Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:46 PM GMT

PDB ID	:	3UZE
Title	:	Crystal structure of the dengue virus serotype 3 envelope protein domain III in complex with the variable domains of Mab 4E11
Authors	:	Cockburn, J.J.B.; Navarro Sanchez, M.E.; Fretes, N.; Urvoas, A.; Staropoli, I.; Kikuti, C.M.; Coffey, L.L.; Arenzana Seisdedos, F.; Bedouelle, H.; Rey, F.A.
Deposited on	:	2011-12-07
Resolution	:	2.04 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:

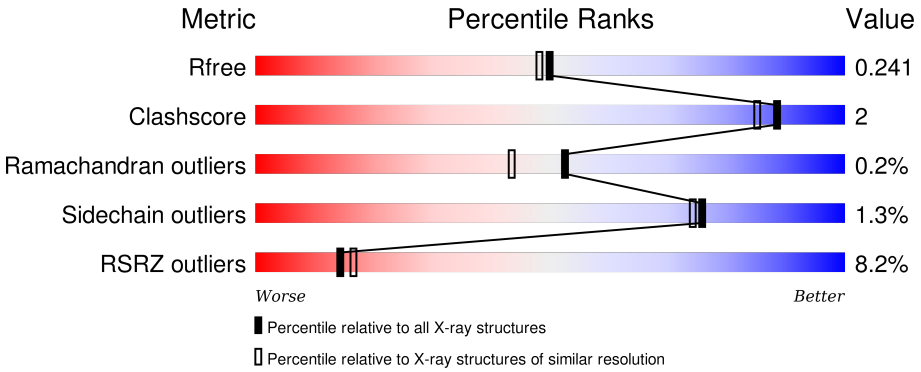
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.04 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	253	2% 83% 8% 9%
1	B	253	3% 83% 6% 11%
2	C	139	9% 60% 8% 32%
2	D	139	19% 48% 5% 47%

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
3	EDO	A	254	-	-	-	X
3	EDO	A	255	-	-	-	X
3	EDO	C	1	-	-	-	X
4	GOL	A	257	-	-	-	X
4	GOL	A	258	-	-	-	X
4	GOL	B	258	-	-	-	X
5	EPE	B	254	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5202 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 Variable domains of murine anti-dengue Mab 4E11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	5	0
			1790	1128	306	347	9			
1	B	226	Total	C	N	O	S	0	4	0
			1759	1111	299	340	9			

