Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 01:37 PM JST

PDB ID	:	5ZC0
Title	:	Crystal structure of Xenopus embryonic epidermal lectin in complex with Samarium ions
Authors	:	Wangkanont, K.
Deposited on	:	2018-02-14
Resolution	:	2.75 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:

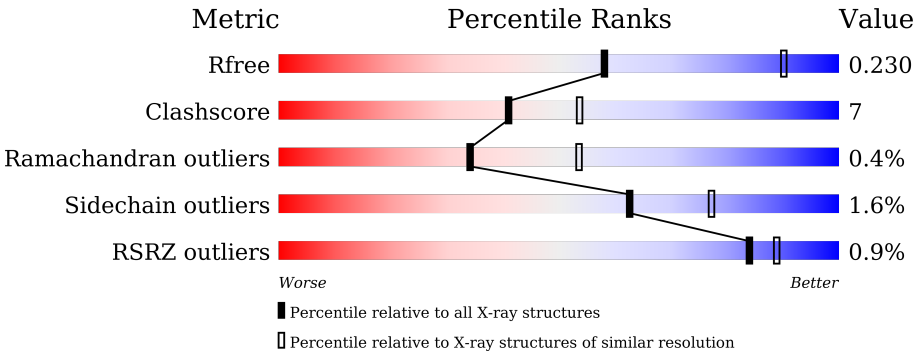
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	289	77% 19%
1	B	289	83% 13%
1	C	289	83% 13%
1	D	289	80% 16%
1	E	289	84% 11%
1	F	289	80% 15%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13325 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 Xenopus Embryonic Epidermal Lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total 2187	C 1370	N 372	O 430	S 15	0	2	0
1	B	281	Total 2187	C 1370	N 372	O 430	S 15	0	2	0
1	C	281	Total 2187	C 1370	N 372	O 430	S 15	0	2	0
1	D	281	Total 2187	C 1370	N 372	O 430	S 15	0	2	0
1	E	281	Total 2187	C 1370	N 372	O 430	S 15	0	2	0
1	F	281	Total 2187	C 1370	N 372	O 430	S 15	0	2	0

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

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

- Molecule 3 is SAMARIUM (III) ION (three-letter code: SM) (formula: Sm).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total Sm 5 5	0	0
3	B	5	Total Sm 5 5	0	0
3	C	5	Total Sm 5 5	0	0
3	D	4	Total Sm 4 4	0	0
3	E	4	Total Sm 4 4	0	0
3	F	4	Total Sm 4 4	0	0

- Molecule 4 is water.

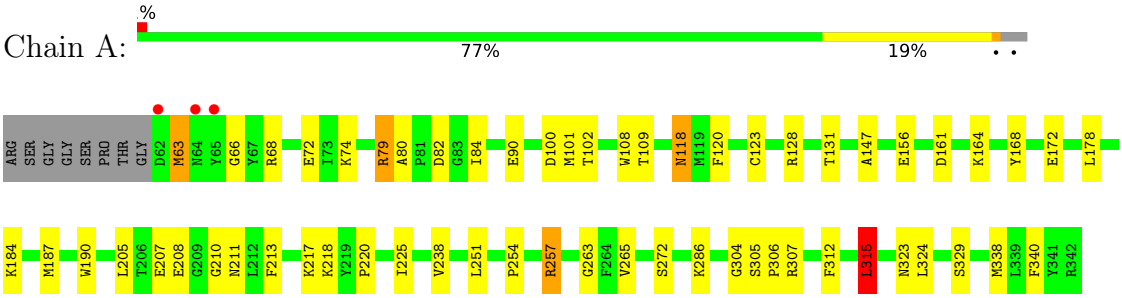
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	34	Total O 34 34	0	0
4	B	21	Total O 21 21	0	0
4	C	29	Total O 29 29	0	0
4	D	25	Total O 25 25	0	0
4	E	26	Total O 26 26	0	0
4	F	29	Total O 29 29	0	0

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.

