Full wwPDB X-ray Structure Validation Report (i)

PDB ID	:	7A0V
Title	:	Crystal structure of the 5-phosphatase domain of Synaptojanin1 in complex with a nanobody
Authors	:	Paesmans, J.; Galicia, C.; Martin, E.; Versees, W.
Deposited on	:	2020-08-11
Resolution	:	2.30 Å(reported)

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

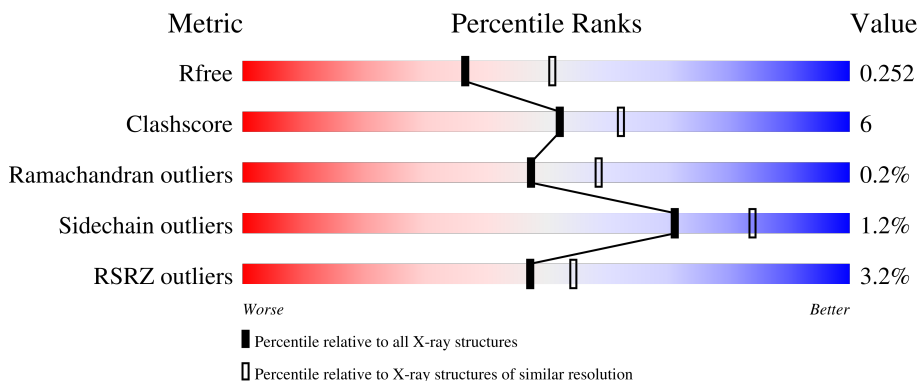|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 2.30 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	Percentile Ranks	Value
Rfree		0.252
Clashscore		6
Ramachandran outliers		0.2%
Sidechain outliers		1.2%
RSRZ outliers		3.2%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 of 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	349	3% 83% 13% 5%
1	C	349	3% 74% 15% 11%
1	E	349	2% 74% 16% 9%
2	B	132	11% 77% 15% • 7%
2	D	132	2% 92% • 5%

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Mol	Chain	Length	Quality of chain
2	F	132	84% 10% 6%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10975 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 Synaptojanin-1.

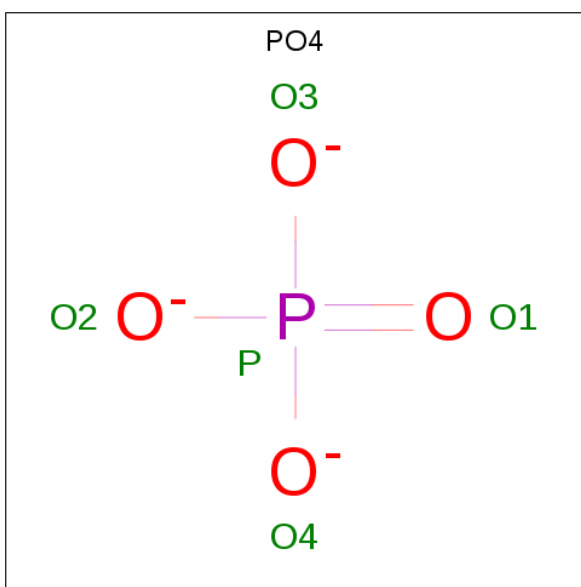| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total 2707	C 1734	N 472	O 490	S 11	0	5	0
1	C	309	Total 2505	C 1610	N 429	O 456	S 10	0	0	0
1	E	317	Total 2538	C 1626	N 444	O 458	S 10	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	525	GLY	-	expression tag	UNP O43426
A	526	ALA	-	expression tag	UNP O43426
A	527	MET	-	expression tag	UNP O43426
C	525	GLY	-	expression tag	UNP O43426
C	526	ALA	-	expression tag	UNP O43426
C	527	MET	-	expression tag	UNP O43426
E	525	GLY	-	expression tag	UNP O43426
E	526	ALA	-	expression tag	UNP O43426
E	527	MET	-	expression tag	UNP O43426

- Molecule 2 is a protein called Nanobody 13015.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	123	Total 917	C 563	N 167	O 183	S 4	0	0	0
2	D	125	Total 952	C 589	N 176	O 183	S 4	0	0	0
2	F	124	Total 955	C 589	N 176	O 186	S 4	0	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	P 1	0	0
3	E	1	Total 5	O 4	P 1	0	0
3	E	1	Total 5	O 4	P 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0
4	E	1	Total 1	Mg 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

C3

OH O3

C1   C2

HO

O1

OH

O2

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

- Molecule 6 is water.