- Molecule 2 is a protein called Envelope protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	94	Total	C	N	O	S	0	0	0
			730	470	123	134	3			
2	D	74	Total	C	N	O	S	0	0	0
			581	377	92	109	3			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	396	PRO	-	EXPRESSION TAG	UNP Q7TGD1
C	397	PHE	-	EXPRESSION TAG	UNP Q7TGD1
C	398	GLU	-	EXPRESSION TAG	UNP Q7TGD1
C	399	ASP	-	EXPRESSION TAG	UNP Q7TGD1
C	400	ASP	-	EXPRESSION TAG	UNP Q7TGD1
C	401	ASP	-	EXPRESSION TAG	UNP Q7TGD1
C	402	ASP	-	EXPRESSION TAG	UNP Q7TGD1
C	403	LYS	-	EXPRESSION TAG	UNP Q7TGD1
C	404	ALA	-	EXPRESSION TAG	UNP Q7TGD1
C	405	GLY	-	EXPRESSION TAG	UNP Q7TGD1
C	406	TRP	-	EXPRESSION TAG	UNP Q7TGD1
C	407	SER	-	EXPRESSION TAG	UNP Q7TGD1
C	408	HIS	-	EXPRESSION TAG	UNP Q7TGD1
C	409	PRO	-	EXPRESSION TAG	UNP Q7TGD1
C	410	GLN	-	EXPRESSION TAG	UNP Q7TGD1
C	411	PHE	-	EXPRESSION TAG	UNP Q7TGD1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	412	GLU	-	EXPRESSION TAG	UNP Q7TGD1
C	413	LYS	-	EXPRESSION TAG	UNP Q7TGD1
C	414	GLY	-	EXPRESSION TAG	UNP Q7TGD1
C	415	GLY	-	EXPRESSION TAG	UNP Q7TGD1
C	416	GLY	-	EXPRESSION TAG	UNP Q7TGD1
C	417	SER	-	EXPRESSION TAG	UNP Q7TGD1
C	418	GLY	-	EXPRESSION TAG	UNP Q7TGD1
C	419	GLY	-	EXPRESSION TAG	UNP Q7TGD1
C	420	GLY	-	EXPRESSION TAG	UNP Q7TGD1
C	421	SER	-	EXPRESSION TAG	UNP Q7TGD1
C	422	GLY	-	EXPRESSION TAG	UNP Q7TGD1
C	423	GLY	-	EXPRESSION TAG	UNP Q7TGD1
C	424	GLY	-	EXPRESSION TAG	UNP Q7TGD1
C	425	SER	-	EXPRESSION TAG	UNP Q7TGD1
C	426	TRP	-	EXPRESSION TAG	UNP Q7TGD1
C	427	SER	-	EXPRESSION TAG	UNP Q7TGD1
C	428	HIS	-	EXPRESSION TAG	UNP Q7TGD1
C	429	PRO	-	EXPRESSION TAG	UNP Q7TGD1
C	430	GLN	-	EXPRESSION TAG	UNP Q7TGD1
C	431	PHE	-	EXPRESSION TAG	UNP Q7TGD1
C	432	GLU	-	EXPRESSION TAG	UNP Q7TGD1
C	433	LYS	-	EXPRESSION TAG	UNP Q7TGD1
D	396	PRO	-	EXPRESSION TAG	UNP Q7TGD1
D	397	PHE	-	EXPRESSION TAG	UNP Q7TGD1
D	398	GLU	-	EXPRESSION TAG	UNP Q7TGD1
D	399	ASP	-	EXPRESSION TAG	UNP Q7TGD1
D	400	ASP	-	EXPRESSION TAG	UNP Q7TGD1
D	401	ASP	-	EXPRESSION TAG	UNP Q7TGD1
D	402	ASP	-	EXPRESSION TAG	UNP Q7TGD1
D	403	LYS	-	EXPRESSION TAG	UNP Q7TGD1
D	404	ALA	-	EXPRESSION TAG	UNP Q7TGD1
D	405	GLY	-	EXPRESSION TAG	UNP Q7TGD1
D	406	TRP	-	EXPRESSION TAG	UNP Q7TGD1
D	407	SER	-	EXPRESSION TAG	UNP Q7TGD1
D	408	HIS	-	EXPRESSION TAG	UNP Q7TGD1
D	409	PRO	-	EXPRESSION TAG	UNP Q7TGD1
D	410	GLN	-	EXPRESSION TAG	UNP Q7TGD1
D	411	PHE	-	EXPRESSION TAG	UNP Q7TGD1
D	412	GLU	-	EXPRESSION TAG	UNP Q7TGD1
D	413	LYS	-	EXPRESSION TAG	UNP Q7TGD1
D	414	GLY	-	EXPRESSION TAG	UNP Q7TGD1
D	415	GLY	-	EXPRESSION TAG	UNP Q7TGD1