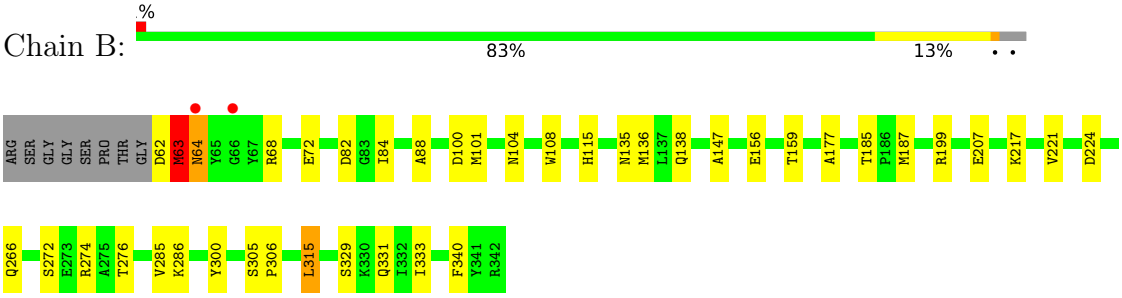
• Molecule 1: Xenopus Embryonic Epidermal Lectin

Chain A:



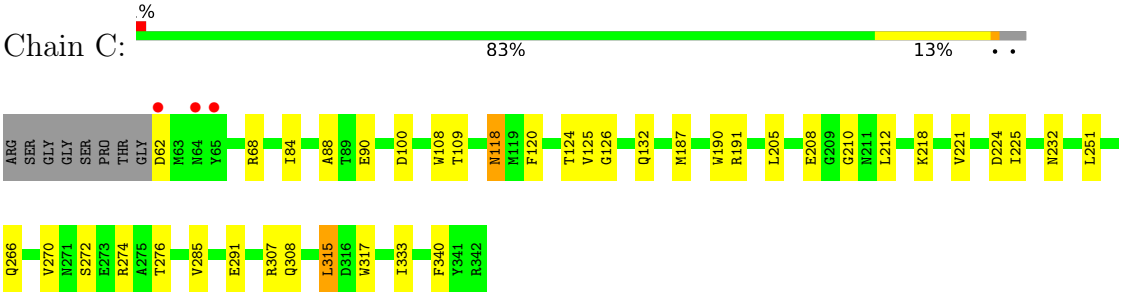
• Molecule 1: Xenopus Embryonic Epidermal Lectin

Chain B:



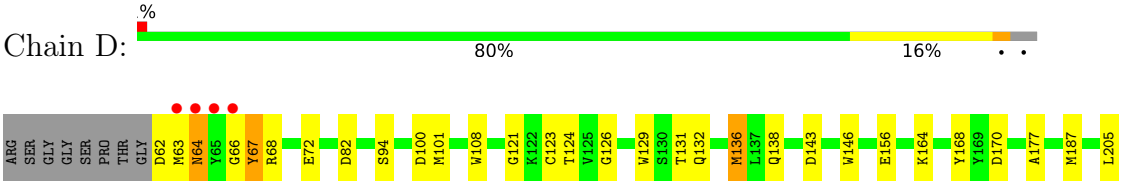
• Molecule 1: Xenopus Embryonic Epidermal Lectin

Chain C:



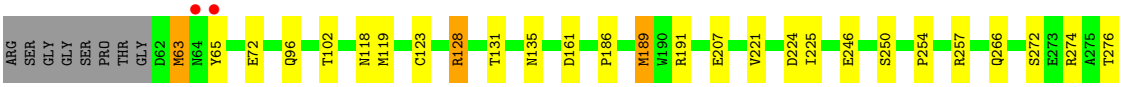
• Molecule 1: Xenopus Embryonic Epidermal Lectin

Chain D:



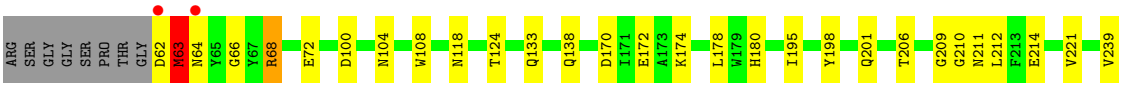
• Molecule 1: Xenopus Embryonic Epidermal Lectin

Chain E:



• Molecule 1: Xenopus Embryonic Epidermal Lectin

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	124.30Å 111.41Å 124.36Å 90.00° 119.94° 90.00°	Depositor
Resolution (Å)	34.19 – 2.75 34.19 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.6 (34.19-2.75) 97.6 (34.19-2.75)	Depositor EDS
R_{merge}	0.46	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 2.76Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.196 , 0.238 0.187 , 0.230	Depositor DCC
R_{free} test set	3954 reflections (5.30%)	wwPDB-VP
Wilson B-factor (Å^2)	15.0	Xtriage
Anisotropy	1.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.085 for -h-l,k,h 0.085 for l,k,-h-l 0.000 for h,-k,-h-l 0.000 for -h-l,-k,l 0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13325	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1220e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

