Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 01:55 PM EST

PDB ID	:	4YXA
Title	:	Complex of SpaO(SPOA1,2 SeMet) and OrgB(APAR)::T4lysozyme fusion protein
Authors	:	Notti, R.Q.; Stebbins, C.E.
Deposited on	:	2015-03-22
Resolution	:	2.35 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

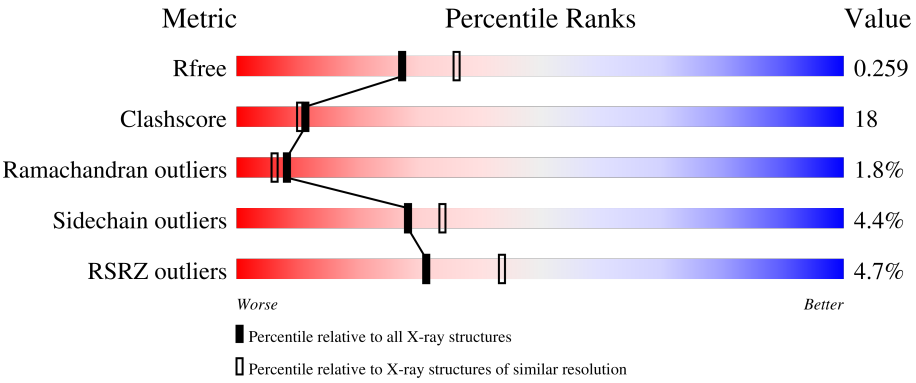
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	73	5% 47% 36% · 15%
1	D	73	3% 63% 22% 15%
2	B	70	4% 47% 43% · · ·
2	E	70	57% 29% 9% 6%
3	C	197	3% 52% 32% · 15%

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Mol	Chain	Length	Quality of chain
3	F	197	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4940 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 Surface presentation of antigens protein SpaO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	62	Total	C	N	O	S	0	0	0
			477	304	87	85	1			
1	D	62	Total	C	N	O	S	0	1	0
			486	311	89	85	1			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P40699
A	2	PRO	-	expression tag	UNP P40699
A	3	VAL	-	expression tag	UNP P40699
A	4	ASP	-	expression tag	UNP P40699
D	1	GLY	-	expression tag	UNP P40699
D	2	PRO	-	expression tag	UNP P40699
D	3	VAL	-	expression tag	UNP P40699
D	4	ASP	-	expression tag	UNP P40699

- Molecule 2 is a protein called Surface presentation of antigens protein SpaO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	67	Total	C	N	O	Se	0	0	0
			522	332	85	102	3			
2	E	66	Total	C	N	O	Se	0	0	0
			515	327	84	101	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLY	-	expression tag	UNP P40699
B	2	PRO	-	expression tag	UNP P40699
B	3	VAL	-	expression tag	UNP P40699
B	4	ASP	-	expression tag	UNP P40699

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1	GLY	-	expression tag	UNP P40699
E	2	PRO	-	expression tag	UNP P40699
E	3	VAL	-	expression tag	UNP P40699
E	4	ASP	-	expression tag	UNP P40699