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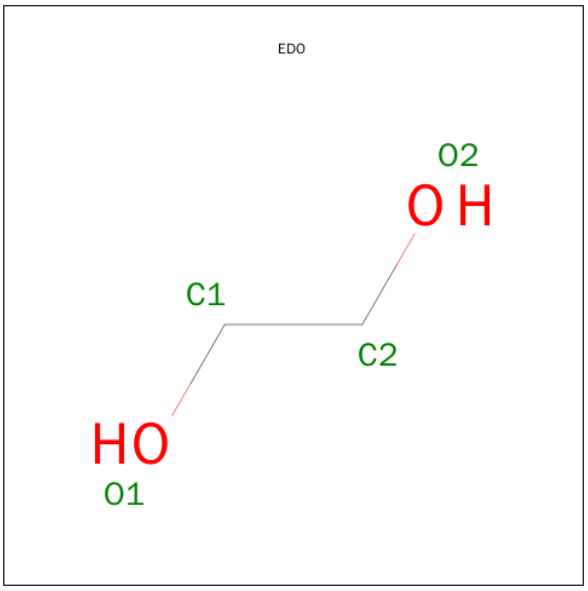
Chain	Residue	Modelled	Actual	Comment	Reference
D	416	GLY	-	EXPRESSION TAG	UNP Q7TGD1
D	417	SER	-	EXPRESSION TAG	UNP Q7TGD1
D	418	GLY	-	EXPRESSION TAG	UNP Q7TGD1
D	419	GLY	-	EXPRESSION TAG	UNP Q7TGD1
D	420	GLY	-	EXPRESSION TAG	UNP Q7TGD1
D	421	SER	-	EXPRESSION TAG	UNP Q7TGD1
D	422	GLY	-	EXPRESSION TAG	UNP Q7TGD1
D	423	GLY	-	EXPRESSION TAG	UNP Q7TGD1
D	424	GLY	-	EXPRESSION TAG	UNP Q7TGD1
D	425	SER	-	EXPRESSION TAG	UNP Q7TGD1
D	426	TRP	-	EXPRESSION TAG	UNP Q7TGD1
D	427	SER	-	EXPRESSION TAG	UNP Q7TGD1
D	428	HIS	-	EXPRESSION TAG	UNP Q7TGD1
D	429	PRO	-	EXPRESSION TAG	UNP Q7TGD1
D	430	GLN	-	EXPRESSION TAG	UNP Q7TGD1
D	431	PHE	-	EXPRESSION TAG	UNP Q7TGD1
D	432	GLU	-	EXPRESSION TAG	UNP Q7TGD1
D	433	LYS	-	EXPRESSION TAG	UNP Q7TGD1

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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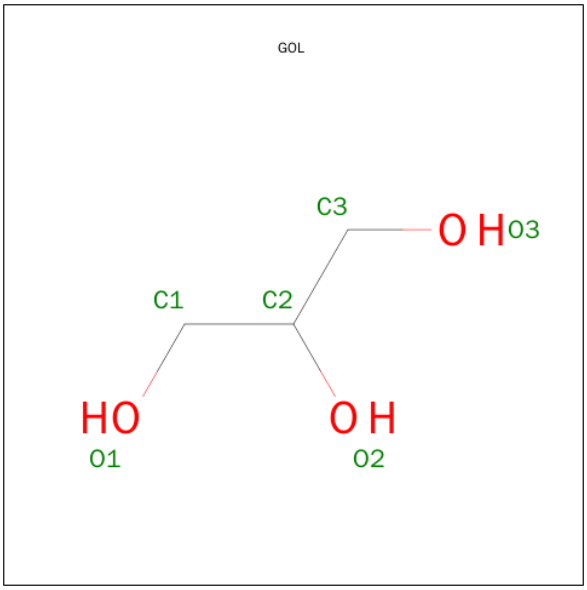
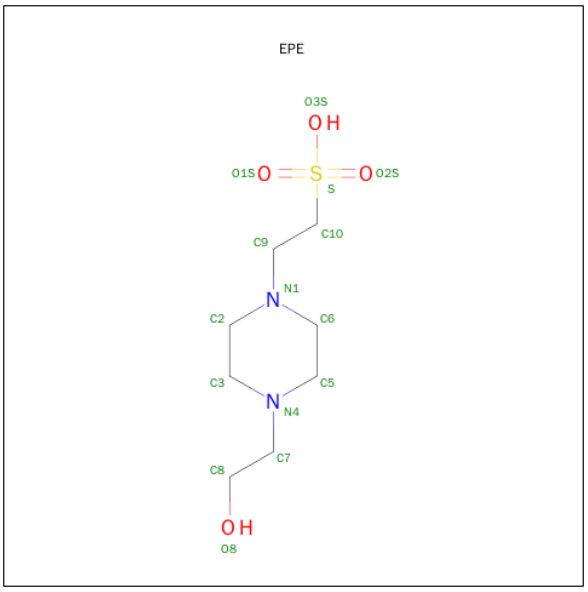
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is water.

