WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2020 – 09:42 pm BST

PDB ID	:	5TR7
Title	:	Crystal structure of a putative D-alanyl-D-alanine carboxypeptidase from Vibrio cholerae O1 biovar eltor str. N16961
Authors	:	Filippova, E.V.; Minasov, G.; Shuvalova, L.; Kiryukhina, O.; Dubrovska, I.; Shatsman, S.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2016-10-25
Resolution	:	2.05 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
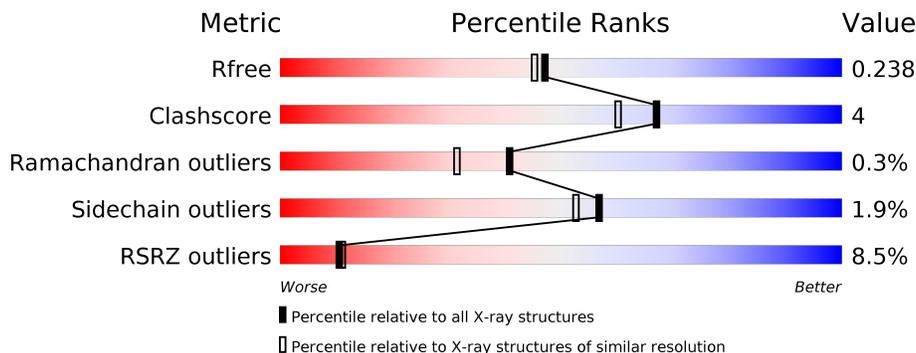
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	341	6% 66% 6% · 26%
1	B	341	6% 64% 9% · 27%
1	C	341	7% 67% 6% · 26%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5902 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 D-alanyl-D-alanine carboxypeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	0	0
			1930	1210	326	382	12			
1	B	249	Total	C	N	O	S	0	0	0
			1912	1200	324	376	12			
1	C	251	Total	C	N	O	S	0	1	0
			1936	1213	327	384	12			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).
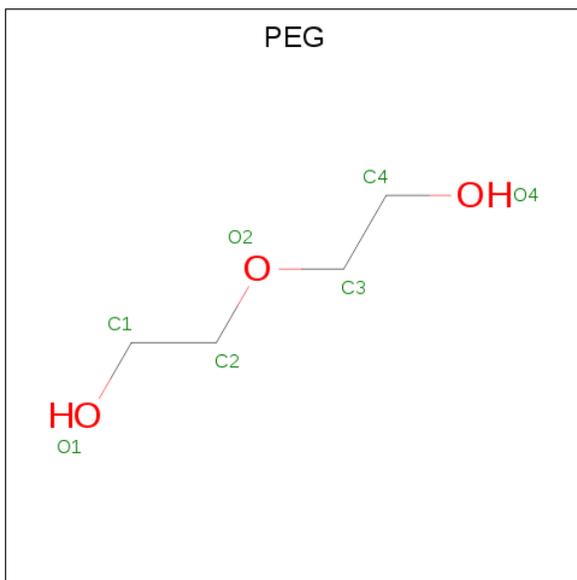
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 3 is NITRITE ION (three-letter code: NO2) (formula: NO_2).
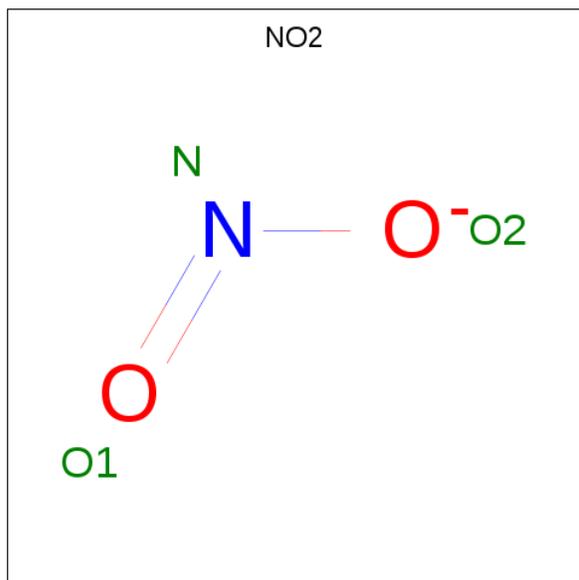
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 3	N 1	O 2	0	0
3	A	1	Total 3	N 1	O 2	0	0
3	C	1	Total 3	N 1	O 2	0	0

