C39-C38-N37	2.43	116.15	111.72
7	C	306	L29	C32-C33-C34	2.62	122.41	119.24
7	B	601	L29	C32-C33-C34	2.71	122.52	119.24
7	B	601	L29	C57-C56-C60	2.96	115.41	111.89
7	B	601	L29	O14-S13-N16	2.98	113.31	106.97
7	B	601	L29	O15-S13-N16	3.41	114.21	106.97
7	C	306	L29	O14-S13-N16	3.67	114.78	106.97
7	C	306	L29	O15-S13-N16	4.05	115.58	106.97
7	B	601	L29	C45-S41-N40	4.27	114.36	107.38
7	C	306	L29	C45-S41-N40	6.11	117.37	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	307	DMS	2	0
6	A	308	PEG	1	0
4	A	309	PGO	1	0
7	B	601	L29	2	0
6	B	607	PEG	2	0
8	B	608	GOL	1	0
6	D	306	PEG	2	0

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	159/159 (100%)	-0.16	3 (1%)	70	78	9, 18, 38, 58	1 (0%)
1	B	159/159 (100%)	-0.01	2 (1%)	79	84	10, 23, 42, 64	0
1	C	156/159 (98%)	-0.13	3 (1%)	70	78	10, 22, 40, 47	1 (0%)
1	D	159/159 (100%)	0.00	3 (1%)	70	78	11, 22, 40, 63	2 (1%)
All	All	633/636 (99%)	-0.07	11 (1%)	73	80	9, 22, 40, 64	4 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	MET	5.2
1	B	105	MET	5.0
1	B	263	GLY	4.9
1	D	154	THR	4.0
1	D	263	GLY	3.9
1	C	263	GLY	3.5
1	C	156	MET	2.8
1	D	156	MET	2.6
1	A	156	MET	2.4
1	A	256	ARG	2.0
1	C	113	TYR	2.0

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	PEG	B	607	7/7	0.86	0.29	11.66	20,33,43,45	0
6	PEG	A	308	7/7	0.80	0.49	11.54	26,28,40,49	0
6	PEG	C	307	7/7	0.79	0.32	8.61	28,33,40,50	0
4	PGO	A	309	5/5	0.95	0.28	6.26	32,37,38,43	0
8	GOL	B	608	6/6	0.83	0.23	5.70	33,37,40,50	0
6	PEG	D	306	7/7	0.86	0.29	4.12	29,41,50,55	0
3	CA	A	305	1/1	1.00	0.11	0.93	14,14,14,14	0
2	ZN	B	602	1/1	1.00	0.10	0.91	16,16,16,16	0
7	L29	B	601	64/64	0.97	0.12	0.84	8,16,22,28	0
5	DMS	A	307	4/4	0.96	0.15	0.53	31,33,33,34	0
3	CA	C	305	1/1	0.99	0.11	0.23	19,19,19,19	0
7	L29	C	306	64/64	0.97	0.12	0.02	8,16,23,27	0
2	ZN	A	302	1/1	1.00	0.11	-0.14	14,14,14,14	0
3	CA	B	605	1/1	0.97	0.11	-0.69	31,31,31,31	0
3	CA	B	606	1/1	0.96	0.10	-0.80	26,26,26,26	0
3	CA	A	304	1/1	0.99	0.09	-0.84	17,17,17,17	0
3	CA	A	303	1/1	0.99	0.06	-1.54	19,19,19,19	0
3	CA	C	304	1/1	0.97	0.08	-1.73	28,28,28,28	0
2	ZN	C	302	1/1	1.00	0.08	-1.78	21,21,21,21	0
3	CA	D	305	1/1	0.98	0.06	-2.22	23,23,23,23	0
2	ZN	D	302	1/1	0.99	0.07	-2.40	24,24,24,24	0
3	CA	D	303	1/1	0.95	0.04	-2.47	26,26,26,26	0
3	CA	C	303	1/1	0.96	0.05	-2.51	27,27,27,27	0
2	ZN	B	603	1/1	0.99	0.07	-2.70	26,26,26,26	0
3	CA	B	604	1/1	0.98	0.04	-3.06	31,31,31,31	0
3	CA	D	304	1/1	0.99	0.04	-5.27	26,26,26,26	0
2	ZN	A	301	1/1	1.00	0.11	-	14,14,14,14	0
2	ZN	C	301	1/1	0.99	0.12	-	16,16,16,16	0
2	ZN	D	301	1/1	1.00	0.08	-	17,17,17,17	0
4	PGO	A	306	5/5	0.82	0.21	-	32,34,38,39	0

6.5 Other polymers

There are no such residues in this entry.