- Molecule 3 is a protein called Oxygen-regulated invasion protein OrgB,Endolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	168	Total	C	N	O	S	0	0	0
			1319	845	236	233	5			
3	F	193	Total	C	N	O	S	0	0	0
			1499	954	266	274	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	GLY	-	expression tag	UNP P0CL45
C	2	PRO	-	expression tag	UNP P0CL45
C	3	VAL	-	expression tag	UNP P0CL45
C	4	ASP	-	expression tag	UNP P0CL45
C	45	GLY	ARG	conflict	UNP P00720
C	53	ASN	ASP	engineered mutation	UNP P00720
C	87	THR	CYS	engineered mutation	UNP P00720
C	130	ALA	CYS	engineered mutation	UNP P00720
C	170	ARG	ILE	conflict	UNP P00720
C	195	ALA	LYS	engineered mutation	UNP P00720
C	196	ALA	ASN	engineered mutation	UNP P00720
C	197	ALA	LEU	engineered mutation	UNP P00720
F	1	GLY	-	expression tag	UNP P0CL45
F	2	PRO	-	expression tag	UNP P0CL45
F	3	VAL	-	expression tag	UNP P0CL45
F	4	ASP	-	expression tag	UNP P0CL45
F	45	GLY	ARG	conflict	UNP P00720
F	53	ASN	ASP	engineered mutation	UNP P00720
F	87	THR	CYS	engineered mutation	UNP P00720
F	130	ALA	CYS	engineered mutation	UNP P00720
F	170	ARG	ILE	conflict	UNP P00720
F	195	ALA	LYS	engineered mutation	UNP P00720
F	196	ALA	ASN	engineered mutation	UNP P00720
F	197	ALA	LEU	engineered mutation	UNP P00720

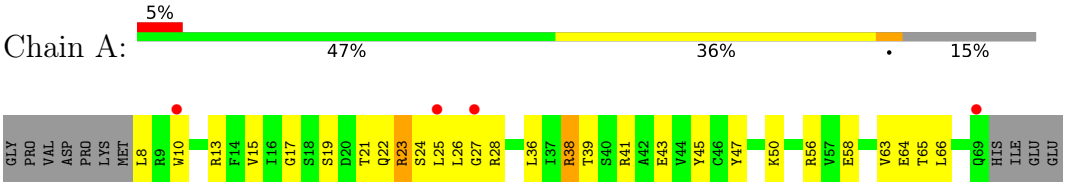
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	10	Total O 10 10	0	0
4	B	10	Total O 10 10	0	0
4	C	47	Total O 47 47	0	0
4	D	10	Total O 10 10	0	0
4	E	13	Total O 13 13	0	0
4	F	32	Total O 32 32	0	0

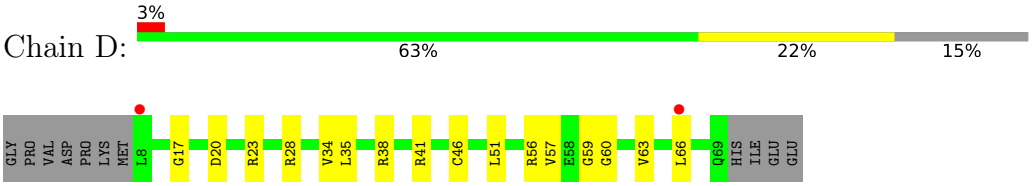
3 Residue-property plots (i)

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.

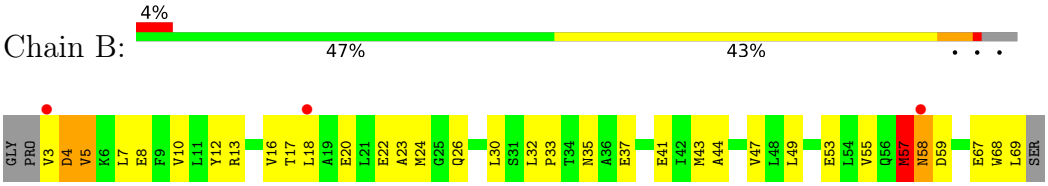
• Molecule 1: Surface presentation of antigens protein SpaO



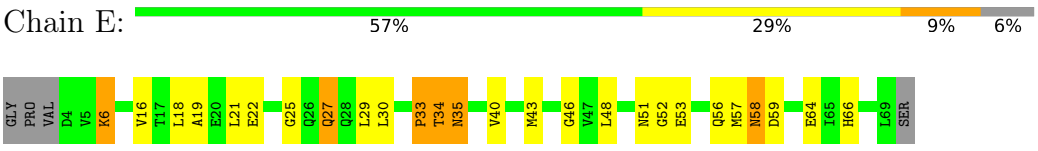
• Molecule 1: Surface presentation of antigens protein SpaO



