Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:16 PM GMT

PDB ID	:	1EV1
Title	:	ECHOVIRUS 1
Authors	:	Wien, M.W.; Filman, D.J.; Hogle, J.M.
Deposited on	:	1997-12-02
Resolution	:	3.55 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

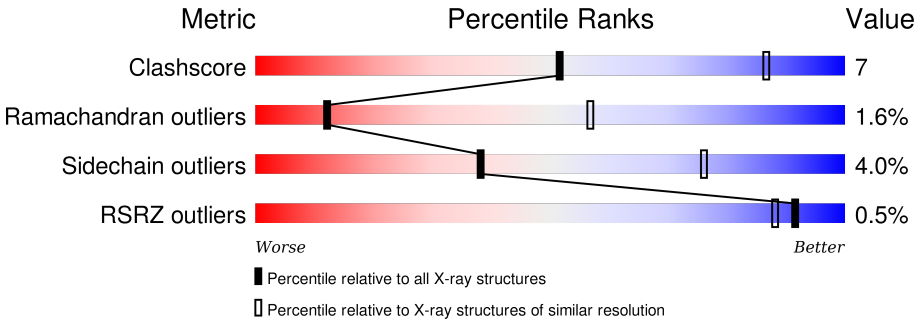
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.55 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))
Clashscore	102246	1057 (3.70-3.42)
Ramachandran outliers	100387	1017 (3.70-3.42)
Sidechain outliers	100360	1017 (3.70-3.42)
RSRZ outliers	91569	1247 (3.72-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	281	80% 16%
2	2	254	74% 21%
3	3	239	% 75% 22%
4	4	68	% 74% 16% 10%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6575 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 ECHOVIRUS 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	281	Total	C	N	O	S	0	0	0
			2227	1402	394	422	9			

- Molecule 2 is a protein called ECHOVIRUS 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	254	Total	C	N	O	S	0	0	0
			1977	1250	336	376	15			

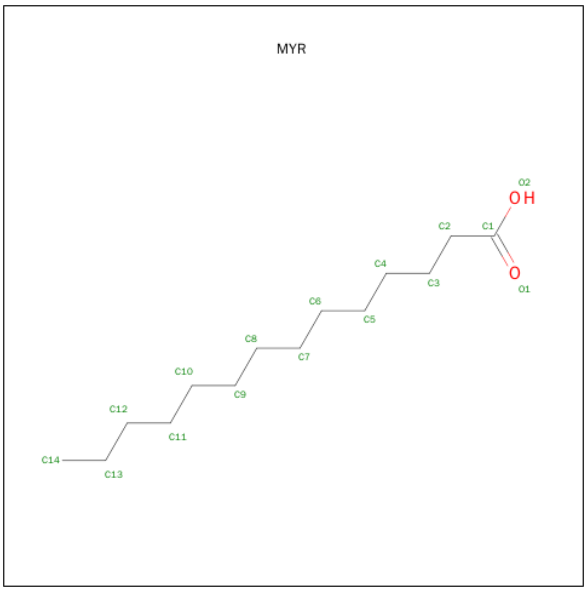
- Molecule 3 is a protein called ECHOVIRUS 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	239	Total	C	N	O	S	0	0	0
			1849	1169	304	355	21			

- Molecule 4 is a protein called ECHOVIRUS 1.

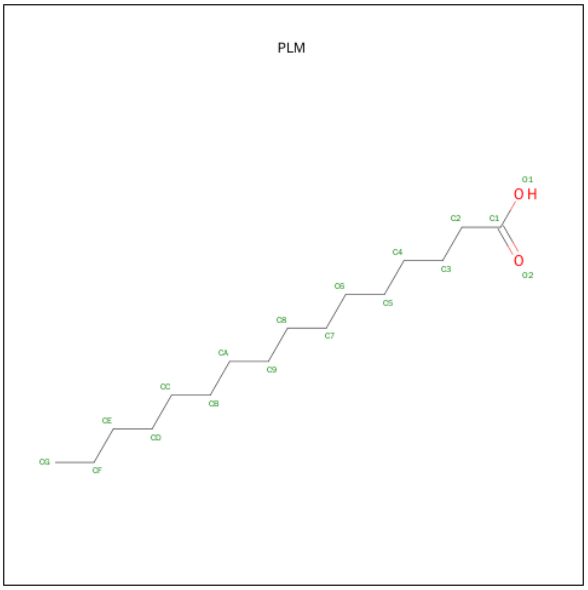
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	61	Total	C	N	O	S	0	0	0
			475	294	82	97	2			

- Molecule 5 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	4	1	Total C O 15 14 1	0	0

- Molecule 6 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	1	1	Total C O 18 16 2	0	0

- Molecule 7 is water.