Bond lengths and bond angles in the following residue types are not validated in this section: CA, SM

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	0.70	1/2244 (0.0%)	0.90	5/3044 (0.2%)
1	B	0.71	0/2244	0.89	1/3044 (0.0%)
1	C	0.70	2/2244 (0.1%)	0.86	2/3044 (0.1%)
1	D	0.70	2/2244 (0.1%)	0.92	4/3044 (0.1%)
1	E	0.68	0/2244	0.90	5/3044 (0.2%)
1	F	0.68	0/2244	0.91	3/3044 (0.1%)
All	All	0.69	5/13464 (0.0%)	0.90	20/18264 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	246	GLU	CD-OE1	-8.55	1.16	1.25
1	D	246	GLU	CD-OE2	-6.99	1.18	1.25
1	C	90	GLU	CB-CG	6.24	1.64	1.52
1	A	257	ARG	CB-CG	-5.71	1.37	1.52
1	C	90	GLU	CG-CD	5.02	1.59	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	128	ARG	CG-CD-NE	-7.41	96.24	111.80
1	F	339	LEU	CA-CB-CG	7.18	131.81	115.30
1	E	286	LYS	CD-CE-NZ	-6.96	95.68	111.70
1	C	191	ARG	NE-CZ-NH1	-6.72	116.94	120.30
1	C	315	LEU	CA-CB-CG	6.63	130.55	115.30
1	A	286	LYS	CD-CE-NZ	-6.16	97.52	111.70
1	E	189	MET	CG-SD-CE	6.16	110.06	100.20
1	D	136	MET	CA-CB-CG	5.65	122.90	113.30
1	A	315	LEU	CA-CB-CG	5.60	128.19	115.30
1	E	207	GLU	CB-CA-C	5.56	121.53	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	72	GLU	CA-CB-CG	5.54	125.58	113.40
1	B	315	LEU	CA-CB-CG	5.49	127.92	115.30
1	E	315	LEU	CB-CG-CD1	5.48	120.32	111.00
1	D	66	GLY	C-N-CA	5.45	135.31	121.70
1	D	315	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	184	LYS	CD-CE-NZ	-5.24	99.65	111.70
1	F	315	LEU	CB-CG-CD1	5.23	119.90	111.00
1	D	143	ASP	CB-CG-OD1	5.14	122.93	118.30
1	F	277	LEU	CA-CB-CG	-5.13	103.50	115.30
1	A	79	ARG	CA-CB-CG	-5.08	102.22	113.40

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	2187	0	2035	34	0
1	B	2187	0	2034	33	0
1	C	2187	0	2035	25	0
1	D	2187	0	2035	36	1
1	E	2187	0	2035	22	0
1	F	2187	0	2035	34	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	5	0	0	0	1
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	4	0	0	0	0
3	E	4	0	0	0	0
3	F	4	0	0	0	0
4	A	34	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	21	0	0	2	0
4	C	29	0	0	2	0
4	D	25	0	0	1	0
4	E	26	0	0	2	0
4	F	29	0	0	0	0
All	All	13325	0	12209	179	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 7.

