Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:34 PM GMT

PDB ID	:	4RU5
Title	:	Crystal Structure of the Pseudomonas phage phi297 tailspike gp61
Authors	:	Browning, C.; Sycheva, L.V.; Shneider, M.M.; Leiman, P.G.
Deposited on	:	2014-11-18
Resolution	:	1.52 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 ⓘ symbol.

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

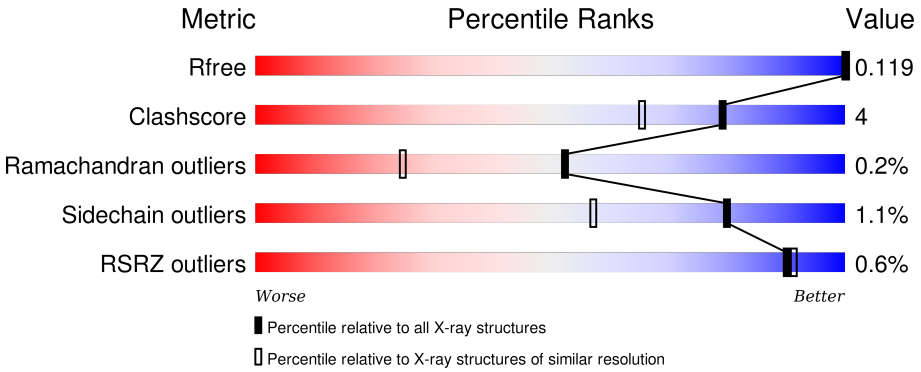
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 1.52 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	2658 (1.54-1.50)
Clashscore	102246	2887 (1.54-1.50)
Ramachandran outliers	100387	2818 (1.54-1.50)
Sidechain outliers	100360	2816 (1.54-1.50)
RSRZ outliers	91569	2660 (1.54-1.50)

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	605	92% 6%
1	B	605	91% 7%
1	C	605	% 93% 6%

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	NA	A	803	-	-	-	X
3	NA	A	804	-	-	-	X
3	NA	A	807	-	-	-	X
3	NA	B	803	-	-	-	X
3	NA	C	803	-	-	-	X
4	EDO	A	811	-	-	-	X
4	EDO	B	807	-	-	-	X
4	EDO	C	805	-	-	-	X
5	ACT	B	810	-	-	X	-
5	ACT	C	812	-	-	-	X
5	ACT	C	813	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17240 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 tailspike gp27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	600	Total	C	N	O	S	0	21	0
			4644	2893	813	913	25			
1	B	600	Total	C	N	O	S	0	29	0
			4696	2925	821	925	25			
1	C	602	Total	C	N	O	S	0	22	0
			4671	2908	814	924	25			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	SER	-	EXPRESSION TAG	UNP H2BD96
B	142	SER	-	EXPRESSION TAG	UNP H2BD96
C	142	SER	-	EXPRESSION TAG	UNP H2BD96

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Na	0	0
			2	2		
3	A	6	Total	Na	0	0
			6	6		

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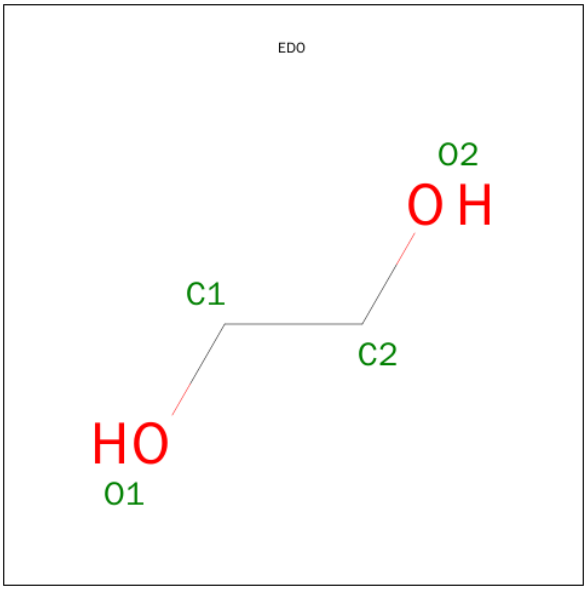
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	2	Total Na 2 2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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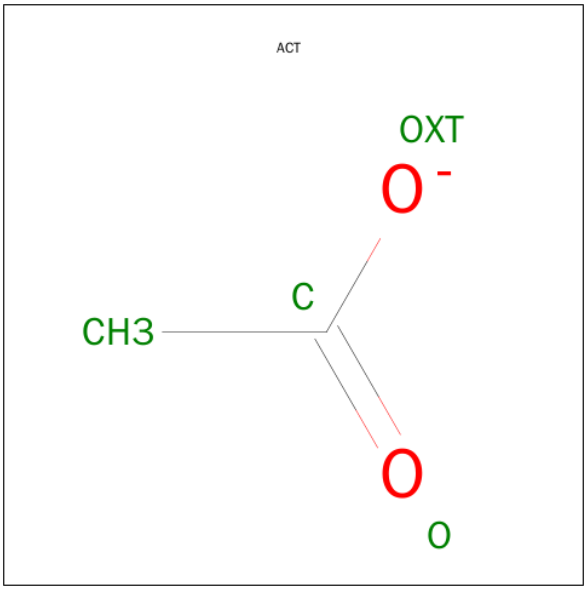
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is water.