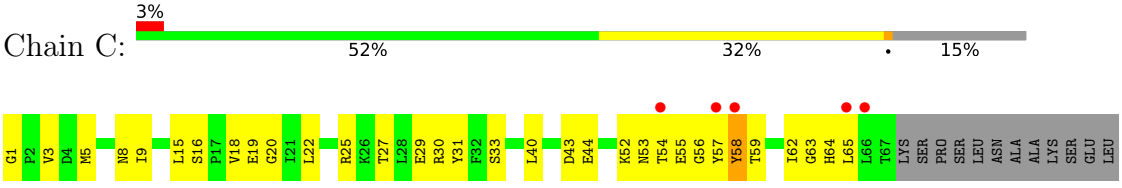
• Molecule 2: Surface presentation of antigens protein SpaO



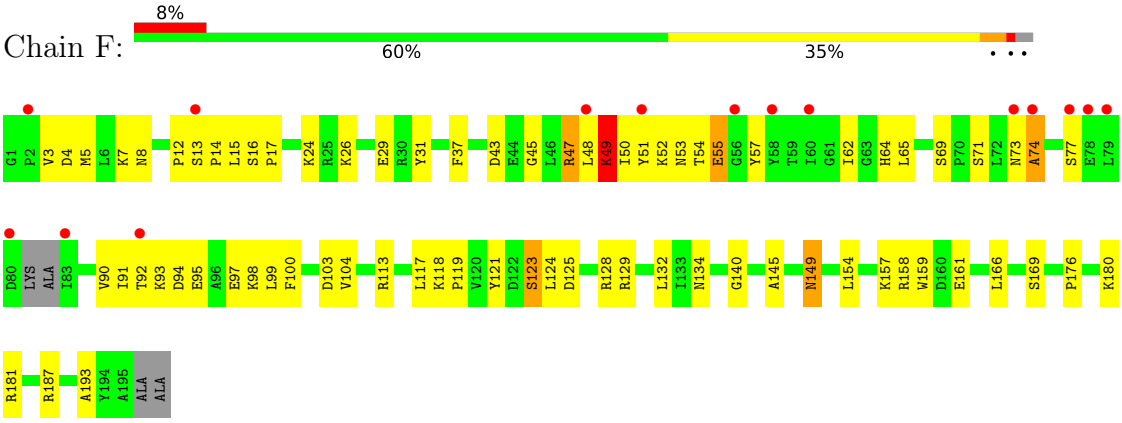
• Molecule 2: Surface presentation of antigens protein SpaO



• Molecule 3: Oxygen-regulated invasion protein OrgB,Endolysin



• Molecule 3: Oxygen-regulated invasion protein OrgB,Endolysin



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.88Å 88.50Å 63.32Å 90.00° 116.07° 90.00°	Depositor
Resolution (Å)	45.80 – 2.35 45.80 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.8 (45.80-2.35) 96.8 (45.80-2.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 2.34Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.198 , 0.262 0.200 , 0.259	Depositor DCC
R_{free} test set	1600 reflections (6.22%)	wwPDB-VP
Wilson B-factor (Å^2)	43.4	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 34.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.248 for l,-k,h	Xtriage
Reported twinning fraction	0.280 for l,-k,h	Depositor
Outliers	1 of 25740 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4940	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.51	0/484	0.72	0/653
1	D	0.44	0/493	0.69	0/666
2	B	0.53	0/524	0.73	0/706
2	E	0.48	0/517	0.80	2/696 (0.3%)
3	C	0.48	0/1343	0.67	1/1817 (0.1%)
3	F	0.51	0/1525	0.72	1/2065 (0.0%)
All	All	0.50	0/4886	0.71	4/6603 (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
2	B	0	1
3	F	0	3
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	34	THR	C-N-CA	6.76	138.61	121.70
3	F	15	LEU	CA-CB-CG	5.80	128.63	115.30
3	C	58	TYR	CA-CB-CG	5.66	124.15	113.40
2	E	34	THR	CA-C-N	5.02	128.25	117.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	57	MSE	Peptide