All (179) 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:D:224:ASP:OD1	1:D:274:ARG:NH1	1.82	1.11
1:F:104:ASN:HD22	1:F:342:ARG:HH22	1.06	0.97
1:F:68:ARG:NH1	1:F:170:ASP:OD2	1.97	0.97
1:C:224:ASP:OD1	1:C:274:ARG:NH1	1.97	0.96
1:D:136:MET:HE1	1:E:118:ASN:HD21	1.36	0.91
1:E:224:ASP:OD1	1:E:274:ARG:NH1	2.05	0.89
1:D:67:TYR:HD1	1:D:72:GLU:HG2	1.44	0.83
1:E:254:PRO:HA	1:E:257:ARG:NH1	1.95	0.81
1:D:62:ASP:N	1:D:68:ARG:HH11	1.80	0.79
1:E:102:THR:HB	1:E:191:ARG:NH1	2.00	0.76
1:B:159:THR:HG21	1:B:185:THR:O	1.85	0.75
1:D:62:ASP:N	1:D:68:ARG:NH1	2.36	0.72
1:D:136:MET:CE	1:E:118:ASN:HD21	2.00	0.71
1:D:126:GLY:H	1:D:132:GLN:HE21	1.38	0.71
1:A:68:ARG:NH1	1:A:90:GLU:HG2	2.06	0.70
1:B:63:MET:HG3	1:B:72:GLU:OE2	1.92	0.69
1:C:126:GLY:H	1:C:132:GLN:HE21	1.37	0.69
1:C:126:GLY:H	1:C:132:GLN:NE2	1.91	0.69
1:F:63:MET:HG2	1:F:66:GLY:O	1.93	0.69
1:F:63:MET:HG3	1:F:72:GLU:OE1	1.93	0.68
1:B:62:ASP:HB2	1:B:68:ARG:NH1	2.09	0.68
1:A:147:ALA:O	1:A:217:LYS:NZ	2.27	0.68
1:B:156:GLU:HG2	1:B:187:MET:HE3	1.76	0.67
1:D:124:THR:HG21	1:F:133:GLN:OE1	1.94	0.67
1:B:224:ASP:OD1	1:B:274:ARG:NE	2.27	0.67
1:E:304:GLY:O	1:E:307:ARG:HG2	1.93	0.67
1:F:104:ASN:ND2	1:F:342:ARG:HH22	1.88	0.67
1:E:128:ARG:NH2	1:E:161:ASP:OD2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ILE:HD11	1:B:187:MET:HE3	1.76	0.66
1:E:246:GLU:H	1:E:246:GLU:CD	1.98	0.66
1:F:209:GLY:O	1:F:214:GLU:HG3	1.97	0.65
1:A:82:ASP:OD1	1:A:101:MET:N	2.30	0.64
1:A:304:GLY:O	1:A:307:ARG:HG2	1.98	0.64
1:D:273:GLU:OE1	4:D:501:HOH:O	2.15	0.64
1:D:126:GLY:H	1:D:132:GLN:NE2	1.97	0.62
1:F:104:ASN:HD22	1:F:342:ARG:NH2	1.88	0.62
1:A:63:MET:HA	1:A:66:GLY:O	2.00	0.61
1:C:315:LEU:HD12	1:C:333:ILE:HG22	1.82	0.61
1:D:227:LYS:NZ	1:D:274:ARG:HH21	1.99	0.61
4:E:522:HOH:O	1:F:124:THR:HB	2.01	0.61
1:B:221:VAL:HA	1:B:276:THR:HG21	1.82	0.60
1:C:225:ILE:HG22	4:C:505:HOH:O	2.01	0.60
1:B:156:GLU:CG	1:B:187:MET:HE3	2.31	0.60
1:B:62:ASP:HB2	1:B:68:ARG:HH11	1.65	0.59
1:F:254:PRO:HA	1:F:257:ARG:HD2	1.84	0.58
1:C:221:VAL:HA	1:C:276:THR:HG21	1.83	0.58
1:E:266:GLN:OE1	1:E:285:VAL:HG22	2.03	0.58
1:A:82:ASP:OD2	1:A:102:THR:OG1	2.21	0.58
1:D:246:GLU:H	1:D:246:GLU:CD	2.06	0.58
1:A:100:ASP:HB3	1:A:108:TRP:HB2	1.84	0.57
1:F:304:GLY:O	1:F:307:ARG:HG2	2.05	0.57
1:C:208:GLU:OE2	1:C:218:LYS:NZ	2.20	0.57
1:F:312:PHE:O	1:F:315:LEU:HD13	2.05	0.57
1:D:156:GLU:HG2	1:D:187:MET:HE3	1.87	0.56
1:D:271:ASN:HB3	1:D:290:VAL:HG22	1.88	0.56
1:B:84:ILE:HD11	1:B:187:MET:CE	2.36	0.55
1:A:128:ARG:NH2	1:A:161:ASP:OD1	2.39	0.55
1:B:63:MET:CG	1:B:72:GLU:OE2	2.54	0.55
1:A:79:ARG:NH1	1:D:318:ASP:OD1	2.35	0.55
1:F:62:ASP:N	1:F:68:ARG:HE	2.03	0.55