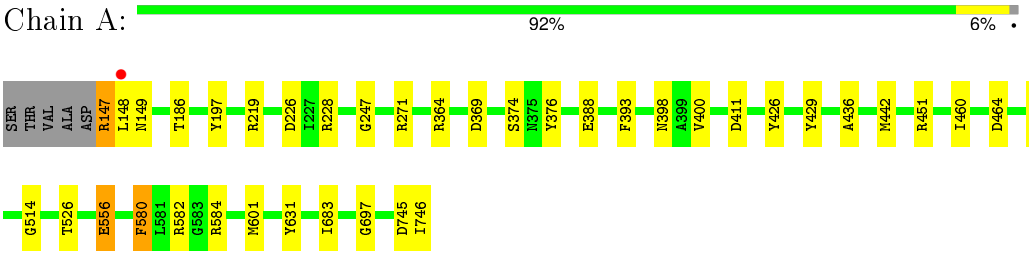
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1003	Total	O	0	0
			1003	1003		
6	B	1120	Total	O	0	0
			1120	1120		
6	C	1010	Total	O	0	0
			1010	1010		

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.

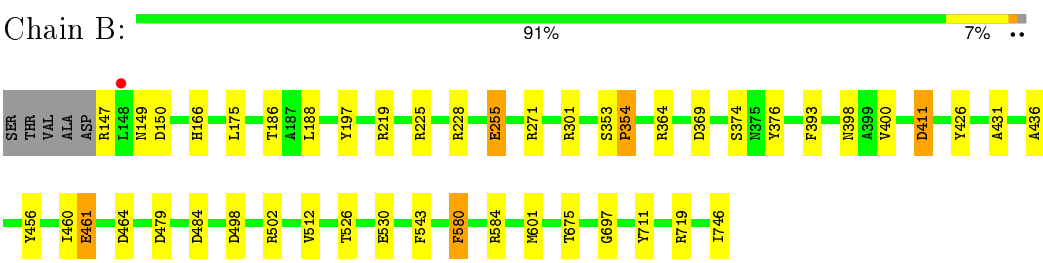
- Molecule 1: tailspike gp27

Chain A:



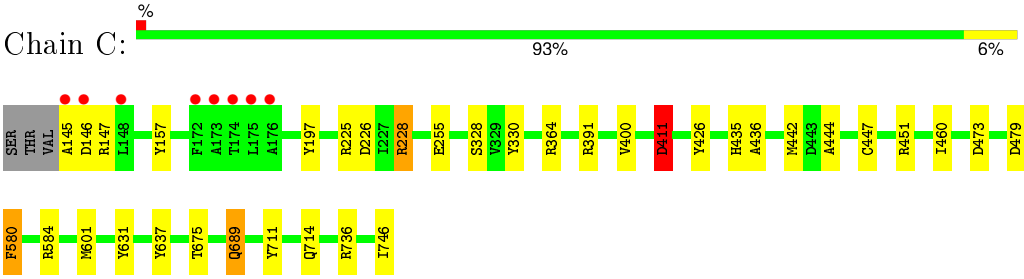
- Molecule 1: tailspike gp27

Chain B:



- Molecule 1: tailspike gp27

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	210.62Å 124.70Å 83.56Å 90.00° 97.93° 90.00°	Depositor
Resolution (Å)	46.37 – 1.52 46.37 – 1.52	Depositor EDS
% Data completeness (in resolution range)	98.0 (46.37-1.52) 98.0 (46.37-1.52)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 1.52Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.079 , 0.120 0.079 , 0.119	Depositor DCC
R_{free} test set	16063 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	13.6	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 66.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	4 of 321302 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.99	EDS
Total number of atoms	17240	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: NA, CA, EDO, ACT

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	0.99	5/4746 (0.1%)	0.94	8/6472 (0.1%)
1	B	0.96	9/4798 (0.2%)	0.94	7/6542 (0.1%)
1	C	0.95	5/4773 (0.1%)	0.95	9/6509 (0.1%)
All	All	0.96	19/14317 (0.1%)	0.95	24/19523 (0.1%)

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	C	0	1
All	All	0	2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	637	TYR	CE1-CZ	-10.76	1.24	1.38
1	A	429	TYR	CE1-CZ	-7.91	1.28	1.38
1	C	228	ARG	CZ-NH1	7.84	1.43	1.33
1	B	426	TYR	CE1-CZ	-7.79	1.28	1.38
1	A	388	GLU	CD-OE1	7.18	1.33	1.25
1	B	255[A]	GLU	CD-OE1	6.95	1.33	1.25
1	B	255[B]	GLU	CD-OE1	6.95	1.33	1.25
1	A	426	TYR	CZ-OH	6.65	1.49	1.37
1	B	426	TYR	CZ-OH	6.19	1.48	1.37
1	B	150	ASP	C-O	6.07	1.34	1.23
1	C	426	TYR	CZ-OH	5.97	1.48	1.37
1	A	147	ARG	CZ-NH2	5.78	1.40	1.33
1	C	426	TYR	CE1-CZ	-5.70	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	225	ARG	CG-CD	-5.45	1.38	1.51
1	B	543	PHE	CG-CD2	-5.36	1.30	1.38
1	B	364	ARG	CB-CG	-5.28	1.38	1.52
1	B	461	GLU	CD-OE2	5.14	1.31	1.25
1	B	225	ARG	CG-CD	-5.09	1.39	1.51
1	A	556	GLU	CD-OE1	-5.01	1.20	1.25

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	228	ARG	NE-CZ-NH2	-11.50	114.55	120.30
1	C	364	ARG	NE-CZ-NH1	-8.08	116.26	120.30
1	C	225	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	B	464	ASP	CB-CG-OD1	7.98	125.48	118.30
1	C	225	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	364	ARG	CG-CD-NE	7.55	127.66	111.80
1	C	580	PHE	CB-CG-CD1	7.31	125.92	120.80
1	A	584	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	A	580	PHE	CB-CG-CD1	7.00	125.70	120.80
1	B	271	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	271	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	C	580	PHE	CB-CG-CD2	-6.13	116.51	120.80
1	A	580	PHE	CB-CG-CD2	-6.12	116.52	120.80
1	A	464	ASP	CB-CG-OD1	5.78	123.50	118.30
1	B	719	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	B	225	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	582	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	C	411	ASP	CB-CG-OD1	5.53	123.28	118.30
1	B	584	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	B	580	PHE	CB-CG-CD1	5.34	124.54	120.80
1	B	225	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	C	584	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	C	736	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	745	ASP	CB-CG-OD2	-5.06	113.74	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	631	TYR	Sidechain
1	C	631	TYR	Sidechain

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	4644	0	4447	26	0
1	B	4696	0	4499	40	0
1	C	4671	0	4462	25	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	6	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	A	16	0	22	0	0
4	B	12	0	15	4	0
4	C	24	0	33	2	0
5	A	4	0	3	1	0
5	B	12	0	9	4	0
5	C	12	0	9	5	0
6	A	1003	0	0	16	3
6	B	1120	0	0	26	1
6	C	1010	0	0	11	2
All	All	17240	0	13499	97	3