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Mol	Chain	Res	Type	Group
3	F	13	SER	Peptide
3	F	74	ALA	Peptide
3	F	93	LYS	Peptide

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	477	0	480	30	1
1	D	486	0	493	18	1
2	B	522	0	529	35	0
2	E	515	0	520	21	0
3	C	1319	0	1348	47	1
3	F	1499	0	1511	51	1
4	A	10	0	0	4	0
4	B	10	0	0	3	0
4	C	47	0	0	5	0
4	D	10	0	0	2	0
4	E	13	0	0	0	0
4	F	32	0	0	5	0
All	All	4940	0	4881	173	2

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 18.

All (173) 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)
3:F:43:ASP:OD1	3:F:181:ARG:NH1	2.03	0.92
3:F:158:ARG:HD2	3:F:161:GLU:OE1	1.79	0.81
3:F:187:ARG:NH1	4:F:201:HOH:O	2.05	0.81
1:A:8:LEU:N	4:A:101:HOH:O	2.14	0.79
3:C:116:LYS:HE2	3:C:148:THR:HG22	1.63	0.79
3:C:62:ILE:O	4:C:201:HOH:O	2.06	0.74
3:C:118:LYS:NZ	3:C:122:ASP:OD2	2.20	0.73
3:F:47:ARG:HB2	3:F:51:TYR:CE2	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:166:LEU:O	3:F:169:SER:OG	2.04	0.73
3:F:154:LEU:O	4:F:202:HOH:O	2.07	0.73
2:E:43:MSE:HG2	2:E:48:LEU:HA	1.70	0.73
2:E:34:THR:OG1	2:E:35:ASN:HB2	1.89	0.72
1:D:66:LEU:HD12	2:E:25:GLY:HA3	1.71	0.72
3:F:176:PRO:O	3:F:180:LYS:HD2	1.92	0.70
1:A:13:ARG:NH2	1:A:47:TYR:O	2.25	0.69
3:F:8:ASN:OD1	4:F:203:HOH:O	2.09	0.69
1:A:23:ARG:HG3	1:A:24:SER:N	2.08	0.69
3:F:71:SER:O	4:F:204:HOH:O	2.10	0.69
2:B:23:ALA:HA	2:B:26:GLN:HE21	1.58	0.68
3:C:53:ASN:OD1	3:C:54:THR:N	2.26	0.68
1:A:21:THR:HG23	2:B:5:VAL:HG13	1.76	0.68
1:A:22:GLN:HG3	1:A:23:ARG:HG2	1.75	0.68
2:B:67:GLU:OE2	4:B:101:HOH:O	2.10	0.68
2:B:4:ASP:OD2	4:B:102:HOH:O	2.12	0.68
2:B:20:GLU:HA	2:B:23:ALA:HB3	1.76	0.67
3:F:181:ARG:HG2	3:F:193:ALA:HB1	1.77	0.67
1:A:10:TRP:N	2:B:16:VAL:O	2.22	0.67
3:C:19:GLU:O	4:C:202:HOH:O	2.12	0.67
3:F:149:ASN:N	3:F:149:ASN:HD22	1.92	0.67
1:A:13:ARG:NH1	2:B:8:GLU:OE1	2.28	0.66
2:B:57:MSE:HE3	3:C:9:ILE:HD12	1.78	0.66
1:A:25:LEU:O	1:A:28:ARG:N	2.18	0.64
3:F:64:HIS:ND1	3:F:103:ASP:OD2	2.25	0.64