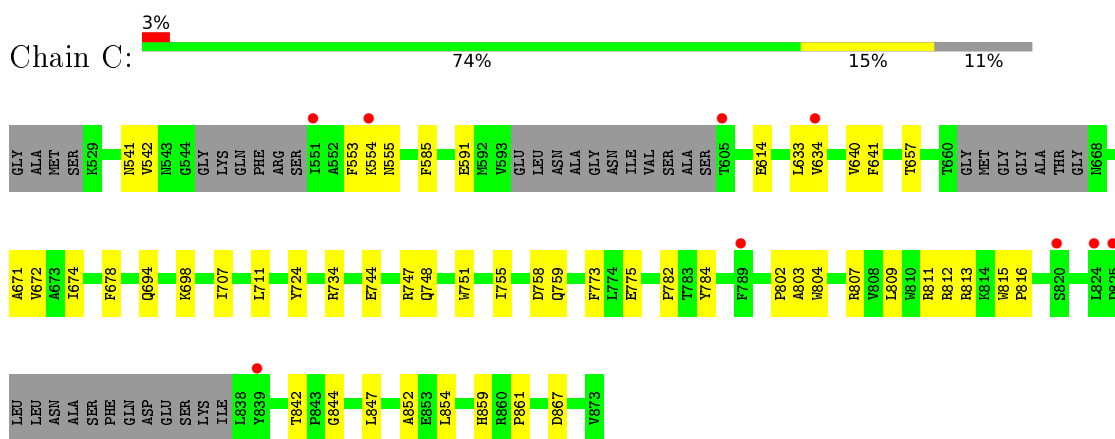| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	147	Total O	147 147	0	0
6	B	10	Total O	10 10	0	0
6	C	68	Total O	68 68	0	0
6	D	21	Total O	21 21	0	0
6	E	68	Total O	68 68	0	0
6	F	45	Total O	45 45	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Synaptojanin-1
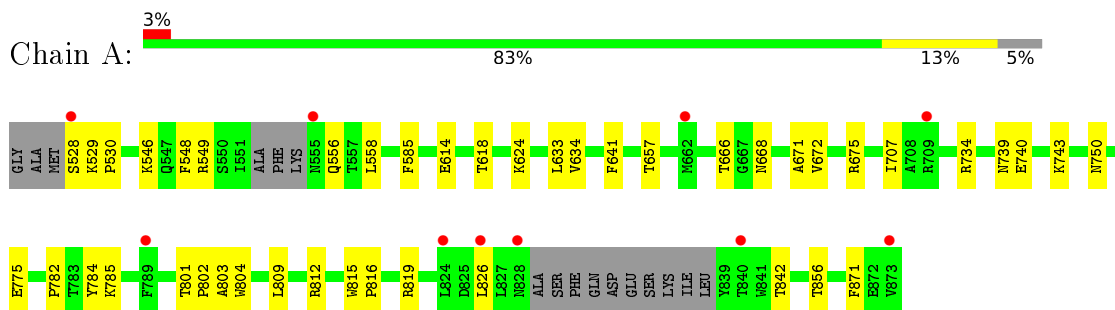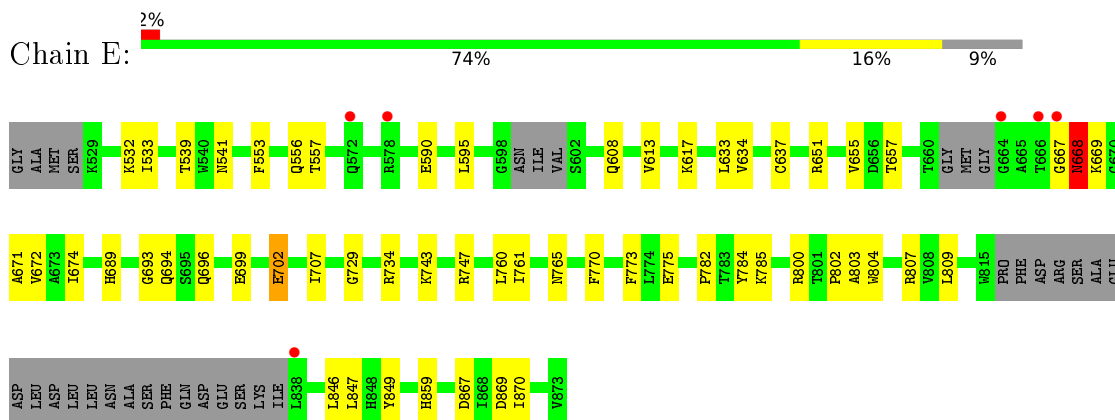
- Molecule 1: Synaptojanin-1