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 (97) 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:B:442[A]:MET:HE3	6:B:1904:HOH:O	1.14	1.27
1:A:601[B]:MET:SD	6:A:1787:HOH:O	1.92	1.25
1:A:601[B]:MET:HE2	6:A:1861:HOH:O	1.28	1.25
1:B:601[B]:MET:SD	6:C:1455:HOH:O	1.97	1.20
1:B:675:THR:H	5:B:810:ACT:H3	1.08	1.17
1:A:186[B]:THR:HG22	6:A:1358:HOH:O	1.42	1.16
1:A:442[B]:MET:SD	6:A:1876:HOH:O	2.09	1.10
1:B:228[B]:ARG:NH1	6:B:1037:HOH:O	1.86	1.08
1:B:186[B]:THR:HG22	6:B:1556:HOH:O	1.57	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:ILE:HB	6:A:1761:HOH:O	1.56	1.03
1:B:442[A]:MET:CE	6:B:1904:HOH:O	1.78	1.03
1:B:147:ARG:N	6:B:1888:HOH:O	1.95	0.98
1:C:442[A]:MET:HE3	6:C:1780:HOH:O	1.63	0.96
1:C:675:THR:H	5:C:813:ACT:H1	1.33	0.94
1:C:442[A]:MET:CE	6:C:1780:HOH:O	2.16	0.90
1:B:301[A]:ARG:NH1	6:B:1741:HOH:O	2.03	0.89
1:B:186[B]:THR:HG21	6:B:1864:HOH:O	1.79	0.81
1:B:675:THR:N	5:B:810:ACT:H3	1.94	0.81
5:B:810:ACT:H2	6:B:1406:HOH:O	1.82	0.80
1:C:145:ALA:HB2	6:C:1662:HOH:O	1.82	0.80
5:C:813:ACT:H3	6:C:1434:HOH:O	1.82	0.79
1:A:442[B]:MET:CE	6:A:1876:HOH:O	2.30	0.78
1:B:255[B]:GLU:OE2	6:B:1930:HOH:O	2.08	0.71
1:B:186[B]:THR:HG23	1:B:219:ARG:HH12	1.56	0.68
1:A:683:ILE:CB	6:A:1761:HOH:O	2.28	0.68
1:A:556:GLU:OE2	6:A:1512:HOH:O	2.13	0.67
4:B:806:EDO:H11	6:B:1617:HOH:O	1.96	0.65
4:B:806:EDO:C1	6:B:1617:HOH:O	2.45	0.64
1:C:675:THR:H	5:C:813:ACT:CH3	2.09	0.64
1:B:442[B]:MET:HE1	6:B:1995:HOH:O	1.99	0.62
1:B:512[B]:VAL:HG21	6:B:1627:HOH:O	2.01	0.60
1:B:442[B]:MET:CG	6:B:1771:HOH:O	2.51	0.58
1:C:228:ARG:NH2	6:C:1891:HOH:O	2.28	0.57
1:B:147:ARG:NH2	6:B:1580:HOH:O	2.38	0.57
1:B:442[B]:MET:SD	6:B:1771:HOH:O	2.58	0.57
5:B:808:ACT:H3	6:B:1167:HOH:O	2.05	0.56
1:A:147:ARG:HD2	1:A:149:ASN:O	2.05	0.56
1:C:255[B]:GLU:HG2	6:C:1678:HOH:O	2.06	0.56
1:C:145:ALA:CB	1:C:147:ARG:HH11	2.19	0.55
1:B:601[B]:MET:HE3	6:B:1815:HOH:O	2.05	0.55
1:C:400:VAL:HB	6:C:1242:HOH:O	2.07	0.54
5:C:811:ACT:H2	6:C:1164:HOH:O	2.08	0.54
1:A:247:GLY:HA2	6:A:1800:HOH:O	2.08	0.52
1:B:147:ARG:CZ	6:B:1580:HOH:O	2.57	0.52
4:B:805:EDO:H22	1:C:226:ASP:HB3	1.91	0.52
1:C:145:ALA:HB3	1:C:147:ARG:HH11	1.74	0.52
1:A:400[B]:VAL:HG13	6:A:1345:HOH:O	2.10	0.52
1:A:228[B]:ARG:NH2	6:A:1804:HOH:O	2.43	0.52
6:A:1423:HOH:O	1:C:689:GLN:HG2	2.09	0.51