3:F:53:ASN:OD1	3:F:57:TYR:HB2	1.97	0.64
2:E:18:LEU:O	2:E:22:GLU:HG3	1.98	0.64
2:B:68:TRP:HD1	1:D:23:ARG:HH12	1.45	0.63
1:D:17:GLY:HA2	1:D:41:ARG:H	1.64	0.63
1:A:23:ARG:HG3	1:A:24:SER:H	1.63	0.63
1:D:59:GLY:O	4:D:101:HOH:O	2.16	0.62
3:F:54:THR:HG23	3:F:55:GLU:HG2	1.81	0.62
3:F:71:SER:OG	3:F:73:ASN:O	2.16	0.62
3:C:43:ASP:OD1	3:C:181:ARG:NH1	2.32	0.62
2:B:57:MSE:O	2:B:59:ASP:N	2.34	0.60
2:E:64:GLU:OE2	3:F:7:LYS:NZ	2.34	0.60
3:C:59:THR:HG23	3:C:65:LEU:N	2.17	0.60
1:A:21:THR:OG1	1:A:25:LEU:HD12	2.03	0.59
2:B:33:PRO:HB2	2:B:35:ASN:HB3	1.84	0.59
3:C:44:GLU:OE1	3:C:63:GLY:HA3	2.02	0.58
3:C:8:ASN:OD1	3:C:127:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:16:VAL:HG21	2:E:21:LEU:HD13	1.86	0.58
2:B:58:ASN:HD22	3:C:126:ALA:H	1.52	0.58
3:F:119:PRO:O	3:F:123:SER:OG	2.22	0.58
3:F:125:ASP:O	3:F:129:ARG:HG3	2.03	0.58
1:D:56:ARG:NH1	1:D:57:VAL:O	2.37	0.57
3:F:95:GLU:HA	3:F:98:LYS:HB3	1.86	0.57
3:F:149:ASN:HD22	3:F:149:ASN:H	1.51	0.57
2:B:17:THR:N	2:B:20:GLU:OE1	2.32	0.56
1:A:15:VAL:HG22	2:B:10:VAL:HG22	1.86	0.56
3:C:109:ARG:NH1	4:C:207:HOH:O	2.38	0.56
3:C:107:ALA:HB2	3:C:137:PHE:HE1	1.70	0.55
1:A:19:SER:OG	1:A:36:LEU:O	2.19	0.55
3:C:121:TYR:CE1	3:C:129:ARG:HD3	2.41	0.55
1:D:34:VAL:HG11	2:E:57:MSE:HE1	1.89	0.54
3:C:18:VAL:N	3:C:22:LEU:O	2.39	0.54
1:A:8:LEU:N	4:A:103:HOH:O	2.40	0.54
3:F:53:ASN:ND2	3:F:54:THR:HG22	2.22	0.54
1:A:45:TYR:OH	1:A:50:LYS:HE3	2.08	0.54
2:B:18:LEU:O	2:B:22:GLU:HG3	2.09	0.53
1:A:38:ARG:NH1	3:C:20:GLY:O	2.41	0.53
3:F:43:ASP:OD2	3:F:134:ASN:ND2	2.38	0.52
3:F:49:LYS:HE2	3:F:50:ILE:H	1.72	0.52
2:E:33:PRO:HB2	2:E:35:ASN:HB3	1.90	0.52
3:F:117:LEU:HD21	3:F:145:ALA:HA	1.91	0.52
3:C:52:LYS:HA	3:C:58:TYR:HA	1.92	0.52
3:C:160:ASP:N	3:C:160:ASP:OD1	2.41	0.52
1:A:22:GLN:HA	2:B:5:VAL:HG12	1.91	0.52
1:A:63:VAL:HG11	1:A:66:LEU:HD13	1.92	0.51
3:F:97:GLU:HA	3:F:100:PHE:HB3	1.92	0.51
3:C:8:ASN:O	3:C:191:TRP:NE1	2.41	0.51
3:F:129:ARG:NH2	4:F:211:HOH:O	2.43	0.51
