



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2018 – 10:58 PM EST

PDB ID : 4RU4
Title : Crystal structure of the tailspike protein gp49 from Pseudomonas phage LKA1
Authors : Browning, C.; Shneider, M.M.; Leiman, P.G.
Deposited on : 2014-11-18
Resolution : 1.90 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030736

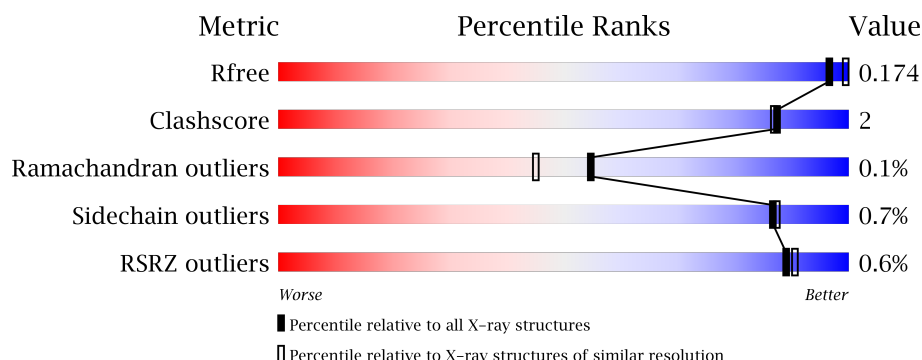
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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 $\leq 5\%$. 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	602	<div> <div>94%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
1	B	602	<div> <div>92%</div> <div>6%</div> <div></div> </div>
1	C	602	<div> <div>%</div> <div>92%</div> <div>6%</div> <div></div> </div>
1	D	602	<div> <div>93%</div> <div>5%</div> <div></div> </div>
1	E	602	<div> <div>93%</div> <div>5%</div> <div></div> </div>

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Mol	Chain	Length	Quality of chain
1	F	602	 .% 92% 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
2	EDO	A	803	-	-	-	X
2	EDO	B	801	-	-	-	X
2	EDO	B	803	-	-	-	X
2	EDO	B	804	-	-	-	X
2	EDO	E	803	-	-	-	X
3	NA	A	804	-	-	-	X
3	NA	A	805	-	-	-	X
3	NA	A	807	-	-	-	X
3	NA	A	810	-	-	-	X
3	NA	B	807	-	-	-	X
3	NA	E	804	-	-	-	X
4	CA	A	811	-	-	-	X
4	CA	A	812	-	-	-	X
4	CA	B	811	-	-	-	X
4	CA	C	805	-	-	-	X
4	CA	D	806	-	-	-	X
4	CA	D	807	-	-	-	X
4	CA	E	808	-	-	-	X
4	CA	F	804	-	-	-	X

2 Entry composition [i](#)

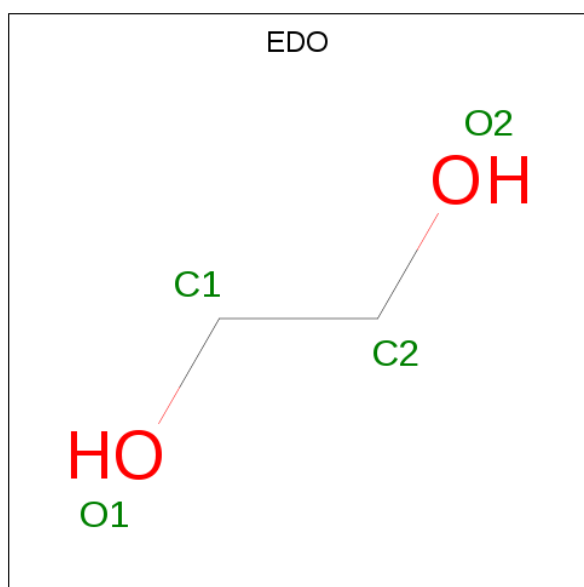
There are 5 unique types of molecules in this entry. The entry contains 32308 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 tail spike protein gp49.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	589	Total	C	N	O	S	0	15	0
			4405	2737	765	886	17			
1	B	590	Total	C	N	O	S	0	18	0
			4426	2747	768	894	17			
1	C	589	Total	C	N	O	S	7	15	0
			4416	2741	769	889	17			
1	D	590	Total	C	N	O	S	0	22	0
			4447	2758	769	902	18			
1	E	590	Total	C	N	O	S	0	20	0
			4442	2757	770	897	18			
1	F	590	Total	C	N	O	S	0	15	0
			4410	2738	765	889	18			

