Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:28 AM GMT

PDB ID	:	3ES5
Title	:	Crystal Structure of Partitivirus (PsV-F)
Authors	:	Pan, J.; Dong, L.; Lin, L.; Ochoa, W.F.; Sinkovits, R.S.; Havens, W.M.; Nibert, M.L.; Baker, T.S.; Ghabrial, S.A.; Tao, Y.J.
Deposited on	:	2008-10-03
Resolution	:	3.30 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:

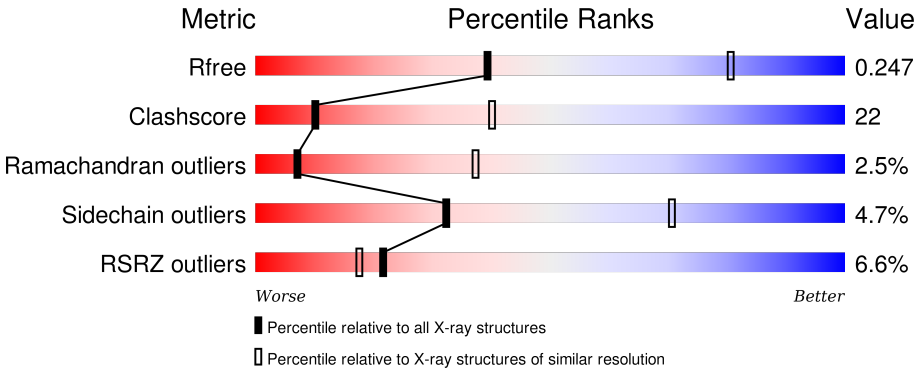
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	A	420	6% 56% 31% • 10%
1	B	420	5% 49% 36% 5% 10%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5919 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 Putative capsid protein.

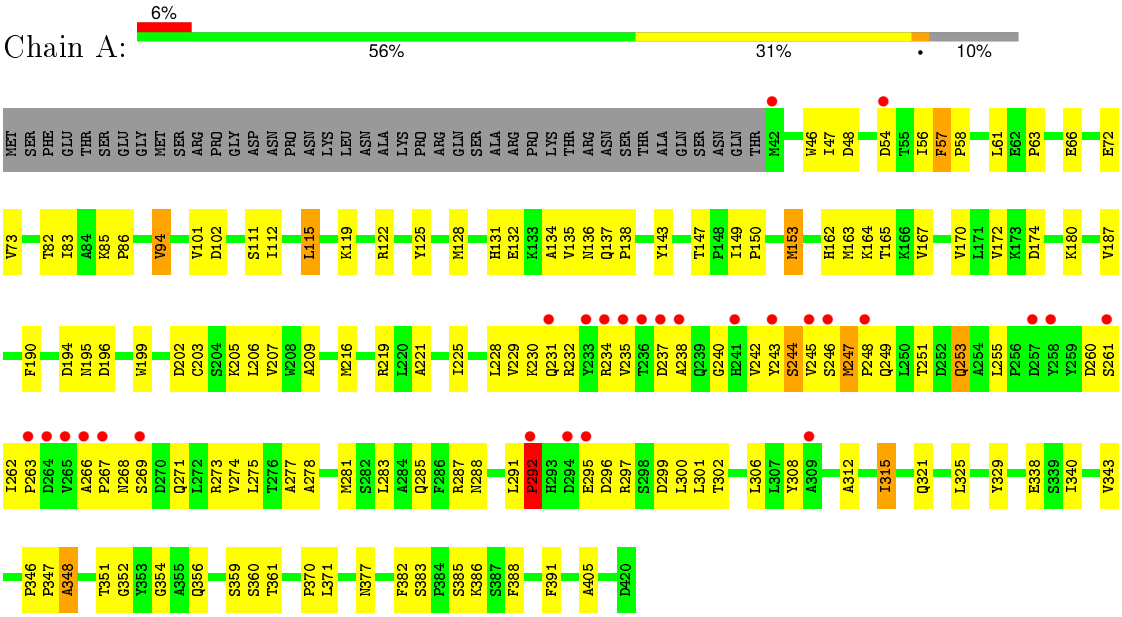
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	0	0
			2964	1884	492	578	10			
1	B	378	Total	C	N	O	S	0	0	0
			2955	1880	491	574	10			

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.