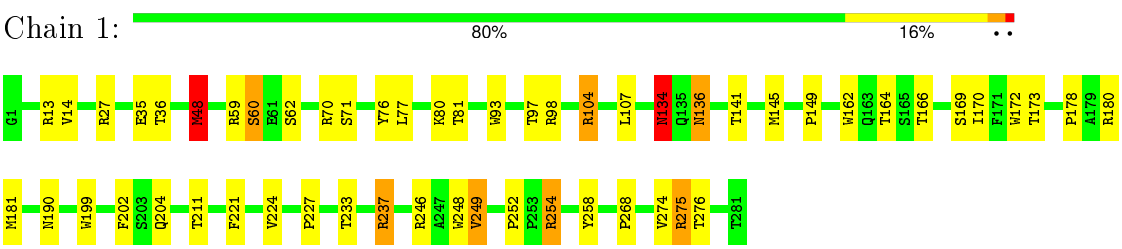
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	1	8	Total O 8 8	3	0
7	2	3	Total O 3 3	0	0
7	3	2	Total O 2 2	0	0
7	4	1	Total O 1 1	1	0

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

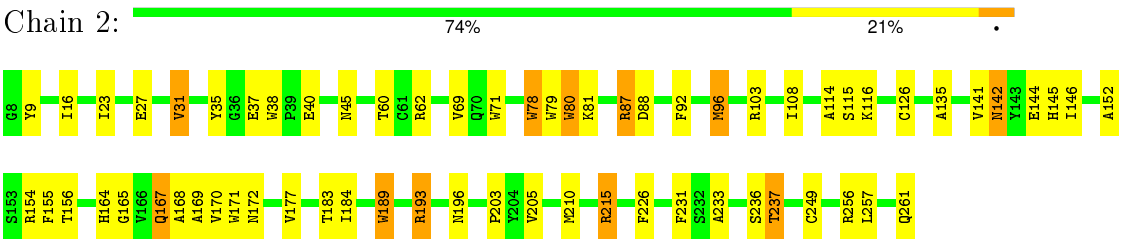
- Molecule 1: ECHOVIRUS 1

Chain 1:



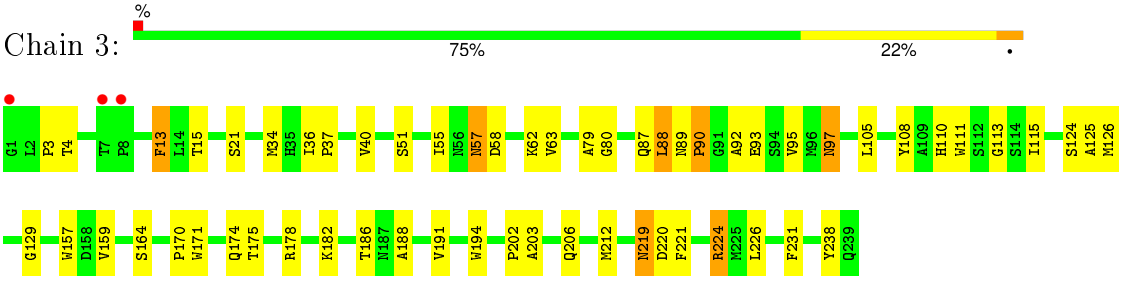
- Molecule 2: ECHOVIRUS 1

Chain 2:



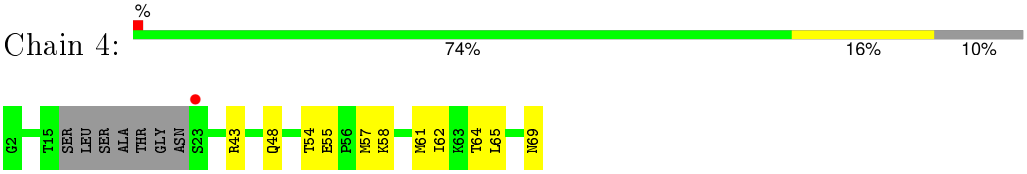
- Molecule 3: ECHOVIRUS 1

Chain 3:



- Molecule 4: ECHOVIRUS 1

Chain 4:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	472.15Å 483.20Å 352.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.55 30.17 – 3.56	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-3.55) 48.8 (30.17-3.56)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.57 (at 3.56Å)	Xtriage
Refinement program	X-PLOR 3.0	Depositor
R, R_{free}	0.263 , (Not available) 0.480 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	28.0	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 31.0	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	4 of 506841 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.03	EDS
Total number of atoms	6575	wwPDB-VP
Average B, all atoms (Å^2)	15.0	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 69.98 % 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 3.3733e-06.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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1	0.78	1/2286 (0.0%)	1.56	29/3123 (0.9%)
2	2	0.78	0/2034	1.51	26/2781 (0.9%)
3	3	0.75	0/1897	1.50	14/2579 (0.5%)
4	4	0.72	0/483	1.35	1/651 (0.2%)
All	All	0.77	1/6700 (0.0%)	1.51	70/9134 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	134	ASN	CG-OD1	6.06	1.37	1.24

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	78	TRP	CD1-CG-CD2	8.72	113.28	106.30
2	2	171	TRP	CD1-CG-CD2	8.61	113.18	106.30
2	2	80	TRP	CD1-CG-CD2	8.54	113.13	106.30
1	1	237	ARG	NE-CZ-NH2	-8.37	116.12	120.30
1	1	199	TRP	CE2-CD2-CG	-8.30	100.66	107.30
1	1	134	ASN	CB-CG-ND2	-8.26	96.88	116.70
3	3	171	TRP	CE2-CD2-CG	-8.22	100.72	107.30
1	1	248	TRP	CD1-CG-CD2	8.22	112.88	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	171	TRP	CD1-CG-CD2	8.18	112.84	106.30
1	1	199	TRP	CD1-CG-CD2	8.17	112.84	106.30
1	1	93	TRP	CD1-CG-CD2	8.12	112.80	106.30
2	2	193	ARG	NE-CZ-NH1	8.06	124.33	120.30
2	2	171	TRP	CE2-CD2-CG	-8.04	100.87	107.30
2	2	38	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	1	172	TRP	CD1-CG-CD2	8.01	112.71	106.30
1	1	180	ARG	NE-CZ-NH1	7.97	124.29	120.30
3	3	111	TRP	CD1-CG-CD2	7.95	112.66	106.30
2	2	189	TRP	CD1-CG-CD2	7.85	112.58	106.30
2	2	78	TRP	CE2-CD2-CG	-7.79	101.07	107.30
3	3	194	TRP	CE2-CD2-CG	-7.78	101.08	107.30
1	1	162	TRP	CE2-CD2-CG	-7.59	101.23	107.30
2	2	80	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	1	162	TRP	CD1-CG-CD2	7.49	112.29	106.30
2	2	189	TRP	CE2-CD2-CG	-7.47	101.33	107.30
3	3	171	TRP	CG-CD2-CE3	7.44	140.60	133.90
3	3	194	TRP	CD1-CG-CD2	7.41	112.23	106.30
1	1	93	TRP	CE2-CD2-CG	-7.37	101.40	107.30
2	2	62	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	1	248	TRP	CE2-CD2-CG	-7.21	101.53	107.30
1	1	172	TRP	CE2-CD2-CG	-7.19	101.55	107.30
3	3	111	TRP	CE2-CD2-CG	-7.17	101.56	107.30
2	2	38	TRP	CE2-CD2-CG	-7.16	101.57	107.30
2	2	79	TRP	CD1-CG-CD2	7.16	112.02	106.30
2	2	71	TRP	CE2-CD2-CG	-7.15	101.58	107.30
2	2	71	TRP	CD1-CG-CD2	7.14	112.01	106.30
2	2	87	ARG	NE-CZ-NH1	7.10	123.85	120.30
3	3	157	TRP	CD1-CG-CD2	6.98	111.89	106.30
2	2	62	ARG	NE-CZ-NH1	6.85	123.73	120.30
3	3	157	TRP	CE2-CD2-CG	-6.70	101.94	107.30
1	1	134	ASN	O-C-N	6.59	133.25	122.70
2	2	79	TRP	CE2-CD2-CG	-6.45	102.14	107.30
1	1	275	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	1	134	ASN	OD1-CG-ND2	6.19	136.14	121.90
2	2	215	ARG	CB-CG-CD	-6.14	95.64	111.60
1	1	246	ARG	NE-CZ-NH2	-6.12	117.24	120.30
3	3	171	TRP	CB-CG-CD1	-6.04	119.15	127.00
1	1	246	ARG	NE-CZ-NH1	6.01	123.31	120.30
3	3	57	ASN	N-CA-CB	-5.92	99.94	110.60
1	1	275	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	1	162	TRP	CG-CD2-CE3	5.78	139.10	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	13	PHE	CB-CG-CD2	-5.74	116.78	120.80
1	1	180	ARG	NE-CZ-NH2	-5.73	117.44	120.30
2	2	154	ARG	NE-CZ-NH1	5.72	123.16	120.30
3	3	224	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	1	13	ARG	NE-CZ-NH2	-5.59	117.50	120.30
2	2	215	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	1	48	MET	CA-CB-CG	5.41	122.49	113.30
2	2	78	TRP	CG-CD2-CE3	5.41	138.77	133.90
2	2	171	TRP	CB-CG-CD1	-5.40	119.98	127.00
2	2	193	ARG	NE-CZ-NH2	-5.36	117.62	120.30
2	2	78	TRP	CG-CD1-NE1	-5.35	104.75	110.10
1	1	48	MET	CB-CA-C	-5.26	99.87	110.40
1	1	254	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	1	237	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	1	104	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	1	70	ARG	NE-CZ-NH1	5.22	122.91	120.30
3	3	194	TRP	CG-CD2-CE3	5.19	138.57	133.90
2	2	78	TRP	CB-CG-CD1	-5.03	120.46	127.00
4	4	43	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	1	136	ASN	OD1-CG-ND2	-5.01	110.39	121.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	134	ASN	Mainchain