1:F:277:LEU:HD13	1:F:290:VAL:HG23	1.88	0.54
1:B:138:GLN:H	1:B:138:GLN:NE2	2.04	0.54
1:F:178:LEU:HD22	1:F:339:LEU:HD13	1.88	0.54
1:D:67:TYR:CD1	1:D:72:GLU:HG2	2.35	0.53
1:D:62:ASP:OD1	1:D:64:ASN:ND2	2.41	0.53
1:B:63:MET:HB2	1:B:72:GLU:OE2	2.09	0.53
1:D:138:GLN:NE2	1:D:138:GLN:H	2.06	0.52
1:B:147:ALA:HB1	1:B:217:LYS:HD3	1.91	0.52
1:F:100:ASP:HB3	1:F:108:TRP:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:ASN:ND2	1:C:270:VAL:H	2.08	0.52
1:B:82:ASP:OD1	1:B:101:MET:N	2.42	0.51
1:E:246:GLU:CD	1:E:246:GLU:N	2.64	0.51
1:F:174:LYS:HG2	1:F:206:THR:CG2	2.41	0.51
1:A:68:ARG:CZ	1:A:90:GLU:HG2	2.40	0.50
1:A:109:THR:O	1:A:340:PHE:HA	2.12	0.50
1:A:208:GLU:OE2	1:A:218:LYS:NZ	2.24	0.50
1:B:159:THR:HG22	4:B:512:HOH:O	2.11	0.50
1:C:109:THR:O	1:C:340:PHE:HA	2.12	0.50
1:E:119:MET:HE2	1:E:316:ASP:HB3	1.94	0.50
1:D:308:GLN:HG2	1:D:314:ALA:HB2	1.93	0.49
1:C:100:ASP:HB3	1:C:108:TRP:HB2	1.94	0.49
1:F:266:GLN:OE1	1:F:285:VAL:HG22	2.11	0.49
1:B:104:ASN:HD22	1:B:199:ARG:NH1	2.10	0.49
1:A:84:ILE:HD11	1:A:187:MET:HE3	1.95	0.49
1:B:68:ARG:HD2	1:B:88:ALA:O	2.12	0.49
1:D:94:SER:H	1:E:96:GLN:HE22	1.59	0.49
1:C:68:ARG:HD2	1:C:88:ALA:O	2.13	0.49
1:E:312:PHE:O	1:E:315:LEU:HD13	2.13	0.49
1:D:82:ASP:OD2	1:D:101:MET:N	2.44	0.49
1:A:118:ASN:HD21	1:A:120:PHE:HB2	1.78	0.48
1:E:221:VAL:HA	1:E:276:THR:HG21	1.95	0.48
1:E:250:SER:HA	1:E:257:ARG:HH21	1.77	0.48
1:B:100:ASP:HB3	1:B:108:TRP:HB2	1.95	0.48
1:F:63:MET:HB2	1:F:72:GLU:OE2	2.14	0.48
1:D:121:GLY:HA3	1:D:124:THR:HG21	1.95	0.48
1:A:312:PHE:O	1:A:315:LEU:HD13	2.13	0.47
1:D:164:LYS:HE3	1:D:168:TYR:CD1	2.49	0.47
1:D:251:LEU:HD22	1:D:332:ILE:HB	1.96	0.47
1:A:74:LYS:NZ	1:A:80:ALA:O	2.47	0.47
1:A:156:GLU:HG2	1:A:187:MET:HE3	1.95	0.47
1:F:329:SER:HB2	1:F:331:GLN:OE1	2.14	0.47
1:E:119:MET:CE	1:E:316:ASP:HB3	2.45	0.47
1:A:323:ASN:ND2	1:A:329:SER:HB3	2.30	0.47
1:B:315:LEU:HD12	1:B:333:ILE:HG22	1.95	0.47
1:C:291:GLU:HG3	1:C:308:GLN:NE2	2.30	0.47
1:A:238:VAL:HG11	1:A:265:VAL:HG23	1.98	0.46
1:F:172:GLU:OE1	1:F:210:GLY:HA3	2.15	0.46
1:A:172:GLU:OE1	1:A:210:GLY:HA3	2.16	0.46
1:B:329:SER:HB2	1:B:331:GLN:OE1	2.15	0.46
1:E:186:PRO:HD2	1:E:189:MET:HE3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ARG:N	1:B:72:GLU:OE1	2.37	0.45
1:C:125:VAL:HA	1:C:132:GLN:HE21	1.81	0.45
1:C:208:GLU:OE2	1:C:208:GLU:HA	2.16	0.45
1:A:305:SER:HA	1:A:306:PRO:HA	1.71	0.45
1:B:286:LYS:HZ2	1:B:286:LYS:HG2	1.73	0.45
1:E:225:ILE:HG22	4:E:504:HOH:O	2.16	0.45
1:D:123:CYS:SG	1:D:131:THR:HG22	2.57	0.45
1:A:211:ASN:OD1	1:A:213:PHE:HB3	2.17	0.45
1:C:84:ILE:HD11	1:C:187:MET:HE1	1.98	0.45
1:A:220:PRO:HB2	1:A:225:ILE:HD13	1.98	0.44