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	5	Total Na 5 5	0	0
3	A	7	Total Na 7 7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	3	Total 3	Na 3	0	0
3	C	2	Total 2	Na 2	0	0
3	E	4	Total 4	Na 4	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total 2	Ca 2	0	0
4	E	1	Total 1	Ca 1	0	0
4	B	1	Total 1	Ca 1	0	0
4	C	1	Total 1	Ca 1	0	0
4	A	2	Total 2	Ca 2	0	0
4	F	1	Total 1	Ca 1	0	0

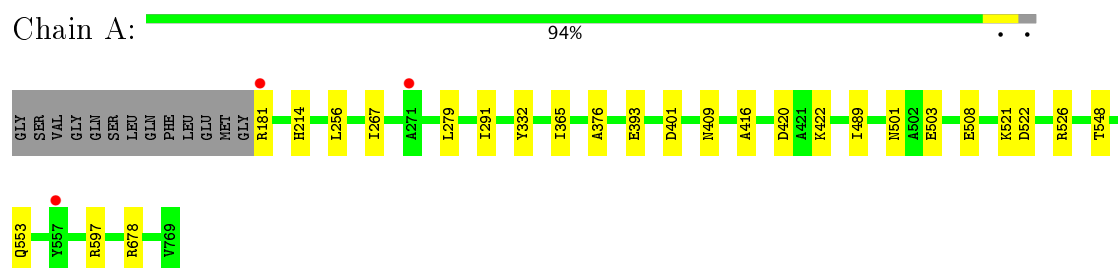
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	981	Total 981	O 981	0	0
5	B	960	Total 960	O 960	0	0
5	C	903	Total 903	O 903	0	0
5	D	968	Total 968	O 968	0	0
5	E	957	Total 957	O 957	0	0
5	F	892	Total 892	O 892	0	0

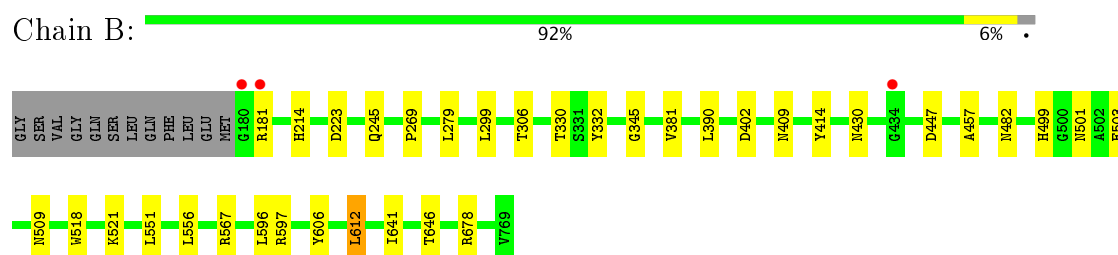
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