- Molecule 1: Synaptojanin-1

• Molecule 2: Nanobody 13015

Chain B:

11%

77%

15%

7%

Q1 V2 S7 G8 G9 A12 G15 L18 R19 L20 T28 R32 G35 Q39 K43 W53 D61 S62 V63 R66 V78 M82 N83 N84 L85 T86 P87 E88 D89 T90 Y94 Q97 D105 T119 V120 H123 HIS HIS HIS HIS HIS

GLU PRO GLU ALA

• Molecule 2: Nanobody 13015

Chain D:

2%

92%

5%

Q1 W53 M82 L85 H125 HIS HIS HIS GLU PRO GLU ALA

• Molecule 2: Nanobody 13015

Chain F:

84%

10%

6%

Q1 V2 T28 F29 R32 W36 W53 R71 V78 M82 L85 A100 D104 H124 HIS HIS HIS HIS GLU PRO GLU ALA
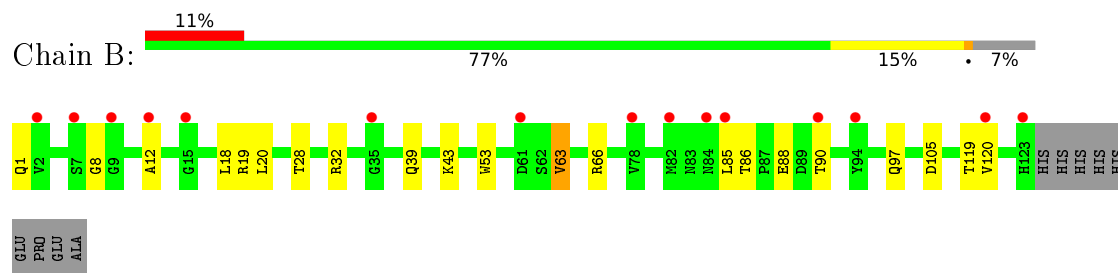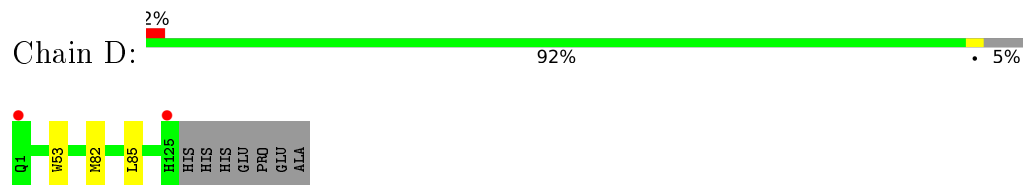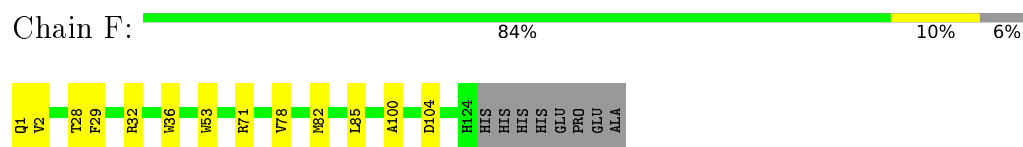
4　Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	168.87Å　　108.79Å　　100.97Å 90.00°　　　120.72°　　　90.00°	Depositor
Resolution (Å)	86.81　–　2.30 87.06　–　2.30	Depositor EDS
% Data completeness (in resolution range)	76.9 (86.81-2.30) 71.8 (87.06-2.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	0.98 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.196　,　0.252 0.196　,　0.252	Depositor DCC
R_{free} test set	2764 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	32.8	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 40.7	EDS
L-test for twinning [2]	$<\vert L\vert> = 0.50$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -1/2*h+1/2*k+l,1/2*h-1/2*k+l,1/2*h+1/2*k 0.003 for -1/2*h-1/2*k+l,-1/2*h-1/2*k-l,1/2*h-1/2*k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10975	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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 $<\vert L\vert>$, $<L^2>$ 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, PO4, MG