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	1	2227	0	2161	36	0
2	2	1977	0	1861	35	0
3	3	1849	0	1781	36	0
4	4	475	0	456	7	0
5	4	15	0	27	0	0
6	1	18	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	1	8	0	0	0	0
7	2	3	0	0	0	0
7	3	2	0	0	0	0
7	4	1	0	0	0	0
All	All	6575	0	6317	88	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 7.

All (88) 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)
1:1:141:THR:HG22	1:1:173:THR:HG22	1.68	0.74
1:1:48:MET:SD	3:3:170:PRO:HG3	2.30	0.72
1:1:36:THR:HG21	4:4:61:MET:SD	2.31	0.71
2:2:193:ARG:HA	3:3:125:ALA:HB2	1.74	0.69
3:3:174:GLN:HG3	3:3:175:THR:HG23	1.74	0.67
2:2:142:ASN:HD21	2:2:144:GLU:HG2	1.59	0.67
2:2:183:THR:HG21	3:3:51:SER:HA	1.76	0.67
2:2:155:PHE:HB3	2:2:170:VAL:HG22	1.78	0.66
2:2:156:THR:HG22	2:2:168:ALA:HB3	1.82	0.62
1:1:164:THR:HG21	1:1:169:SER:OG	2.00	0.62
2:2:103:ARG:HB2	2:2:210:MET:HG2	1.83	0.61
2:2:205:VAL:HG22	3:3:37:PRO:HG2	1.82	0.60
2:2:108:ILE:HD12	2:2:126:CYS:SG	2.42	0.58
3:3:58:ASP:HB2	3:3:62:LYS:HD3	1.86	0.57
4:4:62:ILE:HB	4:4:65:LEU:HD12	1.86	0.57
2:2:116:LYS:HA	3:3:125:ALA:HB3	1.88	0.56
1:1:59:ARG:HD2	4:4:48:GLN:HE22	1.71	0.56
1:1:274:VAL:HG22	3:3:63:VAL:HG21	1.87	0.56
2:2:156:THR:O	2:2:169:ALA:HA	2.06	0.55
2:2:257:LEU:HD23	2:2:257:LEU:H	1.72	0.54
3:3:89:ASN:HD21	3:3:182:LYS:HE2	1.73	0.54
2:2:135:ALA:HA	2:2:167:GLN:HB2	1.89	0.53
2:2:60:THR:HG23	2:2:92:PHE:HD1	1.73	0.52
1:1:178:PRO:HG2	3:3:13:PHE:HB2	1.90	0.52
1:1:141:THR:HG22	1:1:173:THR:CG2	2.38	0.52
2:2:69:VAL:HG21	2:2:78:TRP:NE1	2.24	0.52
1:1:254:ARG:HH21	1:1:258:TYR:HA	1.74	0.52
1:1:275:ARG:HE	3:3:57:ASN:HB3	1.75	0.52
1:1:170:ILE:HD11	1:1:181:MET:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:145:MET:SD	1:1:164:THR:CG2	2.98	0.51
3:3:55:ILE:HG12	3:3:95:VAL:HG13	1.93	0.51
4:4:54:THR:HG23	4:4:55:GLU:HG3	1.94	0.50
2:2:31:VAL:HG13	4:4:58:LYS:HB3	1.93	0.50
1:1:36:THR:HG22	4:4:57:MET:SD	2.52	0.50
1:1:97:THR:HG21	1:1:107:LEU:HD12	1.94	0.50
3:3:89:ASN:HB3	3:3:92:ALA:HB3	1.94	0.50
1:1:252:PRO:HD3	2:2:184:ILE:HG21	1.92	0.50
1:1:62:SER:HA	3:3:108:TYR:OH	2.12	0.50
3:3:126:MET:HG3	3:3:202:PRO:HG2	1.95	0.49
1:1:145:MET:SD	1:1:164:THR:HG22	2.52	0.49
2:2:80:TRP:CZ2	2:2:152:ALA:HB2	2.48	0.49
3:3:89:ASN:ND2	3:3:182:LYS:HE2	2.27	0.49