1:A:186[B]:THR:HG23	1:A:219:ARG:HH12	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442[B]:MET:HG3	6:B:1771:HOH:O	2.12	0.49
1:C:391:ARG:HD3	1:C:447[B]:CYS:SG	2.53	0.49
1:B:442[B]:MET:CE	6:B:1995:HOH:O	2.57	0.48
1:C:145:ALA:HB3	1:C:147:ARG:NH1	2.28	0.48
6:A:1450:HOH:O	1:C:601[B]:MET:HE3	2.12	0.48
1:B:255[B]:GLU:HG2	6:B:1368:HOH:O	2.13	0.47
1:B:400:VAL:HB	6:B:1850:HOH:O	2.13	0.47
1:C:436:ALA:HB3	1:C:460:ILE:HG23	1.96	0.47
1:A:436:ALA:HB3	1:A:460:ILE:HG23	1.96	0.47
1:A:683:ILE:CG1	6:A:1761:HOH:O	2.61	0.47
1:B:436:ALA:HB3	1:B:460:ILE:HG23	1.97	0.47
4:B:806:EDO:H12	6:B:1617:HOH:O	2.11	0.46
1:B:451:ARG:HA	1:B:479:ASP:O	2.16	0.46
1:B:186[B]:THR:OG1	6:B:1120:HOH:O	2.20	0.45
1:C:714:GLN:NE2	6:C:1528:HOH:O	2.49	0.45
1:A:498:ASP:HA	1:A:526:THR:O	2.17	0.45
1:C:328:SER:HB2	1:C:330:TYR:CZ	2.52	0.44
1:A:451:ARG:HA	1:A:479:ASP:O	2.17	0.44
1:A:374:SER:HA	1:A:398[B]:ASN:O	2.17	0.44
1:A:683:ILE:HG21	1:A:683:ILE:HD13	1.69	0.43
5:A:813:ACT:H2	6:A:1124:HOH:O	2.19	0.43
1:C:451:ARG:HA	1:C:479:ASP:O	2.18	0.43
1:A:226:ASP:HB3	4:C:806:EDO:H11	2.01	0.43
1:A:374:SER:HA	1:A:398[A]:ASN:O	2.19	0.42
1:B:374:SER:HA	1:B:398[B]:ASN:O	2.20	0.42
1:C:444:ALA:HA	5:C:812:ACT:H1	2.01	0.42
1:B:376:TYR:HB3	1:B:400:VAL:HG22	2.02	0.41
1:A:400[A]:VAL:HB	6:A:1345:HOH:O	2.19	0.41
1:C:435:HIS:CG	1:C:473:ASP:HB2	2.55	0.41
1:B:175:LEU:CA	1:B:188[B]:LEU:HD11	2.50	0.41
1:C:157:TYR:CZ	4:C:808:EDO:H22	2.54	0.41
1:A:369:ASP:HA	1:A:393:PHE:O	2.20	0.41
1:B:498:ASP:HA	1:B:526:THR:O	2.21	0.41
1:B:601[B]:MET:HA	1:B:601[B]:MET:CE	2.50	0.41
1:A:509:VAL:O	1:A:514:GLY:HA2	2.20	0.41
1:C:508:GLY:HA2	1:C:516:ALA:HA	2.02	0.41
1:A:376:TYR:HB3	1:A:400[A]:VAL:HG22	2.03	0.41
1:B:374:SER:HA	1:B:398[A]:ASN:O	2.20	0.41
1:B:369:ASP:HA	1:B:393:PHE:O	2.20	0.41
1:B:456:TYR:HA	1:B:484:ASP:O	2.21	0.41
1:B:431:ALA:HA	1:B:461:GLU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:697:GLY:HA2	1:C:711:TYR:O	2.21	0.41
1:A:697:GLY:HA2	1:B:711:TYR:O	2.20	0.41
1:B:502:ARG:HA	1:B:530:GLU:O	2.21	0.40
1:C:145:ALA:HA	6:C:1896:HOH:O	2.21	0.40
1:B:166:HIS:HB2	6:B:1994:HOH:O	2.20	0.40
1:B:353:SER:HA	1:B:354:PRO:HD3	1.86	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1630:HOH:O	6:C:1779:HOH:O[4_757]	2.00	0.20
6:A:1518:HOH:O	6:B:1605:HOH:O[1_556]	2.04	0.16
6:A:1784:HOH:O	6:C:1741:HOH:O[4_757]	2.14	0.06