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	0.24	0/2785	0.42	0/3769
1	C	0.24	0/2565	0.43	0/3478
1	E	0.24	0/2595	0.43	0/3510
2	B	0.24	0/935	0.46	0/1267
2	D	0.25	0/973	0.44	0/1314
2	F	0.25	0/976	0.44	0/1317
All	All	0.24	0/10829	0.43	0/14655

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 (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	2707	0	2669	25	0
1	C	2505	0	2433	37	0
1	E	2538	0	2497	33	0
2	B	917	0	837	15	0
2	D	952	0	889	1	0
2	F	955	0	898	7	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	10	0	0	1	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	A	24	0	32	1	0
6	A	147	0	0	1	0
6	B	10	0	0	0	0
6	C	68	0	0	0	0
6	D	21	0	0	0	0
6	E	68	0	0	0	0
6	F	45	0	0	0	0
All	All	10975	0	10255	115	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 6.

All (115) 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:666:THR:HG22	1:A:668:ASN:H	1.41	0.85
1:A:529:LYS:HD3	1:A:530:PRO:HD2	1.60	0.82
1:C:854:LEU:HD12	1:C:861:PRO:HG3	1.65	0.77
1:E:633:LEU:HD22	1:E:657:THR:HB	1.74	0.69
2:B:12:ALA:HA	2:B:120:VAL:HA	1.74	0.68
1:C:758:ASP:OD1	1:C:807:ARG:NH2	2.30	0.65
1:A:558:LEU:HB2	1:A:618:THR:HG21	1.80	0.64
1:E:761:ILE:O	1:E:765:ASN:ND2	2.28	0.64
1:C:852:ALA:HB3	1:C:861:PRO:HG2	1.78	0.64
1:E:699:GLU:OE2	1:E:699:GLU:N	2.31	0.64
2:B:32:ARG:NH2	2:B:97:GLN:OE1	2.30	0.63
1:A:546:LYS:HB3	1:A:549:ARG:HD2	1.80	0.63
1:C:775:GLU:HB2	1:C:809:LEU:HG	1.81	0.61
1:E:633:LEU:HG	1:E:634:VAL:HG22	1.83	0.61
1:C:744:GLU:HA	1:C:747:ARG:NH1	2.16	0.61
1:A:528:SER:HB3	1:A:871:PHE:HB3	1.82	0.60
1:C:744:GLU:OE2	1:C:748:GLN:NE2	2.34	0.60
1:A:556:GLN:HE22	1:A:856:THR:HG23	1.66	0.60
1:A:775:GLU:HB2	1:A:809:LEU:HG	1.83	0.60
1:C:744:GLU:OE1	1:C:747:ARG:NH1	2.35	0.60
2:B:85:LEU:HB3	2:B:120:VAL:HG11	1.84	0.60
1:E:657:THR:HG22	1:E:672:VAL:HG12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:842:THR:HG22	1:C:844:GLY:H	1.68	0.56
1:C:813:ARG:HD2	1:C:815:TRP:NE1	2.20	0.56
1:E:693:GLY:HA3	1:E:696:GLN:HG2	1.87	0.56
1:E:590:GLU:OE2	1:E:729:GLY:HA2	2.06	0.56
1:A:739:ASN:HD21	1:A:743:LYS:HE3	1.72	0.55
1:E:775:GLU:HB2	1:E:809:LEU:HG	1.88	0.55