2:B:58:ASN:ND2	3:C:126:ALA:N	2.59	0.51
3:C:140:GLY:O	3:C:144:VAL:HG23	2.10	0.51
1:A:21:THR:OG1	1:A:22:GLN:N	2.44	0.51
2:B:58:ASN:HD22	3:C:126:ALA:N	2.08	0.50
2:B:69:LEU:HD12	1:D:23:ARG:NH1	2.26	0.50
3:F:118:LYS:N	3:F:119:PRO:HD2	2.26	0.50
2:E:19:ALA:HA	2:E:22:GLU:OE1	2.11	0.50
3:F:47:ARG:HB2	3:F:51:TYR:CD2	2.47	0.50
3:C:176:PRO:HD2	4:C:240:HOH:O	2.11	0.49
3:F:121:TYR:CE2	3:F:129:ARG:HD3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ARG:NH1	2:B:32:LEU:HD12	2.27	0.49
1:D:28:ARG:O	3:F:24:LYS:NZ	2.46	0.49
3:F:53:ASN:CG	3:F:54:THR:N	2.67	0.48
2:E:52:GLY:HA3	2:E:64:GLU:O	2.13	0.48
2:B:13:ARG:NE	2:B:41:GLU:OE1	2.46	0.48
3:F:74:ALA:HA	3:F:77:SER:CB	2.44	0.48
3:C:168:LYS:HG2	4:C:242:HOH:O	2.13	0.48
2:B:24:MSE:C	2:B:26:GLN:H	2.15	0.47
2:B:44:ALA:HB2	2:B:49:LEU:HD11	1.96	0.47
3:F:149:ASN:N	3:F:149:ASN:ND2	2.61	0.47
1:A:43:GLU:OE2	1:A:50:LYS:HE2	2.14	0.47
2:E:57:MSE:HE2	2:E:57:MSE:HB3	1.89	0.47
3:C:118:LYS:HB3	3:C:119:PRO:HD3	1.96	0.47
3:C:111:ILE:HG23	3:C:117:LEU:HB3	1.97	0.47
3:C:64:HIS:CD2	3:C:99:LEU:HD11	2.50	0.47
3:C:135:MET:O	3:C:139:MET:HG2	2.15	0.47
1:A:22:GLN:NE2	4:A:102:HOH:O	2.22	0.46
3:C:9:ILE:HG23	3:C:33:SER:OG	2.15	0.46
1:A:64:GLU:HG3	1:A:65:THR:N	2.31	0.46
3:F:48:LEU:HD22	3:F:91:ILE:O	2.15	0.46
3:F:124:LEU:HD13	3:F:128:ARG:HB3	1.98	0.46
2:B:12:TYR:CE2	2:B:30:LEU:HD21	2.50	0.46
3:C:53:ASN:HB2	3:C:57:TYR:O	2.16	0.45
2:B:53:GLU:O	2:B:55:VAL:HG13	2.16	0.45
3:C:177:ASN:O	3:C:181:ARG:HG3	2.17	0.45
3:F:100:PHE:O	3:F:104:VAL:HG23	2.15	0.45
3:C:40:LEU:HD12	3:C:100:PHE:HZ	1.82	0.45
3:F:95:GLU:O	3:F:99:LEU:N	2.21	0.45
3:C:53:ASN:HB3	3:C:56:GLY:CA	2.46	0.45
1:A:26:LEU:HA	1:A:27:GLY:HA2	1.54	0.44
1:D:63:VAL:O	2:E:27:GLN:HA	2.17	0.44
3:F:12:PRO:HD2	3:F:31:TYR:HE1	1.82	0.44
3:F:16:SER:HA	3:F:17:PRO:HD2	1.76	0.44
3:C:152:ARG:HD2	3:C:156:GLN:NE2	2.32	0.44
3:C:157:LYS:HG2	3:C:159:TRP:CZ2	2.53	0.44
3:F:157:LYS:HA	3:F:159:TRP:CH2	2.53	0.44
1:A:64:GLU:CG	1:A:65:THR:N	2.81	0.44