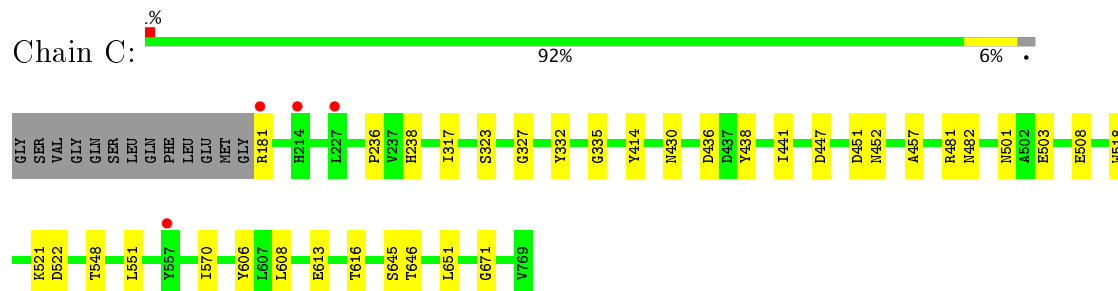
- Molecule 1: tail spike protein gp49



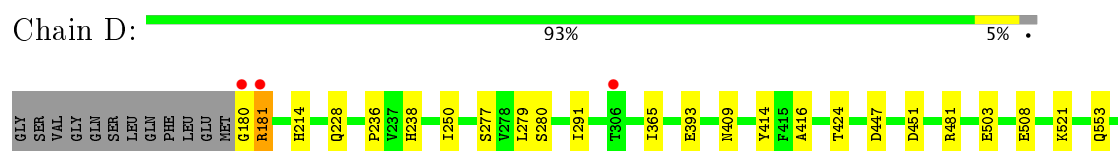
- Molecule 1: tail spike protein gp49



- Molecule 1: tail spike protein gp49



- Molecule 1: tail spike protein gp49

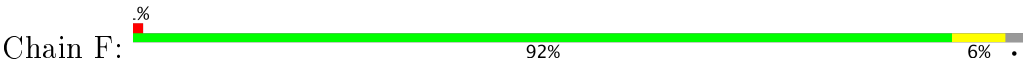




- Molecule 1: tail spike protein gp49



- Molecule 1: tail spike protein gp49



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	114.40Å 148.23Å 117.58Å 90.00° 90.85° 90.00°	Depositor
Resolution (Å)	19.99 – 1.90 19.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.99-1.90) 99.8 (19.99-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 1.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.129 , 0.174 0.129 , 0.174	Depositor DCC
R_{free} test set	15242 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	13.9	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.004 for l,k,-h 0.127 for h,-k,-l 0.013 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	32308	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: NA, CA, 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	0.53	0/4485	0.66	0/6126
1	B	0.54	0/4506	0.67	2/6155 (0.0%)
1	C	0.54	0/4496	0.66	0/6141
1	D	0.54	0/4527	0.66	0/6183
1	E	0.53	0/4522	0.65	1/6178 (0.0%)
1	F	0.53	0/4490	0.65	0/6132
All	All	0.53	0/27026	0.66	3/36915 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	678	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	B	678	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	678	ARG	NE-CZ-NH1	5.04	122.82	120.30

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	4405	0	4291	17	0
1	B	4426	0	4302	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4416	0	4296	20	0
1	D	4447	0	4313	16	0
1	E	4442	0	4317	20	0
1	F	4410	0	4286	27	0
2	A	12	0	18	1	0
2	B	20	0	30	3	0
2	C	8	0	12	1	0
2	D	8	0	12	4	0
2	E	12	0	18	4	0
2	F	12	0	18	1	0
3	A	7	0	0	0	0
3	B	5	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
3	E	4	0	0	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	981	0	0	6	1
5	B	960	0	0	8	0
5	C	903	0	0	8	0
5	D	968	0	0	2	1
5	E	957	0	0	4	0
5	F	892	0	0	9	0
All	All	32308	0	25913	124	1