3:3:110:HIS:HB2	3:3:224:ARG:HB2	1.96	0.48
2:2:231:PHE:CZ	2:2:237:THR:HA	2.50	0.47
3:3:108:TYR:CE2	3:3:226:LEU:HD13	2.50	0.46
2:2:155:PHE:HA	2:2:168:ALA:HB1	1.97	0.46
2:2:40:GLU:HA	2:2:249:CYS:SG	2.56	0.46
1:1:76:TYR:HB3	1:1:237:ARG:HG2	1.97	0.46
2:2:37:GLU:O	2:2:203:PRO:HG3	2.16	0.46
3:3:87:GLN:HG3	3:3:89:ASN:ND2	2.31	0.45
1:1:14:VAL:HG13	3:3:220:ASP:HA	1.98	0.45
3:3:90:PRO:HG3	3:3:115:ILE:HD11	1.98	0.45
3:3:97:ASN:ND2	3:3:231:PHE:HZ	2.14	0.45
2:2:172:ASN:HA	2:2:177:VAL:O	2.16	0.45
2:2:142:ASN:ND2	2:2:144:GLU:HG2	2.30	0.44
1:1:190:ASN:HD22	3:3:34:MET:HB3	1.81	0.44
1:1:80:LYS:HE2	1:1:233:THR:OG1	2.18	0.44
1:1:35:GLU:HA	2:2:189:TRP:HB2	1.99	0.44
1:1:71:SER:O	3:3:15:THR:HG23	2.18	0.44
2:2:69:VAL:HG21	2:2:78:TRP:CD1	2.52	0.44
1:1:190:ASN:ND2	3:3:34:MET:HB3	2.33	0.44
1:1:27:ARG:HB2	4:4:64:THR:HB	2.00	0.44
1:1:97:THR:CG2	1:1:107:LEU:HD12	2.48	0.44
3:3:126:MET:HG3	3:3:202:PRO:CG	2.47	0.44
1:1:14:VAL:CG1	3:3:220:ASP:HA	2.48	0.44
2:2:16:ILE:HD12	2:2:23:ILE:HD11	2.00	0.44
3:3:93:GLU:O	3:3:97:ASN:HB2	2.18	0.43
2:2:145:HIS:HB3	2:2:165:GLY:HA2	1.99	0.43
1:1:81:THR:HG22	1:1:227:PRO:HA	2.01	0.43
3:3:178:ARG:HG2	3:3:186:THR:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:27:GLU:HB2	2:2:196:ASN:ND2	2.34	0.43
1:1:141:THR:OG1	1:1:224:VAL:HB	2.18	0.42
2:2:226:PHE:HB3	3:3:212:MET:HE1	2.00	0.42
1:1:170:ILE:HD11	1:1:181:MET:CG	2.50	0.42
2:2:81:LYS:HE3	2:2:146:ILE:HG23	2.02	0.42
1:1:77:LEU:HD23	1:1:221:PHE:CD1	2.55	0.42
1:1:258:TYR:HB2	3:3:238:TYR:CZ	2.55	0.41
3:3:90:PRO:HB2	3:3:105:LEU:CD1	2.51	0.41
3:3:88:LEU:O	3:3:188:ALA:HB3	2.20	0.41
1:1:268:PRO:HD3	2:2:167:GLN:NE2	2.36	0.41
1:1:98:ARG:HA	1:1:104:ARG:HD2	2.02	0.41
1:1:249:VAL:HG13	2:2:35:TYR:OH	2.21	0.41
3:3:129:GLY:O	3:3:159:VAL:HG12	2.21	0.41
2:2:114:ALA:O	2:2:115:SER:HB3	2.21	0.41
1:1:202:PHE:HA	2:2:215:ARG:HG3	2.02	0.40
2:2:87:ARG:HA	2:2:96:MET:SD	2.61	0.40
3:3:113:GLY:HA3	3:3:221:PHE:HA	2.02	0.40
3:3:206:GLN:HA	3:3:206:GLN:OE1	2.21	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	1	279/281 (99%)	252 (90%)	24 (9%)	3 (1%)	17 64
2	2	252/254 (99%)	215 (85%)	34 (14%)	3 (1%)	16 63
3	3	237/239 (99%)	214 (90%)	16 (7%)	7 (3%)	5 43
4	4	57/68 (84%)	51 (90%)	6 (10%)	0	100 100
All	All	825/842 (98%)	732 (89%)	80 (10%)	13 (2%)	12 57