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	619/605 (102%)	595 (96%)	23 (4%)	1 (0%)	52	25
1	B	627/605 (104%)	603 (96%)	23 (4%)	1 (0%)	52	25
1	C	623/605 (103%)	597 (96%)	25 (4%)	1 (0%)	52	25
All	All	1869/1815 (103%)	1795 (96%)	71 (4%)	3 (0%)	52	25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	411	ASP
1	B	411	ASP
1	C	411	ASP

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	495/478 (104%)	491 (99%)	4 (1%)	86	69
1	B	503/478 (105%)	497 (99%)	6 (1%)	78	53
1	C	498/478 (104%)	492 (99%)	6 (1%)	78	53
All	All	1496/1434 (104%)	1480 (99%)	16 (1%)	80	57

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	LEU
1	A	197	TYR
1	A	580	PHE
1	A	746	ILE
1	B	149	ASN
1	B	197	TYR
1	B	354	PRO
1	B	411	ASP
1	B	580	PHE
1	B	746	ILE
1	C	146	ASP
1	C	197	TYR
1	C	411	ASP
1	C	580	PHE
1	C	689	GLN
1	C	746	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	615	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 36 ligands modelled in this entry, 16 are monoatomic - leaving 20 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	EDO	A	809	-	3,3,3	1.66	1 (33%)	2,2,2	1.63	0
4	EDO	A	810	-	3,3,3	0.65	0	2,2,2	1.35	0
4	EDO	A	811	-	3,3,3	0.50	0	2,2,2	1.03	0
4	EDO	A	812	-	3,3,3	1.25	0	2,2,2	0.70	0
5	ACT	A	813	-	0,3,3	0.00	-	0,3,3	0.00	-
4	EDO	B	805	-	3,3,3	1.22	0	2,2,2	0.81	0
4	EDO	B	806	-	3,3,3	0.98	0	2,2,2	0.69	0
4	EDO	B	807	-	3,3,3	1.54	1 (33%)	2,2,2	0.61	0
5	ACT	B	808	-	0,3,3	0.00	-	0,3,3	0.00	-
5	ACT	B	809	-	0,3,3	0.00	-	0,3,3	0.00	-
5	ACT	B	810	-	0,3,3	0.00	-	0,3,3	0.00	-
4	EDO	C	805	-	3,3,3	0.52	0	2,2,2	0.36	0
4	EDO	C	806	-	3,3,3	1.94	1 (33%)	2,2,2	0.66	0
4	EDO	C	807	-	3,3,3	0.39	0	2,2,2	0.36	0
4	EDO	C	808	-	3,3,3	0.52	0	2,2,2	0.27	0
4	EDO	C	809	-	3,3,3	0.82	0	2,2,2	0.49	0
4	EDO	C	810	-	3,3,3	0.54	0	2,2,2	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	ACT	C	811	-	0,3,3	0.00	-	0,3,3	0.00	-
5	ACT	C	812	-	0,3,3	0.00	-	0,3,3	0.00	-
5	ACT	C	813	-	0,3,3	0.00	-	0,3,3	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
4	EDO	A	809	-	-	0/1/1/1	0/0/0/0
4	EDO	A	810	-	-	0/1/1/1	0/0/0/0
4	EDO	A	811	-	-	0/1/1/1	0/0/0/0
4	EDO	A	812	-	-	0/1/1/1	0/0/0/0
5	ACT	A	813	-	-	0/0/0/0	0/0/0/0
4	EDO	B	805	-	-	0/1/1/1	0/0/0/0
4	EDO	B	806	-	-	0/1/1/1	0/0/0/0
4	EDO	B	807	-	-	0/1/1/1	0/0/0/0
5	ACT	B	808	-	-	0/0/0/0	0/0/0/0
5	ACT	B	809	-	-	0/0/0/0	0/0/0/0
5	ACT	B	810	-	-	0/0/0/0	0/0/0/0
4	EDO	C	805	-	-	0/1/1/1	0/0/0/0
4	EDO	C	806	-	-	0/1/1/1	0/0/0/0
4	EDO	C	807	-	-	0/1/1/1	0/0/0/0
4	EDO	C	808	-	-	0/1/1/1	0/0/0/0
4	EDO	C	809	-	-	0/1/1/1	0/0/0/0
4	EDO	C	810	-	-	0/1/1/1	0/0/0/0
5	ACT	C	811	-	-	0/0/0/0	0/0/0/0
5	ACT	C	812	-	-	0/0/0/0	0/0/0/0
5	ACT	C	813	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	806	EDO	O1-C1	-2.75	1.27	1.42
4	B	807	EDO	O1-C1	-2.60	1.28	1.42
4	A	809	EDO	O2-C2	-2.24	1.30	1.42