1:F:209:GLY:C	1:F:214:GLU:HG3	2.36	0.44
1:B:135:ASN:OD1	1:B:300:TYR:HA	2.17	0.44
1:D:227:LYS:HZ1	1:D:274:ARG:HH21	1.64	0.44
1:F:211:ASN:OD1	1:F:214:GLU:HG2	2.17	0.44
1:B:115:HIS:HD2	4:B:520:HOH:O	2.00	0.44
1:C:307:ARG:NH1	1:C:317:TRP:CH2	2.86	0.44
1:B:62:ASP:OD2	1:B:64:ASN:HB2	2.16	0.44
1:B:207:GLU:H	1:B:207:GLU:HG3	1.57	0.44
1:B:305:SER:HA	1:B:306:PRO:HA	1.83	0.44
1:C:118:ASN:HD21	1:C:120:PHE:HB2	1.83	0.44
1:D:205:LEU:O	1:D:210:GLY:N	2.47	0.44
1:F:221:VAL:HA	1:F:276:THR:HG21	2.00	0.44
1:A:82:ASP:OD1	1:A:100:ASP:HA	2.19	0.43
1:B:62:ASP:HB3	1:B:63:MET:H	1.53	0.43
1:C:124:THR:HB	4:C:514:HOH:O	2.18	0.43
1:C:212:LEU:HA	1:C:212:LEU:HD23	1.58	0.43
1:A:238:VAL:HG22	1:A:263:GLY:C	2.39	0.43
1:A:324:LEU:HA	1:A:324:LEU:HD23	1.73	0.43
1:E:135:ASN:OD1	1:E:300:TYR:HA	2.18	0.43
1:D:68:ARG:NE	1:D:170:ASP:OD2	2.50	0.43
1:D:138:GLN:H	1:D:138:GLN:CD	2.22	0.43
1:F:180:HIS:HE1	1:F:198:TYR:OH	2.01	0.43
1:A:123:CYS:SG	1:A:131:THR:HG22	2.59	0.42
1:C:266:GLN:OE1	1:C:285:VAL:HG22	2.18	0.42
1:D:136:MET:HB3	1:D:138:GLN:NE2	2.33	0.42
1:D:221:VAL:HA	1:D:276:THR:HG21	2.01	0.42
1:C:205:LEU:O	1:C:210:GLY:N	2.51	0.42
1:D:129:TRP:HE3	1:D:146:TRP:CE2	2.36	0.42
1:F:201:GLN:NE2	1:F:239:VAL:HG11	2.34	0.42
1:A:187:MET:HA	1:A:190:TRP:CE2	2.55	0.42
1:C:118:ASN:ND2	1:C:120:PHE:H	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:MET:SD	1:E:72:GLU:OE1	2.78	0.42
1:A:178:LEU:HA	1:A:338:MET:O	2.20	0.42
1:F:138:GLN:NE2	1:F:138:GLN:H	2.17	0.42
1:A:220:PRO:HB2	1:A:225:ILE:CD1	2.50	0.41
1:C:187:MET:HA	1:C:190:TRP:CE2	2.55	0.41
1:D:129:TRP:CE3	1:D:146:TRP:CE2	3.08	0.41
1:F:212:LEU:HA	1:F:212:LEU:HD23	1.88	0.41
1:A:254:PRO:HA	1:A:257:ARG:NH1	2.35	0.41
1:B:63:MET:CB	1:B:72:GLU:OE2	2.68	0.41
1:B:136:MET:HG2	1:B:138:GLN:HE21	1.86	0.41
1:D:100:ASP:HB3	1:D:108:TRP:HB2	2.01	0.41
1:C:221:VAL:HG13	1:C:276:THR:HG22	2.02	0.41
1:D:305:SER:HA	1:D:306:PRO:HA	1.82	0.41
1:B:266:GLN:OE1	1:B:285:VAL:HG22	2.21	0.41
1:C:205:LEU:HD23	1:C:205:LEU:HA	1.88	0.41
1:D:177:ALA:HB3	1:D:340:PHE:HB2	2.02	0.41
1:A:205:LEU:HD23	1:A:205:LEU:HA	1.93	0.41
1:F:195:ILE:HD13	1:F:195:ILE:HG21	1.77	0.41
1:F:271:ASN:HB3	1:F:290:VAL:HG22	2.02	0.41
1:F:305:SER:HA	1:F:306:PRO:HA	1.85	0.41
1:F:329:SER:O	1:F:332:ILE:HG22	2.21	0.41
1:A:207:GLU:H	1:A:207:GLU:HG3	1.58	0.41
1:F:257:ARG:HD2	1:F:257:ARG:HH11	1.68	0.41
1:B:177:ALA:HB3	1:B:340:PHE:HB2	2.02	0.40
1:E:123:CYS:SG	1:E:131:THR:HG22	2.61	0.40
1:E:320:TYR:OH	1:E:334:GLU:OE2	2.26	0.40
1:A:164:LYS:HE3	1:A:168:TYR:CD2	2.57	0.40
1:F:286:LYS:HB3	1:F:286:LYS:HE2	1.91	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)
1:D:207:GLU:OE2	3:A:405:SM:SM[2_657]	1.92	0.28