3:F:45:GLY:O	3:F:62:ILE:HA	2.18	0.44
3:C:43:ASP:OD2	3:C:194:TYR:OH	2.30	0.44
1:D:23:ARG:O	1:D:23:ARG:HG2	2.18	0.44
1:A:13:ARG:NH1	4:A:106:HOH:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:58:ASN:HB3	2:E:59:ASP:H	1.38	0.44
1:A:13:ARG:HD3	2:B:43:MSE:HE1	2.00	0.43
3:C:29:GLU:C	3:C:31:TYR:H	2.22	0.43
3:F:4:ASP:HB2	3:F:5:MET:HE2	2.00	0.43
3:C:53:ASN:HB3	3:C:57:TYR:H	1.84	0.43
1:A:66:LEU:HD12	1:A:66:LEU:HA	1.62	0.43
2:B:47:VAL:HG21	2:E:46:GLY:HA3	2.00	0.43
3:C:64:HIS:HD2	3:C:99:LEU:HD11	1.84	0.43
2:E:56:GLN:HG2	3:F:8:ASN:ND2	2.33	0.43
1:A:23:ARG:HE	2:B:3:VAL:N	2.16	0.43
3:C:59:THR:HG23	3:C:64:HIS:C	2.39	0.43
1:D:46:CYS:HB2	1:D:51:LEU:HD11	2.00	0.43
1:D:60:GLY:HA3	2:E:30:LEU:O	2.19	0.43
3:F:37:PHE:CE2	3:F:62:ILE:HD11	2.54	0.42
3:C:55:GLU:N	3:C:56:GLY:HA2	2.34	0.42
1:D:23:ARG:HE	1:D:23:ARG:HB3	1.51	0.42
3:C:25:ARG:O	3:C:29:GLU:HG3	2.19	0.42
3:F:74:ALA:HA	3:F:77:SER:HB3	2.02	0.42
1:D:35:LEU:HD12	1:D:35:LEU:HA	1.90	0.42
2:E:40:VAL:O	2:E:51:ASN:HB2	2.20	0.42
1:A:21:THR:HG22	2:B:7:LEU:HG	2.02	0.42
2:B:20:GLU:H	2:B:20:GLU:CD	2.23	0.42
2:B:58:ASN:ND2	3:C:126:ALA:H	2.17	0.42
3:C:99:LEU:HD12	3:C:102:GLN:OE1	2.19	0.42
2:E:53:GLU:HB2	2:E:66:HIS:HE1	1.85	0.41
3:F:26:LYS:O	3:F:29:GLU:HB3	2.20	0.41
2:B:49:LEU:O	2:B:69:LEU:N	2.40	0.41
2:E:56:GLN:HG2	3:F:8:ASN:HD21	1.84	0.41
3:F:52:LYS:HA	3:F:57:TYR:O	2.21	0.41
2:B:37:GLU:OE2	4:B:103:HOH:O	2.22	0.41
1:A:17:GLY:HA2	1:A:41:ARG:HG3	2.02	0.41
3:C:27:THR:O	3:C:30:ARG:HB2	2.21	0.41
1:D:20[A]:ASP:HA	2:E:6:LYS:HA	2.03	0.41
3:F:159:TRP:HB3	3:F:187:ARG:HA	2.03	0.40
2:B:24:MSE:C	2:B:26:GLN:N	2.74	0.40
3:C:1:GLY:O	3:C:5:MET:HG2	2.21	0.40
1:D:20[B]:ASP:OD1	2:E:6:LYS:HB2	2.21	0.40
3:F:132:LEU:HA	3:F:132:LEU:HD12	1.87	0.40
2:B:68:TRP:HD1	1:D:23:ARG:NH1	2.16	0.40
3:C:40:LEU:HA	3:C:40:LEU:HD23	1.78	0.40
1:D:41:ARG:O	4:D:102:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:113:ARG:HE	3:F:113:ARG:HB2	1.40	0.40