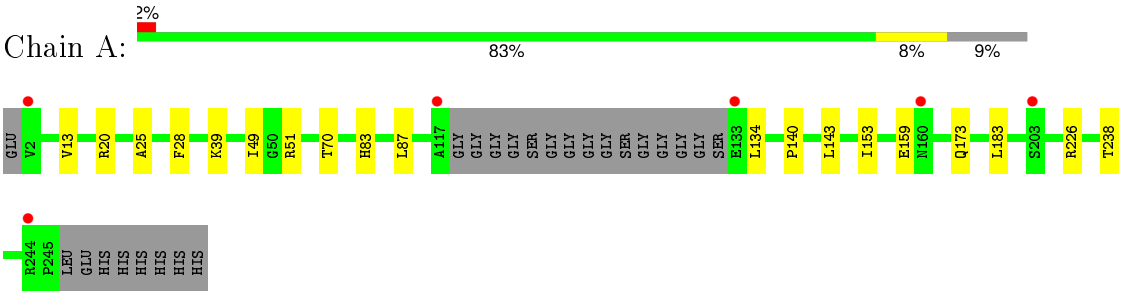
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	144	Total	O	0	0
			144	144		
6	B	90	Total	O	0	0
			90	90		
6	C	35	Total	O	0	0
			35	35		
6	D	8	Total	O	0	0
			8	8		

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.

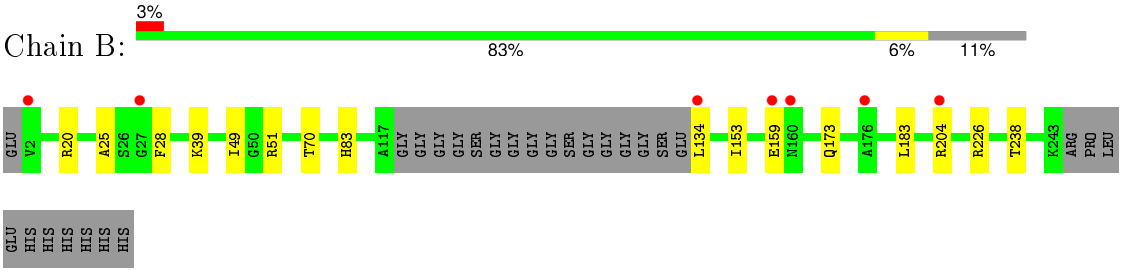
- Molecule 1: Variable domains of murine anti-dengue Mab 4E11

Chain A:



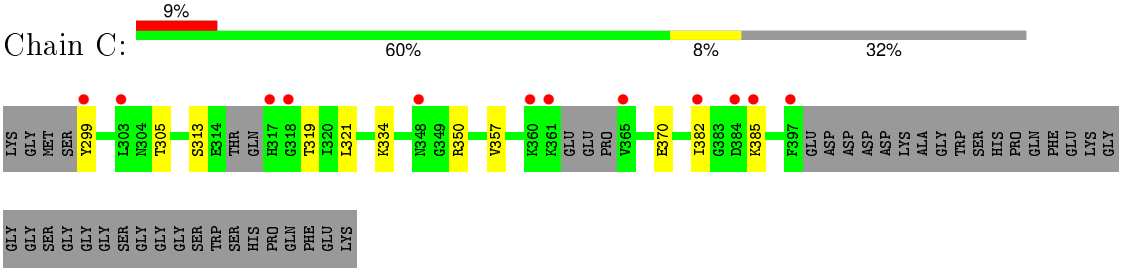
- Molecule 1: Variable domains of murine anti-dengue Mab 4E11