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 (124) 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:F:214:HIS:HB2	2:F:803:EDO:H21	1.61	0.81
1:C:181:ARG:HD3	1:C:236:PRO:HD2	1.63	0.81
1:F:553:GLN:OE1	5:F:1730:HOH:O	2.01	0.79
1:E:214:HIS:HB2	2:E:803:EDO:H12	1.67	0.77
1:D:180:GLY:HA3	1:D:238:HIS:HB2	1.68	0.74
1:E:553:GLN:OE1	5:E:1857:HOH:O	2.05	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:553:GLN:NE2	5:F:1717:HOH:O	2.22	0.73
1:A:214:HIS:HB2	2:A:803:EDO:H21	1.71	0.72
1:B:402[A]:ASP:OD2	5:B:1600:HOH:O	2.10	0.69
1:B:567[A]:ARG:NH2	5:B:1182:HOH:O	2.26	0.68
1:F:180:GLY:HA2	1:F:236:PRO:HB2	1.75	0.68
1:A:256:LEU:HD21	1:A:279[B]:LEU:HD22	1.76	0.67
1:D:250:ILE:HB	1:D:279:LEU:HD12	1.77	0.67
1:C:451:ASP:OD2	5:C:1676:HOH:O	2.13	0.67
1:E:597[A]:ARG:NH2	5:E:1853:HOH:O	2.28	0.66
1:F:567[A]:ARG:NH1	5:F:1488:HOH:O	2.29	0.63
1:F:613[B]:GLU:OE2	5:F:1354:HOH:O	2.15	0.63
1:D:553:GLN:NE2	1:F:552:ASP:OD2	2.33	0.61
1:F:597[A]:ARG:NH2	5:F:1727:HOH:O	2.34	0.60
1:E:250:ILE:HB	1:E:279:LEU:HD23	1.84	0.60
1:A:597:ARG:NH1	5:A:1311:HOH:O	2.24	0.59
1:E:478[B]:VAL:HG22	1:E:505:CYS:SG	2.43	0.59
1:C:613:GLU:OE2	5:C:1365:HOH:O	2.16	0.58
1:B:345:GLY:O	5:B:1782:HOH:O	2.17	0.58
1:C:436:ASP:OD2	5:C:1211:HOH:O	2.17	0.57
1:B:214:HIS:HB2	2:B:804:EDO:H21	1.87	0.56
1:C:481[A]:ARG:NH1	1:C:508:GLU:OE1	2.38	0.56
1:F:181:ARG:NH2	5:F:1581:HOH:O	2.39	0.55
1:C:481[A]:ARG:NH2	5:C:1538:HOH:O	2.22	0.55
1:E:635:LYS:HG2	1:E:664:THR:HB	1.88	0.55
1:F:250:ILE:HB	1:F:279:LEU:HD12	1.88	0.55
1:B:597[A]:ARG:NH2	5:B:1332:HOH:O	2.40	0.55
1:E:180:GLY:HA3	1:E:238:HIS:HB2	1.90	0.54
1:D:214:HIS:HB2	2:D:801:EDO:H11	1.90	0.54
1:D:228:GLN:HB3	2:D:801:EDO:H22	1.88	0.54
1:C:238:HIS:HE1	5:C:1680:HOH:O	1.89	0.54
1:F:279:LEU:HB3	1:F:390[B]:LEU:HD23	1.90	0.54
1:B:567[B]:ARG:NH1	5:B:1356:HOH:O	2.40	0.53
1:F:181:ARG:HE	1:F:236:PRO:HD2	1.74	0.53
1:C:481[B]:ARG:NH1	5:C:1800:HOH:O	2.40	0.52
1:D:214:HIS:HB2	2:D:801:EDO:C1	2.39	0.52
1:E:181[A]:ARG:NH1	5:E:1757:HOH:O	2.42	0.51
1:D:733:ASN:HD21	2:E:802:EDO:C2	2.23	0.51
1:B:503:GLU:HA	1:B:521:LYS:O	2.11	0.51
1:E:721:SER:H	2:E:802:EDO:H21	1.75	0.51
1:B:509:ASN:ND2	5:B:1744:HOH:O	2.45	0.50
1:E:332:TYR:CD1	1:E:501:ASN:HB3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:390[B]:LEU:HD12	1:F:413:VAL:HG22	1.94	0.49
1:A:420:ASP:OD1	1:A:422[B]:LYS:HE3	2.13	0.49
1:A:508:GLU:HG2	1:A:526:ARG:HB2	1.95	0.49
1:E:181[B]:ARG:HD3	5:F:1645:HOH:O	2.13	0.49
2:E:802:EDO:H22	5:E:1296:HOH:O	2.12	0.49
1:D:424:THR:HG22	1:D:451:ASP:HB3	1.94	0.48
1:F:503:GLU:HA	1:F:521:LYS:O	2.13	0.48
1:A:332:TYR:CD1	1:A:501:ASN:HB3	2.48	0.48
1:E:522:ASP:HA	1:E:548:THR:O	2.13	0.48
1:F:635:LYS:HG2	1:F:664:THR:HB	1.96	0.48
1:B:612:LEU:HD22	1:B:641:ILE:HG12	1.94	0.48
1:B:518:TRP:CZ2	1:B:551:LEU:HG	2.49	0.48
1:B:482:ASN:HB3	5:C:1800:HOH:O	2.13	0.47