All (2) 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)
3:C:56:GLY:O	1:D:38:ARG:NH1[2_455]	2.18	0.02
1:A:39:THR:OG1	3:F:55:GLU:OE1[2_554]	2.19	0.01

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	60/73 (82%)	48 (80%)	10 (17%)	2 (3%)	4 2
1	D	61/73 (84%)	55 (90%)	6 (10%)	0	100 100
2	B	65/70 (93%)	55 (85%)	8 (12%)	2 (3%)	4 2
2	E	64/70 (91%)	60 (94%)	2 (3%)	2 (3%)	4 2
3	C	164/197 (83%)	150 (92%)	13 (8%)	1 (1%)	25 27
3	F	189/197 (96%)	171 (90%)	14 (7%)	4 (2%)	7 4
All	All	603/680 (89%)	539 (89%)	53 (9%)	11 (2%)	8 6

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
2	B	58	ASN
3	F	14	PRO
3	F	94	ASP
2	E	35	ASN
3	F	49	LYS

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Mol	Chain	Res	Type
2	B	4	ASP
1	A	58	GLU
2	E	33	PRO
3	F	140	GLY
3	C	16	SER

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	49/63 (78%)	48 (98%)	1 (2%)	55 66
1	D	50/63 (79%)	50 (100%)	0	100 100
2	B	58/57 (102%)	56 (97%)	2 (3%)	37 46
2	E	57/57 (100%)	53 (93%)	4 (7%)	15 15
3	C	136/165 (82%)	131 (96%)	5 (4%)	34 42
3	F	155/165 (94%)	145 (94%)	10 (6%)	17 18
All	All	505/570 (89%)	483 (96%)	22 (4%)	28 34

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
2	B	5	VAL
2	B	57	MSE
3	C	3	VAL
3	C	15	LEU
3	C	98	LYS
3	C	123	SER
3	C	160	ASP
2	E	6	LYS
2	E	27	GLN
2	E	29	LEU
2	E	58	ASN
3	F	3	VAL

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Mol	Chain	Res	Type
3	F	47	ARG
3	F	49	LYS
3	F	55	GLU
3	F	65	LEU
3	F	69	SER
3	F	90	VAL
3	F	92	THR
3	F	123	SER
3	F	149	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	26	GLN
2	B	58	ASN
3	F	149	ASN
3	F	165	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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

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	62/73 (84%)	0.46	4 (6%) 18 27	29, 52, 66, 73	0
1	D	62/73 (84%)	0.27	2 (3%) 47 59	31, 47, 65, 75	0
2	B	64/70 (91%)	0.33	3 (4%) 31 44	27, 43, 69, 77	0
2	E	63/70 (90%)	0.09	0 100 100	31, 42, 62, 69	0
3	C	168/197 (85%)	0.20	5 (2%) 50 61	23, 37, 69, 84	0
3	F	193/197 (97%)	0.41	15 (7%) 13 19	26, 49, 76, 87	0
All	All	612/680 (90%)	0.30	29 (4%) 31 44	23, 45, 73, 87	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	58	TYR	8.5
2	B	18	LEU	6.9
3	F	56	GLY	5.4
1	A	69	GLN	4.7
1	D	66	LEU	4.6
3	C	54	THR	3.9
2	B	3	VAL	3.8
1	A	27	GLY	3.8
3	F	51	TYR	3.7
3	F	13	SER	3.6
1	D	8	LEU	3.4
3	F	79	LEU	3.3
3	F	77	SER	3.1
3	F	58	TYR	3.0
3	C	66	LEU	2.8
3	F	83	ILE	2.5
3	F	78	GLU	2.5
3	C	65	LEU	2.5
3	F	74	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
3	F	80	ASP	2.4
3	F	92	THR	2.4
3	C	57	TYR	2.3
2	B	58	ASN	2.3
3	F	60	ILE	2.3
3	F	2	PRO	2.2
1	A	25	LEU	2.2
3	F	73	ASN	2.1
1	A	10	TRP	2.1
3	F	48	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.