Chain B:



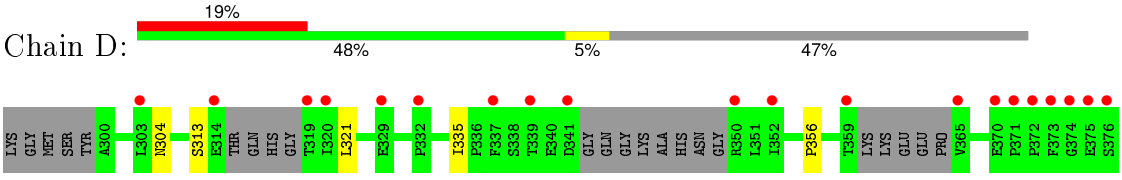
- Molecule 2: Envelope protein

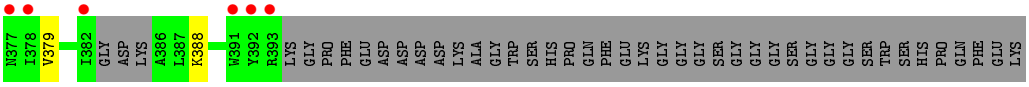
Chain C:



- Molecule 2: Envelope protein

Chain D:




N377
I378
V379
I382
GLY
ASP
LYS
A386
L387
K388
W391
Y392
R393
LYS
GLY
PRO
PHE
GLU
ASP
ASP
ASP
LYS
ALA
GLY
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS
GLY
GLY
GLY
SER
GLY
GLY
GLY
SER
GLY
GLY
GLY
GLY
SER
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.05Å 74.67Å 86.89Å 90.00° 104.49° 90.00°	Depositor
Resolution (Å)	40.80 – 2.04 42.06 – 2.04	Depositor EDS
% Data completeness (in resolution range)	94.6 (40.80-2.04) 94.5 (42.06-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 2.03Å)	Xtriage
Refinement program	BUSTER 2.9.3	Depositor
R, R_{free}	0.218 , 0.234 0.224 , 0.241	Depositor DCC
R_{free} test set	1981 reflections (5.15%)	DCC
Wilson B-factor (Å^2)	27.8	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 40584 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5202	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.61% 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, EPE, EDO

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	0.35	0/1846	0.60	0/2504
1	B	0.35	0/1811	0.59	0/2457
2	C	0.35	0/744	0.58	0/1001
2	D	0.35	0/588	0.53	0/793
All	All	0.35	0/4989	0.58	0/6755

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	1790	0	1746	9	0
1	B	1759	0	1718	7	0
2	C	730	0	740	5	0
2	D	581	0	593	3	0
3	A	8	0	12	0	0
3	B	8	0	12	0	0
3	C	4	0	6	0	0
4	A	18	0	24	1	0
4	B	12	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	15	0	18	0	0
6	A	144	0	0	0	0
6	B	90	0	0	0	0
6	C	35	0	0	0	0
6	D	8	0	0	0	0
All	All	5202	0	4885	24	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 2.