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	281/289 (97%)	267 (95%)	14 (5%)	0	100	100
1	B	281/289 (97%)	267 (95%)	13 (5%)	1 (0%)	34	53
1	C	281/289 (97%)	268 (95%)	13 (5%)	0	100	100
1	D	281/289 (97%)	265 (94%)	14 (5%)	2 (1%)	22	39
1	E	281/289 (97%)	266 (95%)	13 (5%)	2 (1%)	22	39
1	F	281/289 (97%)	267 (95%)	13 (5%)	1 (0%)	34	53
All	All	1686/1734 (97%)	1600 (95%)	80 (5%)	6 (0%)	34	53

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	63	MET
1	D	63	MET
1	F	63	MET
1	E	63	MET
1	D	67	TYR
1	E	65	TYR

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	229/232 (99%)	224 (98%)	5 (2%)	52	70
1	B	229/232 (99%)	226 (99%)	3 (1%)	69	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	229/232 (99%)	225 (98%)	4 (2%)	60 76
1	D	229/232 (99%)	226 (99%)	3 (1%)	69 81
1	E	229/232 (99%)	227 (99%)	2 (1%)	78 87
1	F	229/232 (99%)	224 (98%)	5 (2%)	52 70
All	All	1374/1392 (99%)	1352 (98%)	22 (2%)	62 77

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

Mol	Chain	Res	Type
1	A	63	MET
1	A	118	ASN
1	A	251	LEU
1	A	272	SER
1	A	315	LEU
1	B	63	MET
1	B	64	ASN
1	B	272	SER
1	C	62	ASP
1	C	118	ASN
1	C	251	LEU
1	C	272	SER
1	D	64	ASN
1	D	272	SER
1	D	315	LEU
1	E	272	SER
1	E	315	LEU
1	F	63	MET
1	F	64	ASN
1	F	68	ARG
1	F	118	ASN
1	F	315	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	192	ASN
1	A	323	ASN
1	B	64	ASN
1	B	104	ASN

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Mol	Chain	Res	Type
1	B	115	HIS
1	B	133	GLN
1	B	138	GLN
1	C	71	ASN
1	C	118	ASN
1	C	132	GLN
1	C	133	GLN
1	C	183	ASN
1	C	192	ASN
1	C	232	ASN
1	D	132	GLN
1	D	138	GLN
1	D	192	ASN
1	E	71	ASN
1	E	96	GLN
1	E	118	ASN
1	E	133	GLN
1	E	192	ASN
1	E	201	GLN
1	F	64	ASN
1	F	104	ASN
1	F	118	ASN
1	F	138	GLN
1	F	180	HIS
1	F	308	GLN