1:D:481[A]:ARG:NH1	1:D:508:GLU:OE1	2.35	0.47
1:A:291:ILE:HG23	1:A:365:ILE:HG13	1.96	0.47
1:C:438:TYR:CE2	1:C:441:ILE:HD12	2.49	0.47
1:D:503:GLU:HA	1:D:521:LYS:O	2.15	0.47
1:E:503:GLU:HA	1:E:521:LYS:O	2.15	0.47
1:D:181:ARG:NH1	5:D:1600:HOH:O	2.48	0.46
1:B:306:THR:HG23	5:B:1782:HOH:O	2.15	0.46
1:D:181:ARG:HB3	1:D:236:PRO:O	2.15	0.46
1:B:612:LEU:HD21	1:B:646:THR:HB	1.98	0.45
1:C:570:ILE:O	1:C:608:LEU:HA	2.16	0.45
1:A:489:ILE:HG21	1:B:299:LEU:HD13	1.97	0.45
1:C:503:GLU:HA	1:C:521:LYS:O	2.17	0.45
1:E:279:LEU:HB2	1:E:390[B]:LEU:HD23	1.99	0.45
1:A:503:GLU:HA	1:A:521:LYS:O	2.18	0.44
1:A:181:ARG:HG3	5:C:1720:HOH:O	2.17	0.44
1:D:393:GLU:HA	1:D:416:ALA:O	2.18	0.44
1:A:522:ASP:HA	1:A:548:THR:O	2.18	0.44
1:F:339:GLU:HG2	1:F:351:ARG:HD2	2.00	0.44
1:F:522:ASP:HA	1:F:548:THR:O	2.18	0.44
1:F:181:ARG:NE	1:F:236:PRO:HD2	2.33	0.43
1:C:518:TRP:CZ2	1:C:551:LEU:HG	2.53	0.43
1:F:646:THR:O	1:F:671:GLY:HA3	2.19	0.43
1:C:332:TYR:CD1	1:C:501:ASN:HB3	2.54	0.43
1:E:184:PRO:HG3	1:E:227[B]:LEU:HD13	2.01	0.43
1:C:430:ASN:O	1:C:457:ALA:HA	2.18	0.43
1:C:522:ASP:HA	1:C:548:THR:O	2.19	0.43
1:E:390[B]:LEU:HD12	1:E:413:VAL:HG22	2.01	0.43
1:D:277[B]:SER:OG	1:D:280:SER:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:692:THR:HA	1:E:752:PHE:O	2.19	0.43
1:A:376:ALA:HA	1:A:401:ASP:O	2.19	0.43
1:D:616:THR:HA	1:D:645:SER:O	2.19	0.42
1:A:553:GLN:OE1	5:A:1876:HOH:O	2.20	0.42
1:B:332:TYR:CD1	1:B:501:ASN:HB3	2.54	0.42
1:E:280:SER:HA	1:E:391:LEU:O	2.20	0.42
1:C:452:ASN:HA	1:C:482:ASN:O	2.19	0.42
1:A:267:ILE:HD13	1:A:279[A]:LEU:HD11	2.01	0.42
5:A:1377:HOH:O	1:B:181:ARG:HD3	2.20	0.42
1:B:556:LEU:HB2	1:B:596[B]:LEU:HD13	2.02	0.42
1:B:214:HIS:HB2	2:B:804:EDO:C2	2.50	0.42
1:B:269:PRO:HD2	1:B:381:VAL:O	2.20	0.42
1:E:181[A]:ARG:HB3	1:E:235:ALA:HB1	2.02	0.42
1:A:678[A]:ARG:HD3	5:A:1589:HOH:O	2.20	0.41
1:B:279:LEU:HB3	1:B:390[B]:LEU:HD23	2.01	0.41
1:B:430:ASN:O	1:B:457:ALA:HA	2.19	0.41
1:C:646:THR:O	1:C:671:GLY:HA3	2.20	0.41
1:B:330[A]:THR:HB	5:B:1738:HOH:O	2.20	0.41
5:D:1864:HOH:O	1:F:181:ARG:HB3	2.19	0.41
1:C:323:SER:HB3	1:C:327:GLY:HA2	2.03	0.41
1:B:499:HIS:CD2	2:B:803:EDO:H12	2.55	0.41
1:C:616:THR:HA	1:C:645:SER:O	2.20	0.41
1:F:388:ASN:HA	1:F:411:ALA:O	2.21	0.41
5:A:1075:HOH:O	2:C:801:EDO:H21	2.20	0.41
1:F:611:ARG:NH1	1:F:613[A]:GLU:OE2	2.43	0.41
1:E:299:LEU:HD13	1:F:489:ILE:HG21	2.02	0.41
1:A:597:ARG:NH2	5:A:1445:HOH:O	2.25	0.41
1:F:290:ASN:ND2	5:F:1359:HOH:O	2.33	0.41
1:B:223:ASP:HB2	1:B:245:GLN:O	2.20	0.41
1:A:393:GLU:HA	1:A:416:ALA:O	2.20	0.41
1:D:291:ILE:HG23	1:D:365:ILE:HG13	2.03	0.41
2:D:802:EDO:H21	5:F:1224:HOH:O	2.21	0.41
1:F:518:TRP:CZ2	1:F:551:LEU:HG	2.57	0.40
1:F:393:GLU:HA	1:F:416:ALA:O	2.21	0.40
1:C:317:ILE:O	1:C:335:GLY:HA3	2.21	0.40
1:F:616:THR:HA	1:F:645:SER:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1029:HOH:O	5:D:1784:HOH:O[2_646]	2.00	0.20