All (24) 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:A:134:LEU:HD12	1:A:159:GLU:HB2	1.80	0.62
1:B:134:LEU:HD12	1:B:159:GLU:HB2	1.81	0.61
4:A:258:GOL:H31	1:B:20:ARG:HB2	1.84	0.59
1:B:173:GLN:HB2	1:B:183:LEU:HD11	1.91	0.52
2:C:319:THR:HG22	2:C:370:GLU:HB3	1.92	0.51
1:A:70:THR:HB	1:A:83:HIS:HB2	1.93	0.51
1:A:153:ILE:HG12	1:A:238:THR:HG21	1.93	0.50
2:C:305:THR:HB	2:C:385:LYS:HB3	1.96	0.47
1:A:20:ARG:HB2	4:B:258:GOL:H11	1.96	0.47
1:B:153:ILE:HG12	1:B:238:THR:HG21	1.97	0.46
2:C:334:LYS:HA	2:C:357:VAL:HG12	1.96	0.46
2:D:379:VAL:HG22	2:D:388:LYS:HG2	1.96	0.46
1:B:39:LYS:HB2	1:B:49:ILE:HD11	1.97	0.46
1:A:173:GLN:HB2	1:A:183:LEU:HD11	1.98	0.45
1:A:13:VAL:HG21	1:A:87:LEU:HD13	1.99	0.44
2:D:313:SER:HB2	2:D:321:LEU:HB2	2.00	0.43
1:A:25:ALA:HB1	1:A:28:PHE:CE2	2.54	0.43
1:B:25:ALA:HB1	1:B:28:PHE:CE2	2.53	0.43
2:D:335:ILE:HB	2:D:356:PRO:HB2	2.01	0.43
1:B:70:THR:HB	1:B:83:HIS:HB2	2.01	0.43
2:C:313:SER:HB2	2:C:321:LEU:HB2	2.02	0.41
1:A:39:LYS:HB2	1:A:49:ILE:HD11	2.03	0.41
2:C:350:ARG:HB3	2:C:370:GLU:CG	2.52	0.40
1:A:140:PRO:HG2	1:A:143:LEU:HB2	2.02	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	230/253 (91%)	224 (97%)	6 (3%)	0	100 100
1	B	226/253 (89%)	219 (97%)	6 (3%)	1 (0%)	39 28
2	C	88/139 (63%)	86 (98%)	2 (2%)	0	100 100
2	D	64/139 (46%)	63 (98%)	1 (2%)	0	100 100
All	All	608/784 (78%)	592 (97%)	15 (2%)	1 (0%)	52 43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	204	ARG

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	194/201 (96%)	192 (99%)	2 (1%)	82 81
1	B	190/201 (94%)	188 (99%)	2 (1%)	80 79
2	C	79/112 (70%)	77 (98%)	2 (2%)	55 48
2	D	66/112 (59%)	65 (98%)	1 (2%)	72 70
All	All	529/626 (84%)	522 (99%)	7 (1%)	76 74

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ARG
1	A	226	ARG
1	B	51	ARG
1	B	226	ARG
2	C	299	TYR
2	C	382	ILE
2	D	304	ASN

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

11 ligands are modelled in this entry.