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

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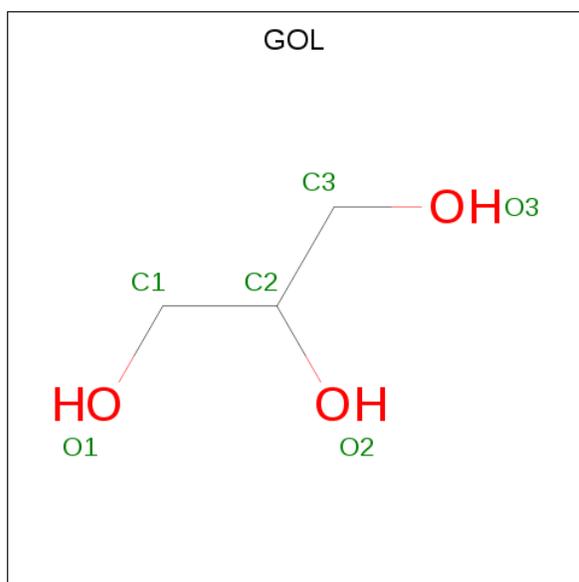
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 6	C 3	O 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total 26	O 26	0	0
5	B	38	Total 38	O 38	0	0
5	C	17	Total 17	O 17	0	0

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 the various outlier classes 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: D-alanyl-D-alanine carboxypeptidase
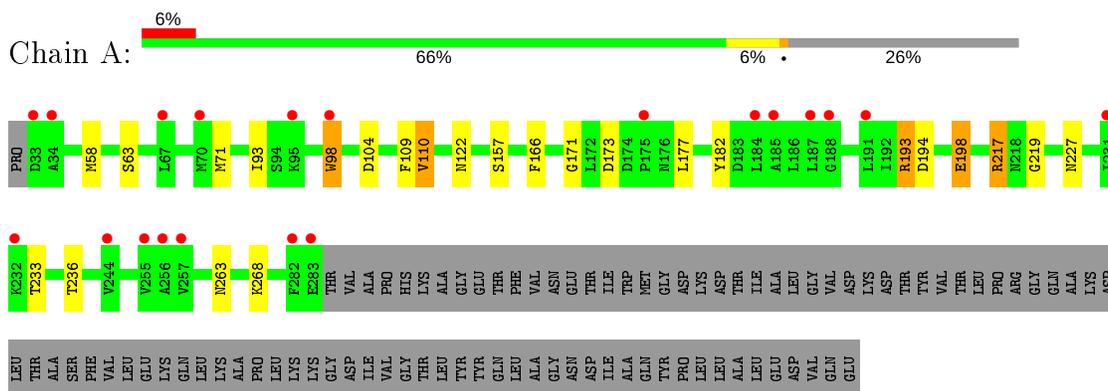
- Molecule 1: D-alanyl-D-alanine carboxypeptidase
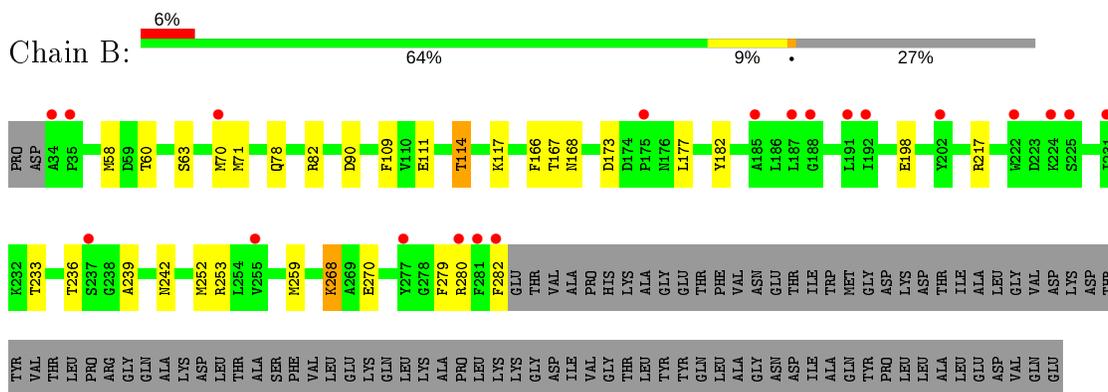
- Molecule 1: D-alanyl-D-alanine carboxypeptidase

THR ALA SER PHE VAL LEU GLU LYS GLN LEU LYS ALA PRO LEU LYS LYS GLY ASP ILE VAL GLY THR LEU TYR TYR GLN LEU ALA GLY ASN ASP ILE ALA GLN TYR PRO LEU LEU ALA LEU GLU ASP VAL GLN GLU