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	602/602 (100%)	579 (96%)	22 (4%)	1 (0%)	51	41
1	B	606/602 (101%)	586 (97%)	19 (3%)	1 (0%)	51	41
1	C	603/602 (100%)	580 (96%)	23 (4%)	0	100	100
1	D	610/602 (101%)	588 (96%)	21 (3%)	1 (0%)	51	41
1	E	608/602 (101%)	582 (96%)	26 (4%)	0	100	100
1	F	603/602 (100%)	584 (97%)	19 (3%)	0	100	100
All	All	3632/3612 (101%)	3499 (96%)	130 (4%)	3 (0%)	55	45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	409	ASN
1	B	409	ASN
1	A	409	ASN

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	474/469 (101%)	474 (100%)	0	100	100
1	B	477/469 (102%)	473 (99%)	4 (1%)	85	85
1	C	475/469 (101%)	471 (99%)	4 (1%)	85	85
1	D	481/469 (103%)	475 (99%)	6 (1%)	75	75
1	E	479/469 (102%)	476 (99%)	3 (1%)	89	90
1	F	474/469 (101%)	471 (99%)	3 (1%)	89	90
All	All	2860/2814 (102%)	2840 (99%)	20 (1%)	87	87

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	414	TYR
1	B	447	ASP
1	B	606	TYR
1	B	612	LEU
1	C	414	TYR
1	C	447	ASP
1	C	606	TYR
1	C	651	LEU
1	D	181	ARG
1	D	414	TYR
1	D	447	ASP
1	D	606	TYR
1	D	651[A]	LEU
1	D	651[B]	LEU
1	E	181[A]	ARG
1	E	181[B]	ARG
1	E	447	ASP
1	F	414	TYR
1	F	447	ASP
1	F	489	ILE