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	EDO	A	254	-	3,3,3	0.48	0	2,2,2	0.38	0
3	EDO	A	255	-	3,3,3	0.49	0	2,2,2	0.32	0
4	GOL	A	256	-	5,5,5	0.34	0	5,5,5	0.23	0
4	GOL	A	257	-	5,5,5	0.30	0	5,5,5	0.59	0
4	GOL	A	258	-	5,5,5	0.37	0	5,5,5	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EPE	B	254	-	14,15,15	0.86	0	18,20,20	2.71	8 (44%)
4	GOL	B	255	-	5,5,5	0.24	0	5,5,5	0.35	0
3	EDO	B	256	-	3,3,3	0.47	0	2,2,2	0.43	0
3	EDO	B	257	-	3,3,3	0.45	0	2,2,2	0.46	0
4	GOL	B	258	-	5,5,5	0.28	0	5,5,5	0.25	0
3	EDO	C	1	-	3,3,3	0.48	0	2,2,2	0.39	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
3	EDO	A	254	-	-	0/1/1/1	0/0/0/0
3	EDO	A	255	-	-	0/1/1/1	0/0/0/0
4	GOL	A	256	-	-	0/4/4/4	0/0/0/0
4	GOL	A	257	-	-	0/4/4/4	0/0/0/0
4	GOL	A	258	-	-	0/4/4/4	0/0/0/0
5	EPE	B	254	-	-	0/9/19/19	0/1/1/1
4	GOL	B	255	-	-	0/4/4/4	0/0/0/0
3	EDO	B	256	-	-	0/1/1/1	0/0/0/0
3	EDO	B	257	-	-	0/1/1/1	0/0/0/0
4	GOL	B	258	-	-	0/4/4/4	0/0/0/0
3	EDO	C	1	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	254	EPE	O3S-S-O2S	-3.94	102.45	111.61
5	B	254	EPE	O3S-S-O1S	-3.17	104.22	111.61
5	B	254	EPE	C9-N1-C2	-2.79	104.12	111.27
5	B	254	EPE	C6-C5-N4	2.09	114.37	110.63
5	B	254	EPE	O2S-S-O1S	2.27	121.74	113.48
5	B	254	EPE	C3-C2-N1	2.39	114.91	110.63
5	B	254	EPE	O2S-S-C10	5.25	111.38	106.91
5	B	254	EPE	O1S-S-C10	6.33	112.31	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	258	GOL	1	0
4	B	258	GOL	1	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	229/253 (90%)	0.23	6 (2%) 59 65	16, 26, 46, 78	0
1	B	226/253 (89%)	0.32	7 (3%) 52 60	22, 33, 54, 85	0
2	C	94/139 (67%)	0.64	12 (12%) 5 5	22, 34, 59, 88	0
2	D	74/139 (53%)	2.08	26 (35%) 0 0	39, 61, 88, 105	0
All	All	623/784 (79%)	0.55	51 (8%) 14 16	16, 33, 67, 105	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	303	LEU	11.2
2	C	397	PHE	9.6
2	D	392	TYR	9.1
2	D	374	GLY	6.9
1	A	244	ARG	6.2
2	D	391	TRP	6.1
2	C	317	HIS	6.0
1	B	2	VAL	5.7
2	D	376	SER	5.6
2	C	384	ASP	5.6
2	D	375	GLU	5.1
2	D	373	PHE	4.8
2	D	370	GLU	4.7
1	A	133	GLU	4.4
2	D	372	PRO	4.3
1	A	2	VAL	4.3
2	D	393	ARG	3.9
2	D	350	ARG	3.9
2	D	319	THR	3.9
2	D	332	PRO	3.9
2	C	365	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	134	LEU	3.8
2	D	341	ASP	3.6
1	B	160	ASN	3.6
2	C	385	LYS	3.4
2	D	365	VAL	3.4
2	D	329	GLU	3.3
2	D	382	ILE	3.3
2	C	318	GLY	3.1
2	D	339	THR	3.0
1	A	160	ASN	3.0
1	B	176	ALA	2.9
2	D	377	ASN	2.8
2	D	320	ILE	2.7
1	B	27	GLY	2.7
1	B	204	ARG	2.7
2	C	299	TYR	2.7
2	D	371	PRO	2.7
2	D	359	THR	2.6
1	A	117	ALA	2.6
1	B	159	GLU	2.5
2	D	337	PHE	2.4
2	C	361	LYS	2.4
2	C	382	ILE	2.3
1	A	203	SER	2.2
2	D	314	GLU	2.2
2	C	360	LYS	2.1
2	C	348	ASN	2.1
2	D	352	ILE	2.1
2	D	378	ILE	2.0
2	C	303	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no 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
3	EDO	C	1	4/4	0.77	0.41	16.78	52,54,55,57	0
4	GOL	B	258	6/6	0.52	0.28	11.39	73,74,74,75	0
5	EPE	B	254	15/15	0.90	0.26	5.97	48,50,52,55	0
4	GOL	A	258	6/6	0.63	0.27	5.06	47,48,48,49	0
4	GOL	A	257	6/6	0.88	0.18	4.64	31,33,34,34	0
3	EDO	A	254	4/4	0.74	0.24	4.63	35,37,39,39	0
3	EDO	A	255	4/4	0.67	0.19	2.35	39,40,41,43	0
4	GOL	B	255	6/6	0.91	0.18	1.00	36,36,37,37	0
3	EDO	B	257	4/4	0.91	0.15	0.21	42,44,46,47	0
4	GOL	A	256	6/6	0.73	0.20	-	55,55,55,56	0
3	EDO	B	256	4/4	0.80	0.23	-	66,68,70,71	0

6.5 Other polymers

There are no such residues in this entry.