4 Data and refinement statistics (i)
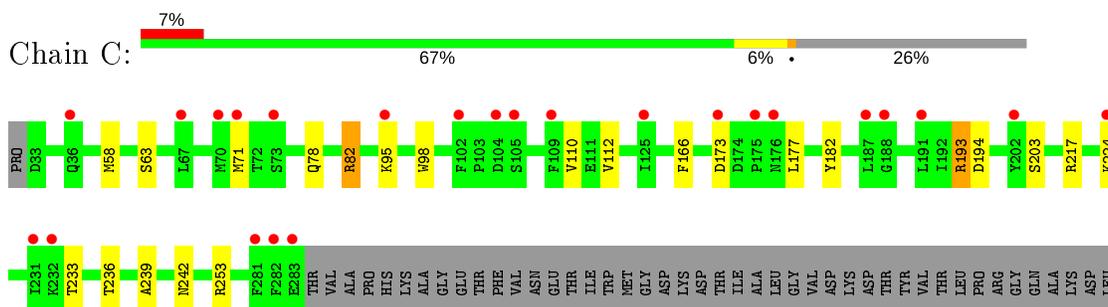
Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	88.75Å　　88.75Å　　85.42Å 90.00°　　90.00°　　120.00°	Depositor
Resolution (Å)	30.00　－　2.05 29.05　－　2.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.05) 100.0 (29.05-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.02 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.191　,　0.238 0.193　,　0.238	Depositor DCC
R_{free} test set	2246 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å^2)	48.6	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.1	EDS
L-test for twinning[2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l 0.043 for h,-h-k,-l 0.024 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5902	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ 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: GOL, PEG, NO2

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	0.95	2/1965 (0.1%)	1.10	8/2656 (0.3%)
1	B	0.87	1/1947 (0.1%)	1.02	5/2631 (0.2%)
1	C	0.91	1/1971 (0.1%)	1.08	6/2664 (0.2%)
All	All	0.91	4/5883 (0.1%)	1.07	19/7951 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	GLU	CD-OE1	8.36	1.34	1.25
1	A	157	SER	CB-OG	-5.99	1.34	1.42
1	B	198	GLU	CD-OE1	5.67	1.31	1.25
1	C	203	SER	CB-OG	-5.58	1.35	1.42

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	193	ARG	NE-CZ-NH1	13.54	127.07	120.30
1	A	193	ARG	NE-CZ-NH1	13.41	127.00	120.30
1	C	193	ARG	NE-CZ-NH2	-11.95	114.33	120.30
1	A	173	ASP	CB-CA-C	-9.37	91.67	110.40
1	A	198	GLU	CG-CD-OE2	-8.19	101.92	118.30
1	A	217	ARG	NE-CZ-NH2	7.27	123.93	120.30
1	A	193	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	C	82	ARG	NE-CZ-NH2	6.39	123.50	120.30
1	A	71	MET	CG-SD-CE	-6.33	90.08	100.20
1	C	253	ARG	NE-CZ-NH1	-6.19	117.20	120.30
1	C	71	MET	CG-SD-CE	-6.00	90.59	100.20
1	A	173	ASP	N-CA-C	5.80	126.67	111.00
1	C	253	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	B	71	MET	CG-SD-CE	-5.71	91.06	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	253	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	A	98	TRP	CA-CB-CG	5.45	124.06	113.70
1	B	259	MET	CA-CB-CG	-5.17	104.50	113.30
1	B	280	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	268	LYS	CB-CG-CD	5.04	124.70	111.60