2:B:1:GLN:HE22	2:F:71:ARG:H	1.55	0.55
1:C:751:TRP:O	1:C:755:ILE:HG13	2.06	0.54
1:C:698:LYS:H	1:C:698:LYS:HD2	1.72	0.54
2:B:63:VAL:HA	2:B:66:ARG:HD3	1.90	0.54
1:A:585:PHE:HB2	1:A:641:PHE:HB2	1.89	0.53
1:A:812:ARG:NH1	1:A:842:THR:O	2.41	0.53
1:A:739:ASN:HD22	1:A:801:THR:HA	1.74	0.53
1:E:760:LEU:HD13	1:E:807:ARG:HG3	1.90	0.53
2:B:105:ASP:OD1	2:B:105:ASP:N	2.41	0.52
1:A:624:LYS:H	5:A:905:GOL:H11	1.74	0.52
1:A:740:GLU:H	1:A:740:GLU:CD	2.13	0.52
1:E:655:VAL:HG12	1:E:674:ILE:HG12	1.91	0.52
1:C:694:GLN:HA	1:C:734:ARG:HG3	1.93	0.51
1:A:556:GLN:NE2	1:A:856:THR:HG23	2.26	0.51
2:F:28:THR:O	2:F:32:ARG:HG3	2.10	0.51
1:E:667:GLY:O	1:E:669:LYS:N	2.43	0.51
1:E:595:LEU:HD12	1:E:668:ASN:HB3	1.91	0.51
1:E:847:LEU:HD11	1:E:867:ASP:OD2	2.11	0.51
1:E:532:LYS:HE2	1:E:869:ASP:OD2	2.11	0.50
1:C:633:LEU:HG	1:C:634:VAL:HG22	1.92	0.50
1:C:633:LEU:HD22	1:C:657:THR:HB	1.94	0.50
1:C:744:GLU:HA	1:C:747:ARG:HH12	1.76	0.50
2:F:82:MET:HB3	2:F:85:LEU:HD21	1.93	0.49
1:C:657:THR:HG22	1:C:672:VAL:HG22	1.95	0.49
1:E:846:LEU:HD21	1:E:849:TYR:HB2	1.94	0.49
1:C:758:ASP:CG	1:C:807:ARG:HH22	2.17	0.49
1:A:819[B]:ARG:NH1	6:A:1006:HOH:O	2.45	0.48
2:B:90:THR:HG22	2:B:120:VAL:H	1.77	0.48
2:F:36:TRP:HE1	2:F:78:VAL:HG12	1.79	0.48
1:C:724:TYR:CE2	1:C:812:ARG:HG3	2.49	0.48
1:C:804:TRP:HB2	1:C:807:ARG:HH21	1.79	0.47
2:B:63:VAL:HG22	2:B:66:ARG:HB2	1.97	0.47
1:E:541:ASN:HB3	1:E:859:HIS:CG	2.50	0.47
1:A:815:TRP:CG	1:A:816:PRO:HD3	2.50	0.47
1:C:671:ALA:HB2	1:C:707:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:699:GLU:O	1:E:702:GLU:HG3	2.14	0.47
1:C:734:ARG:HA	1:C:803:ALA:HB1	1.96	0.46
1:E:533:ILE:HG13	1:E:870:ILE:HG12	1.97	0.46
2:F:1:GLN:HG2	2:F:2:VAL:HG23	1.98	0.46
1:C:813:ARG:HD2	1:C:815:TRP:HE1	1.81	0.46
1:E:613:VAL:O	1:E:617:LYS:HG3	2.16	0.46
2:F:29:PHE:HZ	2:F:78:VAL:HG23	1.80	0.46
1:E:553:PHE:HA	1:E:556:GLN:HG2	1.96	0.46
1:A:633:LEU:HD22	1:A:657:THR:HB	1.98	0.45
1:A:784:TYR:HA	1:A:785:LYS:HA	1.76	0.45
1:E:770:PHE:HB3	1:E:773:PHE:HB2	1.98	0.45
1:C:553:PHE:CE1	1:C:614:GLU:HG3	2.51	0.45
1:E:800:ARG:HH12	3:E:901:PO4:P	2.40	0.45