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

Of 39 ligands modelled in this entry, 39 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	281/289 (97%)	-0.55	3 (1%)	80	86	6, 17, 31, 69	0
1	B	281/289 (97%)	-0.55	2 (0%)	87	91	6, 18, 32, 76	0
1	C	281/289 (97%)	-0.62	3 (1%)	80	86	7, 16, 30, 68	0
1	D	281/289 (97%)	-0.53	4 (1%)	75	82	7, 18, 34, 74	0
1	E	281/289 (97%)	-0.53	2 (0%)	87	91	7, 18, 32, 82	0
1	F	281/289 (97%)	-0.55	2 (0%)	87	91	6, 17, 31, 72	0
All	All	1686/1734 (97%)	-0.55	16 (0%)	84	89	6, 17, 32, 82	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	64	ASN	4.9
1	D	63	MET	4.8
1	F	64	ASN	4.6
1	A	64	ASN	4.4
1	B	64	ASN	4.4
1	D	64	ASN	3.8
1	C	64	ASN	3.7
1	D	66	GLY	3.3
1	D	65	TYR	3.2
1	E	65	TYR	3.2
1	C	65	TYR	3.0
1	A	62	ASP	2.7
1	F	62	ASP	2.6
1	A	65	TYR	2.3
1	C	62	ASP	2.2
1	B	66	GLY	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, 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	B-factors(Å^2)	Q<0.9
3	SM	F	406	1/1	0.84	0.09	75,75,75,75	1
3	SM	B	406	1/1	0.85	0.18	90,90,90,90	1
3	SM	C	407	1/1	0.88	0.16	71,71,71,71	1
3	SM	D	405	1/1	0.91	0.14	87,87,87,87	1
3	SM	F	405	1/1	0.93	0.16	85,85,85,85	1
3	SM	A	406	1/1	0.93	0.16	86,86,86,86	1
3	SM	C	406	1/1	0.95	0.11	90,90,90,90	1
3	SM	E	405	1/1	0.96	0.19	84,84,84,84	1
3	SM	B	407	1/1	0.96	0.10	67,67,67,67	1
3	SM	D	406	1/1	0.96	0.08	63,63,63,63	1
3	SM	E	406	1/1	0.97	0.09	68,68,68,68	1
2	CA	F	402	1/1	0.98	0.08	8,8,8,8	0
3	SM	A	407	1/1	0.98	0.10	74,74,74,74	1
3	SM	B	403	1/1	0.99	0.05	25,25,25,25	0
2	CA	B	402	1/1	0.99	0.05	6,6,6,6	0
2	CA	C	401	1/1	0.99	0.06	10,10,10,10	0
2	CA	D	401	1/1	0.99	0.04	7,7,7,7	0
2	CA	D	402	1/1	0.99	0.07	12,12,12,12	0
2	CA	E	402	1/1	0.99	0.06	8,8,8,8	0
2	CA	F	401	1/1	0.99	0.04	7,7,7,7	0
2	CA	A	401	1/1	0.99	0.04	7,7,7,7	0
3	SM	A	404	1/1	0.99	0.04	35,35,35,35	0
2	CA	A	402	1/1	0.99	0.06	8,8,8,8	0
2	CA	B	401	1/1	0.99	0.05	18,18,18,18	0
3	SM	C	405	1/1	1.00	0.05	25,25,25,25	0
3	SM	A	403	1/1	1.00	0.05	22,22,22,22	0
2	CA	E	401	1/1	1.00	0.06	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SM	D	403	1/1	1.00	0.05	22,22,22,22	0
3	SM	D	404	1/1	1.00	0.04	29,29,29,29	0
3	SM	B	404	1/1	1.00	0.04	34,34,34,34	0
3	SM	B	405	1/1	1.00	0.06	28,28,28,28	0
3	SM	E	403	1/1	1.00	0.05	25,25,25,25	0
3	SM	E	404	1/1	1.00	0.04	31,31,31,31	0
3	SM	A	405	1/1	1.00	0.06	26,26,26,26	0
2	CA	C	402	1/1	1.00	0.06	9,9,9,9	0
3	SM	F	403	1/1	1.00	0.06	22,22,22,22	0
3	SM	F	404	1/1	1.00	0.03	31,31,31,31	0
3	SM	C	403	1/1	1.00	0.06	18,18,18,18	0
3	SM	C	404	1/1	1.00	0.04	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.