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	813	ACT	1	0
4	B	805	EDO	1	0
4	B	806	EDO	3	0
5	B	808	ACT	1	0
5	B	810	ACT	3	0
4	C	806	EDO	1	0
4	C	808	EDO	1	0
5	C	811	ACT	1	0
5	C	812	ACT	1	0
5	C	813	ACT	3	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	600/605 (99%)	-0.84	1 (0%)	95	95	9, 14, 23, 54	0
1	B	600/605 (99%)	-0.75	1 (0%)	95	95	9, 13, 21, 76	0
1	C	602/605 (99%)	-0.70	8 (1%)	79	82	9, 15, 27, 109	0
All	All	1802/1815 (99%)	-0.76	10 (0%)	90	91	9, 14, 24, 109	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	148	LEU	6.7
1	C	146	ASP	6.1
1	C	145	ALA	6.0
1	A	148	LEU	3.7
1	C	176	ALA	2.7
1	C	175	LEU	2.5
1	C	172	PHE	2.5
1	B	148	LEU	2.4
1	C	174	THR	2.2
1	C	173	ALA	2.1

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 (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. 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	NA	A	803	1/1	0.89	0.16	16.60	60,60,60,60	0
3	NA	B	803	1/1	0.94	0.19	14.84	70,70,70,70	0
3	NA	A	807	1/1	0.96	0.13	8.39	64,64,64,64	0
4	EDO	C	805	4/4	0.99	0.06	4.90	17,18,19,24	0
3	NA	A	804	1/1	0.94	0.10	4.06	58,58,58,58	0
4	EDO	B	807	4/4	0.95	0.13	3.66	25,28,41,47	0
4	EDO	A	811	4/4	0.98	0.08	3.04	17,32,34,38	0
3	NA	C	803	1/1	0.97	0.07	2.94	38,38,38,38	0
5	ACT	C	812	4/4	0.95	0.10	2.80	28,31,32,57	0
4	EDO	A	810	4/4	0.96	0.06	1.84	21,27,36,42	0
4	EDO	C	810	4/4	0.96	0.12	1.63	23,40,41,44	0
4	EDO	C	806	4/4	0.98	0.06	1.00	21,21,23,26	0
4	EDO	B	805	4/4	0.99	0.06	0.35	20,20,25,29	0
4	EDO	A	809	4/4	0.97	0.07	0.13	19,24,32,33	0
2	CA	B	802	1/1	1.00	0.05	-0.67	17,17,17,17	0
2	CA	C	802	1/1	1.00	0.05	-0.86	18,18,18,18	0
2	CA	A	802	1/1	1.00	0.04	-1.16	18,18,18,18	0
2	CA	B	801	1/1	1.00	0.03	-1.59	15,15,15,15	0
2	CA	C	801	1/1	1.00	0.04	-1.63	19,19,19,19	0
2	CA	A	801	1/1	1.00	0.04	-2.51	17,17,17,17	0
3	NA	A	805	1/1	0.94	0.22	-	67,67,67,67	0
5	ACT	A	813	4/4	0.99	0.08	-	27,27,28,29	0
5	ACT	B	810	4/4	0.93	0.13	-	17,31,55,59	0
4	EDO	C	809	4/4	0.99	0.11	-	19,28,29,34	0
3	NA	A	808	1/1	0.96	0.22	-	55,55,55,55	0
5	ACT	B	808	4/4	0.99	0.05	-	23,24,33,34	0
5	ACT	C	813	4/4	0.93	0.19	-	17,36,64,70	0
3	NA	A	806	1/1	0.98	0.07	-	44,44,44,44	0
5	ACT	C	811	4/4	0.95	0.09	-	25,31,33,37	0
3	NA	C	804	1/1	0.95	0.32	-	50,50,50,50	0
4	EDO	B	806	4/4	0.99	0.08	-	17,23,30,39	0
5	ACT	B	809	4/4	0.97	0.16	-	49,49,49,52	0
3	NA	B	804	1/1	0.97	0.14	-	54,54,54,54	0
4	EDO	C	807	4/4	0.96	0.17	-	36,43,47,82	0
4	EDO	C	808	4/4	0.95	0.10	-	38,43,57,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	EDO	A	812	4/4	0.84	0.22	-	40,41,44,45	0

6.5 Other polymers (i)

There are no such residues in this entry.