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	1930	0	1885	11	0
1	B	1912	0	1871	22	0
1	C	1936	0	1889	15	0
2	A	7	0	10	0	0
2	B	14	0	20	0	0
2	C	7	0	10	0	0
3	A	6	0	0	0	0
3	C	3	0	0	0	0
4	B	6	0	8	0	0
5	A	26	0	0	2	0
5	B	38	0	0	1	0
5	C	17	0	0	0	0
All	All	5902	0	5693	45	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 (45) 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:193:ARG:HD2	1:A:194:ASP:OD1	1.73	0.89
1:C:193:ARG:HD2	1:C:194:ASP:OD1	1.79	0.82
1:B:114:THR:HG21	5:B:512:HOH:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:THR:HB	1:C:224:LYS:HE2	1.67	0.76
1:C:217:ARG:HB2	1:C:233:THR:HG21	1.71	0.72
1:B:63:SER:O	1:B:236:THR:HG21	1.90	0.72
1:A:217:ARG:HB2	1:A:233:THR:HG21	1.74	0.69
1:B:236:THR:HG23	1:B:242:ASN:HD21	1.60	0.67
1:C:236:THR:HG23	1:C:242:ASN:HD21	1.61	0.66
1:B:217:ARG:HB2	1:B:233:THR:HG21	1.78	0.65
1:B:252:MET:HE3	1:B:282:PHE:CE1	2.32	0.64
1:C:98:TRP:CG	1:C:112:VAL:HG23	2.33	0.63
1:B:90:ASP:OD1	1:B:117:LYS:CE	2.47	0.62
1:C:58:MET:HG2	1:C:182:TYR:HB2	1.87	0.55
1:A:58:MET:HG2	1:A:182:TYR:HB2	1.89	0.53
1:C:78:GLN:O	1:C:82:ARG:HG3	2.09	0.53
1:B:58:MET:HG2	1:B:182:TYR:HB2	1.91	0.53
1:B:111:GLU:O	1:B:114:THR:HG22	2.10	0.52
1:B:252:MET:HE2	1:B:279:PHE:HA	1.92	0.51
1:C:236:THR:HG23	1:C:242:ASN:ND2	2.26	0.51
1:B:78:GLN:O	1:B:82:ARG:HG3	2.10	0.50
1:B:63:SER:O	1:B:236:THR:CG2	2.60	0.49
1:B:236:THR:HG23	1:B:242:ASN:ND2	2.27	0.48
1:A:227:ASN:HB3	5:A:524:HOH:O	2.14	0.48
1:C:98:TRP:CD2	1:C:112:VAL:HG23	2.49	0.47
1:C:236:THR:OG1	1:C:239:ALA:HB3	2.15	0.47
1:A:263:ASN:HB2	5:A:508:HOH:O	2.16	0.46
1:C:58:MET:CG	1:C:182:TYR:HB2	2.46	0.46
1:A:93:ILE:HG21	1:A:110:VAL:HG13	1.98	0.45
1:B:236:THR:OG1	1:B:239:ALA:HB3	2.16	0.45
1:C:63:SER:O	1:C:236:THR:HG21	2.17	0.45
1:B:270:GLU:OE1	1:B:270:GLU:HA	2.18	0.44
1:B:90:ASP:OD1	1:B:117:LYS:HE2	2.15	0.44
1:B:168:ASN:HD22	1:C:224:LYS:NZ	2.16	0.44
1:B:252:MET:CE	1:B:282:PHE:CD1	3.02	0.43
1:A:58:MET:CG	1:A:182:TYR:HB2	2.48	0.42
1:C:166:PHE:HA	1:C:177:LEU:HD13	2.02	0.42
1:B:167:THR:CB	1:C:224:LYS:HE2	2.45	0.42
1:B:58:MET:CG	1:B:182:TYR:HB2	2.49	0.42
1:A:219:GLY:HA3	1:A:268:LYS:HD3	2.02	0.42
1:A:171:GLY:HA2	1:A:177:LEU:HD21	2.03	0.41
1:B:70:MET:HB3	1:B:70:MET:HE2	1.98	0.41
1:A:63:SER:HB3	1:A:236:THR:HG23	2.03	0.40
1:B:166:PHE:HA	1:B:177:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:PHE:HA	1:A:177:LEU:HD13	2.03	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	249/341 (73%)	244 (98%)	4 (2%)	1 (0%)	34	24
1	B	247/341 (72%)	241 (98%)	5 (2%)	1 (0%)	34	24
1	C	250/341 (73%)	244 (98%)	6 (2%)	0	100	100
All	All	746/1023 (73%)	729 (98%)	15 (2%)	2 (0%)	41	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	PHE
1	B	109	PHE

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	209/283 (74%)	204 (98%)	5 (2%)	49	42
1	B	207/283 (73%)	203 (98%)	4 (2%)	57	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	210/283 (74%)	207 (99%)	3 (1%)	67	65
All	All	626/849 (74%)	614 (98%)	12 (2%)	57	53

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	TRP
1	A	104	ASP
1	A	110	VAL
1	A	122	ASN
1	A	198	GLU
1	B	60	THR
1	B	114	THR
1	B	173	ASP
1	B	268	LYS
1	C	95	LYS
1	C	110	VAL
1	C	173	ASP

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

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates (i)

There are no carbohydrates in this entry.

5.6   Ligand geometry (i)

8 ligands are modelled in this entry.