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 47 ligands modelled in this entry, 29 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EDO	A	801	-	3,3,3	0.40	0	2,2,2	0.19	0
2	EDO	A	802	-	3,3,3	0.47	0	2,2,2	0.49	0
2	EDO	A	803	-	3,3,3	0.42	0	2,2,2	0.70	0
2	EDO	B	801	-	3,3,3	0.34	0	2,2,2	0.49	0
2	EDO	B	802	-	3,3,3	0.46	0	2,2,2	0.31	0
2	EDO	B	803	-	3,3,3	0.41	0	2,2,2	0.40	0
2	EDO	B	804	-	3,3,3	0.31	0	2,2,2	0.72	0
2	EDO	B	805	-	3,3,3	0.47	0	2,2,2	0.20	0
2	EDO	C	801	-	3,3,3	0.39	0	2,2,2	0.46	0
2	EDO	C	802	-	3,3,3	0.49	0	2,2,2	0.16	0
2	EDO	D	801	-	3,3,3	0.30	0	2,2,2	0.68	0
2	EDO	D	802	-	3,3,3	0.36	0	2,2,2	0.44	0
2	EDO	E	801	-	3,3,3	0.45	0	2,2,2	0.32	0
2	EDO	E	802	-	3,3,3	0.41	0	2,2,2	0.33	0
2	EDO	E	803	-	3,3,3	0.35	0	2,2,2	0.81	0
2	EDO	F	801	-	3,3,3	0.41	0	2,2,2	0.33	0
2	EDO	F	802	-	3,3,3	0.43	0	2,2,2	0.56	0
2	EDO	F	803	-	3,3,3	0.40	0	2,2,2	0.58	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
2	EDO	A	801	-	-	0/1/1/1	0/0/0/0
2	EDO	A	802	-	-	0/1/1/1	0/0/0/0
2	EDO	A	803	-	-	0/1/1/1	0/0/0/0
2	EDO	B	801	-	-	0/1/1/1	0/0/0/0
2	EDO	B	802	-	-	0/1/1/1	0/0/0/0
2	EDO	B	803	-	-	0/1/1/1	0/0/0/0
2	EDO	B	804	-	-	0/1/1/1	0/0/0/0
2	EDO	B	805	-	-	0/1/1/1	0/0/0/0
2	EDO	C	801	-	-	0/1/1/1	0/0/0/0
2	EDO	C	802	-	-	0/1/1/1	0/0/0/0
2	EDO	D	801	-	-	0/1/1/1	0/0/0/0
2	EDO	D	802	-	-	0/1/1/1	0/0/0/0
2	EDO	E	801	-	-	0/1/1/1	0/0/0/0
2	EDO	E	802	-	-	0/1/1/1	0/0/0/0
2	EDO	E	803	-	-	0/1/1/1	0/0/0/0
2	EDO	F	801	-	-	0/1/1/1	0/0/0/0
2	EDO	F	802	-	-	0/1/1/1	0/0/0/0
2	EDO	F	803	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	803	EDO	1	0
2	B	803	EDO	1	0
2	B	804	EDO	2	0
2	C	801	EDO	1	0
2	D	801	EDO	3	0
2	D	802	EDO	1	0
2	E	802	EDO	3	0
2	E	803	EDO	1	0
2	F	803	EDO	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, 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	589/602 (97%)	-0.33	3 (0%) 90 92	6, 11, 19, 54	0
1	B	590/602 (98%)	-0.32	3 (0%) 90 92	6, 10, 18, 65	0
1	C	589/602 (97%)	-0.30	4 (0%) 87 89	6, 11, 21, 50	0
1	D	590/602 (98%)	-0.29	3 (0%) 90 92	6, 11, 20, 73	0
1	E	590/602 (98%)	-0.28	3 (0%) 90 92	6, 11, 19, 58	0
1	F	590/602 (98%)	-0.21	5 (0%) 86 87	6, 12, 23, 69	0
All	All	3538/3612 (97%)	-0.29	21 (0%) 89 90	6, 11, 21, 73	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	180	GLY	5.8
1	E	180	GLY	5.7
1	F	180	GLY	5.4
1	D	181	ARG	3.5
1	B	180	GLY	3.1
1	B	181	ARG	3.1
1	E	254	GLY	3.0
1	F	214	HIS	2.6
1	A	271	ALA	2.5
1	E	557[A]	TYR	2.5
1	F	557[A]	TYR	2.5
1	A	557[A]	TYR	2.4