1:A:826:LEU:HD11	1:C:811:ARG:NH2	2.33	0.44
1:E:533:ILE:CG1	1:E:870:ILE:HG12	2.47	0.44
2:B:8:GLY:HA2	2:B:20:LEU:HA	1.99	0.44
1:A:657:THR:HG22	1:A:672:VAL:HG22	1.98	0.44
1:C:542:VAL:O	1:C:591:GLU:HB2	2.17	0.44
1:C:734:ARG:O	1:C:759:GLN:HG3	2.17	0.44
1:E:784:TYR:HA	1:E:785:LYS:HA	1.70	0.43
1:C:815:TRP:CG	1:C:816:PRO:HD3	2.54	0.43
1:C:782:PRO:HA	1:C:804:TRP:CD1	2.54	0.43
1:E:651:ARG:HG2	2:F:100:ALA:HB2	2.00	0.43
2:B:39:GLN:NE2	2:B:43:LYS:O	2.50	0.43
1:C:784:TYR:O	1:C:802:PRO:HA	2.18	0.43
1:A:734:ARG:HA	1:A:803:ALA:HB1	2.00	0.43
1:A:784:TYR:O	1:A:802:PRO:HA	2.19	0.43
1:E:608:GLN:HG3	1:E:637:CYS:SG	2.59	0.42
1:C:541:ASN:HB3	1:C:859:HIS:CG	2.55	0.42
1:E:671:ALA:HB2	1:E:707:ILE:HD13	2.01	0.42
1:A:671:ALA:HB2	1:A:707:ILE:HD13	2.01	0.42
1:C:847:LEU:HD11	1:C:867:ASP:OD2	2.19	0.42
2:B:90:THR:HG22	2:B:119:THR:HA	2.02	0.42
2:D:82:MET:HB3	2:D:85:LEU:HD21	2.01	0.42
1:A:782:PRO:HA	1:A:804:TRP:CD1	2.55	0.42
2:B:86:THR:HG23	2:B:88:GLU:H	1.84	0.41
1:E:743:LYS:O	1:E:747:ARG:HG3	2.20	0.41
1:A:548:PHE:CD1	1:A:614:GLU:HG3	2.56	0.41
1:C:585:PHE:HB2	1:C:641:PHE:HB2	2.03	0.41
2:B:8:GLY:HA3	2:B:20:LEU:HG	2.02	0.41
1:E:634:VAL:HB	1:E:668:ASN:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:694:GLN:HA	1:E:734:ARG:HG3	2.02	0.41
1:E:782:PRO:HA	1:E:804:TRP:CD1	2.56	0.41
1:E:734:ARG:HA	1:E:803:ALA:HB1	2.03	0.41
1:C:640:VAL:HG23	1:C:674:ILE:HD12	2.01	0.41
2:B:18:LEU:HA	2:B:18:LEU:HD12	1.94	0.41
1:C:554:LYS:HB3	1:C:555:ASN:H	1.56	0.41
1:C:711:LEU:HA	1:C:711:LEU:HD23	1.95	0.41
1:E:784:TYR:O	1:E:802:PRO:HA	2.21	0.40
1:C:804:TRP:HB3	1:C:807:ARG:HE	1.87	0.40
2:B:28:THR:O	2:B:32:ARG:HD2	2.21	0.40
1:C:773:PHE:HA	1:C:811:ARG:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	332/349 (95%)	322 (97%)	9 (3%)	1 (0%)	41	50
1	C	299/349 (86%)	289 (97%)	10 (3%)	0	100	100
1	E	309/349 (88%)	292 (94%)	16 (5%)	1 (0%)	41	50
2	B	121/132 (92%)	107 (88%)	13 (11%)	1 (1%)	19	23
2	D	123/132 (93%)	119 (97%)	4 (3%)	0	100	100
2	F	122/132 (92%)	122 (100%)	0	0	100	100
All	All	1306/1443 (90%)	1251 (96%)	52 (4%)	3 (0%)	47	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	668	ASN