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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	$\#|Z| > 2$
2	PEG	B	402	-	6,6,6	0.47	0	5,5,5	0.32	0
3	NO2	A	402	-	1,2,2	0.14	0	0,1,1	0.00	-
3	NO2	C	402	-	1,2,2	0.10	0	0,1,1	0.00	-
2	PEG	B	401	-	6,6,6	0.48	0	5,5,5	0.41	0
2	PEG	C	401	-	6,6,6	0.46	0	5,5,5	0.28	0
4	GOL	B	403	-	5,5,5	0.31	0	5,5,5	0.48	0
2	PEG	A	401	-	6,6,6	0.55	0	5,5,5	0.31	0
3	NO2	A	403	-	1,2,2	0.06	0	0,1,1	0.00	-

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
2	PEG	C	401	-	-	2/4/4/4	-
2	PEG	B	401	-	-	1/4/4/4	-
2	PEG	B	402	-	-	1/4/4/4	-
4	GOL	B	403	-	-	0/4/4/4	-
2	PEG	A	401	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	PEG	O1-C1-C2-O2
2	B	402	PEG	O2-C3-C4-O4
2	A	401	PEG	O2-C3-C4-O4
2	A	401	PEG	C1-C2-O2-C3
2	C	401	PEG	O2-C3-C4-O4
2	B	401	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
2	A	401	PEG	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	251/341 (73%)	0.15	20 (7%)	12	13	46, 61, 87, 125	0
1	B	249/341 (73%)	0.20	20 (8%)	12	13	42, 61, 93, 125	0
1	C	251/341 (73%)	0.27	24 (9%)	8	8	51, 64, 93, 109	0
All	All	751/1023 (73%)	0.20	64 (8%)	10	11	42, 62, 92, 125	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	34	ALA	6.7
1	B	231	ILE	4.9
1	B	175	PRO	4.6
1	A	244	VAL	4.1
1	C	231	ILE	4.1
1	A	33	ASP	4.0
1	A	34	ALA	4.0
1	A	98	TRP	3.8
1	C	102	PHE	3.4
1	A	191	LEU	3.4
1	C	191	LEU	3.2
1	A	282	PHE	3.2
1	C	71	MET	3.2
1	B	185	ALA	3.1
1	B	222	TRP	3.1
1	C	224	LYS	2.9
1	B	188	GLY	2.9
1	A	283	GLU	2.9
1	A	70	MET	2.9
1	C	105	SER	2.8
1	B	281	PHE	2.7
1	B	191	LEU	2.7
1	C	36	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	255	VAL	2.7
1	A	67	LEU	2.6
1	C	104	ASP	2.6
1	B	35	PRO	2.6
1	A	185	ALA	2.6
1	A	231	ILE	2.6
1	C	282	PHE	2.5
1	C	67	LEU	2.5
1	C	125	ILE	2.5
1	A	257	VAL	2.4
1	B	237	SER	2.4
1	C	281	PHE	2.3
1	B	277	TYR	2.3
1	C	232	LYS	2.3
1	C	176	ASN	2.3
1	B	280	ARG	2.3
1	C	175	PRO	2.3
1	A	184	LEU	2.3
1	C	70	MET	2.2
1	C	188	GLY	2.2
1	A	187	LEU	2.2
1	C	109	PHE	2.2
1	A	175	PRO	2.2
1	A	95	LYS	2.2
1	B	70	MET	2.2
1	C	95	LYS	2.2
1	C	202	TYR	2.2
1	C	283	GLU	2.2
1	C	73	SER	2.2
1	B	202	TYR	2.2
1	A	256	ALA	2.2
1	B	282	PHE	2.1
1	B	224	LYS	2.1
1	A	255	VAL	2.1
1	C	187	LEU	2.1
1	B	225	SER	2.1
1	B	187	LEU	2.1
1	A	232	LYS	2.0
1	A	188	GLY	2.0
1	C	173	ASP	2.0
1	B	192	ILE	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 (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NO2	A	402	3/3	0.71	0.18	80,80,87,100	0
2	PEG	B	402	7/7	0.73	0.33	89,95,100,100	0
2	PEG	A	401	7/7	0.81	0.26	78,90,103,104	0
3	NO2	C	402	3/3	0.87	0.09	87,87,89,92	0
4	GOL	B	403	6/6	0.88	0.13	73,82,86,87	0
2	PEG	B	401	7/7	0.91	0.12	52,64,69,75	0
2	PEG	C	401	7/7	0.91	0.07	67,70,72,72	0
3	NO2	A	403	3/3	0.91	0.13	68,68,72,72	0

6.5 Other polymers (i)

There are no such residues in this entry.