1	F	227[A]	LEU	2.4
1	F	181	ARG	2.4
1	D	306	THR	2.3
1	A	181	ARG	2.1
1	C	214	HIS	2.1
1	C	557[A]	TYR	2.1
1	B	434	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	227[A]	LEU	2.1
1	C	181	ARG	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	CA	A	811	1/1	0.65	0.36	22.43	70,70,70,70	0
4	CA	D	806	1/1	0.90	0.30	19.82	74,74,74,74	0
4	CA	A	812	1/1	0.94	0.29	17.95	88,88,88,88	0
4	CA	D	807	1/1	0.89	0.39	14.95	59,59,59,59	0
4	CA	C	805	1/1	0.98	0.31	14.19	52,52,52,52	0
4	CA	E	808	1/1	0.98	0.35	13.52	59,59,59,59	0
4	CA	B	811	1/1	0.93	0.35	13.06	57,57,57,57	0
2	EDO	B	803	4/4	0.90	0.17	9.79	28,28,30,31	0
4	CA	F	804	1/1	0.94	0.25	9.24	59,59,59,59	0
3	NA	A	810	1/1	1.00	0.18	8.42	3,3,3,3	0
2	EDO	E	803	4/4	0.93	0.16	4.13	22,22,24,28	0
2	EDO	A	803	4/4	0.94	0.16	3.78	26,27,28,31	0
3	NA	A	804	1/1	0.98	0.12	3.25	15,15,15,15	0
2	EDO	B	804	4/4	0.92	0.17	2.92	20,26,29,32	0
3	NA	B	807	1/1	0.98	0.12	2.88	12,12,12,12	0
3	NA	E	804	1/1	0.99	0.12	2.59	10,10,10,10	0
3	NA	A	807	1/1	0.99	0.11	2.58	12,12,12,12	0
3	NA	A	805	1/1	0.88	0.15	2.14	46,46,46,46	0
2	EDO	B	801	4/4	0.93	0.12	2.04	23,25,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	EDO	D	801	4/4	0.95	0.13	1.87	19,26,31,33	0
2	EDO	B	802	4/4	0.95	0.11	1.84	11,11,14,18	0
3	NA	B	808	1/1	0.99	0.12	1.80	4,4,4,4	0
2	EDO	F	802	4/4	0.96	0.10	1.32	17,22,25,27	0
2	EDO	F	801	4/4	0.98	0.09	1.06	11,14,15,19	0
3	NA	E	805	1/1	0.99	0.10	0.98	11,11,11,11	0
3	NA	D	803	1/1	0.99	0.09	0.35	13,13,13,13	0
3	NA	E	807	1/1	0.79	0.11	0.33	40,40,40,40	0
2	EDO	D	802	4/4	0.95	0.09	0.30	20,22,29,33	0
2	EDO	C	801	4/4	0.96	0.10	0.21	21,22,23,26	0
2	EDO	E	801	4/4	0.96	0.10	-0.11	18,21,23,23	0
2	EDO	A	801	4/4	0.97	0.08	-0.49	14,15,16,16	0
2	EDO	F	803	4/4	0.96	0.10	-0.63	31,31,33,33	0
2	EDO	C	802	4/4	0.97	0.08	-0.86	13,16,17,18	0
3	NA	D	804	1/1	0.99	0.07	-0.94	9,9,9,9	0
2	EDO	A	802	4/4	0.97	0.08	-1.40	10,13,13,17	0
3	NA	C	803	1/1	0.93	0.20	-	43,43,43,43	0
2	EDO	B	805	4/4	0.85	0.18	-	46,48,48,49	0
3	NA	A	808	1/1	0.99	0.09	-	12,12,12,12	0
3	NA	A	809	1/1	1.00	0.16	-	6,6,6,6	0
3	NA	B	806	1/1	0.95	0.14	-	29,29,29,29	0
3	NA	C	804	1/1	0.98	0.12	-	25,25,25,25	0
3	NA	D	805	1/1	0.98	0.08	-	12,12,12,12	0
3	NA	B	809	1/1	0.98	0.10	-	13,13,13,13	0
3	NA	B	810	1/1	0.99	0.09	-	24,24,24,24	0
3	NA	A	806	1/1	0.99	0.12	-	7,7,7,7	0
3	NA	E	806	1/1	1.00	0.10	-	12,12,12,12	0
2	EDO	E	802	4/4	0.92	0.14	-	28,28,30,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.