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Mol	Chain	Res	Type
1	A	634	VAL
2	B	63	VAL

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	290/302 (96%)	288 (99%)	2 (1%)	84	92
1	C	268/302 (89%)	267 (100%)	1 (0%)	91	96
1	E	269/302 (89%)	264 (98%)	5 (2%)	57	73
2	B	90/105 (86%)	88 (98%)	2 (2%)	52	69
2	D	95/105 (90%)	94 (99%)	1 (1%)	73	86
2	F	98/105 (93%)	96 (98%)	2 (2%)	55	72
All	All	1110/1221 (91%)	1097 (99%)	13 (1%)	71	84

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	675	ARG
1	A	750	ASN
2	B	19	ARG
2	B	53	TRP
1	C	678	PHE
2	D	53	TRP
1	E	539	THR
1	E	557	THR
1	E	668	ASN
1	E	689	HIS
1	E	702	GLU
2	F	53	TRP
2	F	104	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	739	ASN
2	B	1	GLN
2	B	117	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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	#$|Z| > 2$
3	PO4	E	901	4	4,4,4	0.91	0	6,6,6	0.44	0
3	PO4	A	901	-	4,4,4	0.91	0	6,6,6	0.43	0
5	GOL	A	904	-	5,5,5	0.37	0	5,5,5	0.24	0
3	PO4	E	902	-	4,4,4	0.90	0	6,6,6	0.43	0
5	GOL	A	903	-	5,5,5	0.38	0	5,5,5	0.25	0
5	GOL	A	906	-	5,5,5	0.37	0	5,5,5	0.28	0
5	GOL	A	905	-	5,5,5	0.37	0	5,5,5	0.28	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
5	GOL	A	904	-	-	1/4/4/4	-
5	GOL	A	906	-	-	2/4/4/4	-
5	GOL	A	903	-	-	1/4/4/4	-
5	GOL	A	905	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	906	GOL	O1-C1-C2-C3
5	A	903	GOL	O1-C1-C2-C3
5	A	905	GOL	O1-C1-C2-C3
5	A	906	GOL	O1-C1-C2-O2
5	A	905	GOL	O1-C1-C2-O2
5	A	904	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	901	PO4	1	0
5	A	905	GOL	1	0

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	333/349 (95%)	-0.09	10 (3%)	50	57	23, 36, 69, 90	0
1	C	309/349 (88%)	0.03	9 (2%)	51	58	33, 47, 75, 91	0
1	E	317/349 (90%)	0.05	6 (1%)	66	73	29, 46, 77, 91	0
2	B	123/132 (93%)	0.78	15 (12%)	4	6	33, 69, 96, 102	0
2	D	125/132 (94%)	-0.10	2 (1%)	72	77	34, 44, 66, 89	0
2	F	124/132 (93%)	-0.17	0	100	100	28, 36, 57, 82	0
All	All	1331/1443 (92%)	0.04	42 (3%)	47	54	23, 44, 81, 102	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	15	GLY	4.4
2	B	12	ALA	4.1
1	E	664	GLY	4.0
1	A	873	VAL	4.0
1	A	789	PHE	3.9
2	D	125	HIS	3.8
2	B	2	VAL	3.7
1	E	666	THR	3.6
2	B	82	MET	3.3
1	E	667	GLY	3.3
2	B	90	THR	3.0
1	C	824	LEU	3.0
1	A	824	LEU	3.0
1	C	554	LYS	2.7
1	C	551	ILE	2.7
2	B	35	GLY	2.7
2	B	7	SER	2.6
1	C	789	PHE	2.5
1	C	820	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	662	MET	2.4
1	C	634	VAL	2.4
1	E	572	GLN	2.4
2	B	123	HIS	2.3
2	B	85	LEU	2.3
1	A	528	SER	2.3
2	B	84	ASN	2.3
1	A	828	ASN	2.3
1	A	826	LEU	2.2
2	D	1	GLN	2.2
1	E	838	LEU	2.2
2	B	94	TYR	2.2
1	C	839	TYR	2.2
2	B	61	ASP	2.2
1	A	555	ASN	2.2
1	A	840	THR	2.1
2	B	9	GLY	2.0
1	C	825	ASP	2.0
2	B	78	VAL	2.0
1	C	605	THR	2.0
1	E	578	ARG	2.0
2	B	120	VAL	2.0
1	A	709	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 monosaccharides 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
5	GOL	A	905	6/6	0.76	0.24	52,60,64,73	0
3	PO4	E	901	5/5	0.81	0.15	75,78,86,106	0
5	GOL	A	903	6/6	0.86	0.15	56,58,61,64	0
3	PO4	E	902	5/5	0.87	0.40	70,76,89,97	0
5	GOL	A	906	6/6	0.93	0.20	46,50,52,55	0
5	GOL	A	904	6/6	0.94	0.12	48,51,52,58	0
3	PO4	A	901	5/5	0.94	0.15	61,71,74,93	0
4	MG	E	903	1/1	0.95	0.06	67,67,67,67	0
4	MG	A	902	1/1	0.95	0.09	46,46,46,46	0
4	MG	C	901	1/1	0.96	0.09	71,71,71,71	0

6.5 Other polymers ⓘ

There are no such residues in this entry.