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	236	SER
2	2	233	ALA
3	3	36	ILE
3	3	203	ALA
3	3	219	ASN
2	2	9	TYR
3	3	79	ALA
1	1	60	SER
3	3	3	PRO
3	3	88	LEU
1	1	149	PRO
1	1	249	VAL
3	3	80	GLY

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	1	250/250 (100%)	242 (97%)	8 (3%)	46	81
2	2	212/212 (100%)	201 (95%)	11 (5%)	29	69
3	3	208/208 (100%)	199 (96%)	9 (4%)	35	75
4	4	52/57 (91%)	51 (98%)	1 (2%)	65	88
All	All	722/727 (99%)	693 (96%)	29 (4%)	38	76

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	48	MET
1	1	60	SER
1	1	134	ASN
1	1	136	ASN
1	1	166	THR
1	1	204	GLN
1	1	211	THR
1	1	276	THR
2	2	31	VAL

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Mol	Chain	Res	Type
2	2	45	ASN
2	2	88	ASP
2	2	96	MET
2	2	141	VAL
2	2	142	ASN
2	2	164	HIS
2	2	167	GLN
2	2	237	THR
2	2	256	ARG
2	2	261	GLN
3	3	4	THR
3	3	21	SER
3	3	40	VAL
3	3	90	PRO
3	3	97	ASN
3	3	124	SER
3	3	164	SER
3	3	191	VAL
3	3	219	ASN
4	4	69	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	52	HIS
1	1	56	ASN
1	1	134	ASN
1	1	176	ASN
1	1	223	HIS
2	2	55	GLN
2	2	167	GLN
2	2	261	GLN
3	3	42	ASN
3	3	76	ASN
3	3	89	ASN
3	3	97	ASN
3	3	205	ASN
3	3	219	ASN
4	4	42	ASN

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

2 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
6	PLM	1	0	-	14,17,17	0.17	0	14,17,17	1.03	0
5	MYR	4	1	4	14,14,15	0.31	0	12,13,15	1.17	2 (16%)

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
6	PLM	1	0	-	-	0/13/15/15	0/0/0/0
5	MYR	4	1	4	-	0/11/12/13	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	4	1	MYR	C7-C6-C5	-2.59	101.16	114.53
5	4	1	MYR	C12-C11-C10	-2.26	102.84	114.53

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	1	281/281 (100%)	-0.19	0	100	100	15, 15, 15, 15	0
2	2	254/254 (100%)	-0.17	0	100	100	15, 15, 15, 15	0
3	3	239/239 (100%)	-0.14	3 (1%)	79	71	15, 15, 15, 15	0
4	4	61/68 (89%)	0.38	1 (1%)	74	66	15, 15, 15, 15	0
All	All	835/842 (99%)	-0.13	4 (0%)	91	88	15, 15, 15, 15	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	4	23	SER	2.4
3	3	1	GLY	2.3
3	3	8	PRO	2.2
3	3	7	THR	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	PLM	1	0	18/18	0.92	0.24	1.93	15,15,15,15	0
5	MYR	4	1	15/16	0.91	0.70	-	15,15,15,15	0

6.5 Other polymers (i)

There are no such residues in this entry.