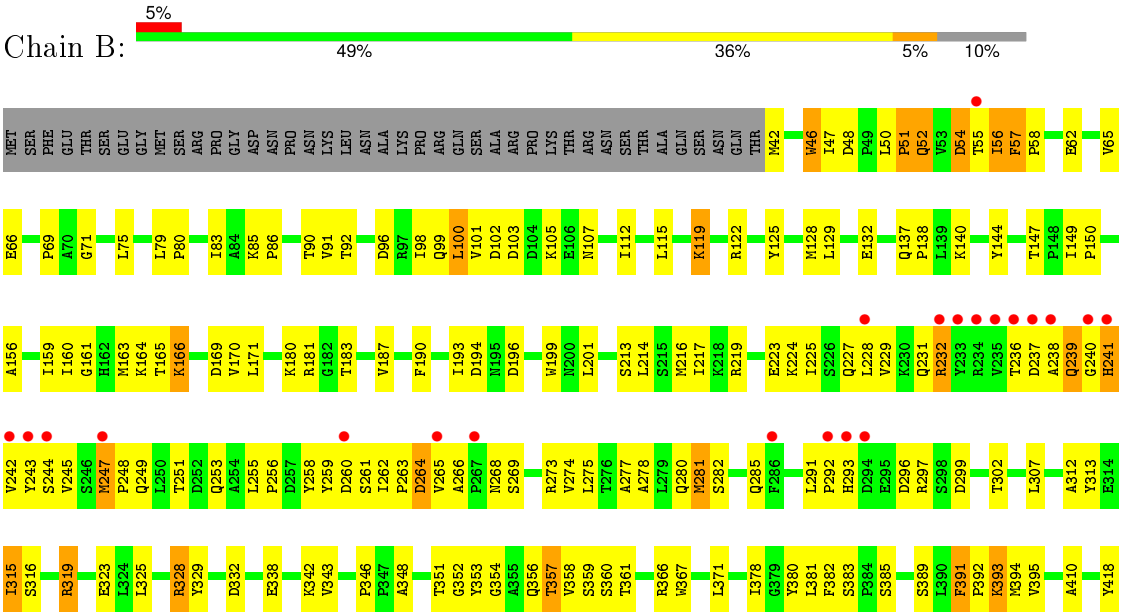
- Molecule 1: Putative capsid protein

Chain A:



- Molecule 1: Putative capsid protein

Chain B:




A419
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	F 2 3	Depositor
Cell constants a, b, c, α, β, γ	459.27Å 459.27Å 459.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.96 – 3.30 77.63 – 3.30	Depositor EDS
% Data completeness (in resolution range)	74.9 (48.96-3.30) 74.9 (77.63-3.30)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 3.33Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.248 , 0.267 0.243 , 0.247	Depositor DCC
R_{free} test set	4539 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	61.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 57.7	EDS
Estimated twinning fraction	0.020 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 89413 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	5919	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.40	0/3032	0.65	0/4119
1	B	0.41	0/3023	0.67	1/4108 (0.0%)
All	All	0.40	0/6055	0.66	1/8227 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	342	LYS	N-CA-C	-5.31	96.67	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2964	0	2908	131	1
1	B	2955	0	2904	145	2
All	All	5919	0	5812	256	3

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 22.

All (256) 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:253:GLN:H	1:A:253:GLN:NE2	1.67	0.90
1:B:163:MET:HA	1:B:351:THR:HG23	1.54	0.90
1:A:94:VAL:HB	1:A:340:ILE:HG23	1.54	0.89
1:B:231:GLN:HE22	1:B:268:ASN:HD22	1.21	0.89
1:A:253:GLN:H	1:A:253:GLN:HE21	0.91	0.88
1:A:253:GLN:N	1:A:253:GLN:HE21	1.73	0.87
1:B:100:LEU:HD22	1:B:105:LYS:HA	1.61	0.83
1:B:299:ASP:HA	1:B:302:THR:HG22	1.61	0.82
1:A:245:VAL:HG22	1:A:246:SER:H	1.46	0.80
1:A:263:PRO:HG2	1:A:266:ALA:HB2	1.64	0.79
1:A:299:ASP:HA	1:A:302:THR:HG22	1.65	0.79
1:B:236:THR:OG1	1:B:242:VAL:HG12	1.84	0.78
1:B:278:ALA:HA	1:B:281:MET:HG3	1.65	0.78
1:B:119:LYS:HG3	1:B:346:PRO:HB3	1.63	0.78
1:B:285:GLN:HE22	1:B:292:PRO:HG3	1.49	0.78
1:B:219:ARG:O	1:B:223:GLU:HG2	1.84	0.77
1:B:65:VAL:HA	1:B:394:MET:HE2	1.66	0.77
1:A:356:GLN:O	1:A:385:SER:HB3	1.85	0.77
1:B:180:LYS:HD3	1:B:315:ILE:HD11	1.66	0.76
1:B:98:ILE:HG22	1:B:99:GLN:H	1.49	0.76
1:B:229:VAL:HG13	1:B:247:MET:O	1.85	0.75
1:A:115:LEU:HD23	1:A:149:ILE:HG22	1.67	0.75
1:A:247:MET:SD	1:A:248:PRO:HD2	2.30	0.72
1:B:356:GLN:O	1:B:385:SER:HB3	1.91	0.71
1:A:163:MET:HA	1:A:351:THR:HG23	1.75	0.67
1:B:85:LYS:HB3	1:B:86:PRO:HD3	1.75	0.67
1:B:232:ARG:HH11	1:B:232:ARG:HB2	1.60	0.67
1:A:232:ARG:HD3	1:B:248:PRO:HB3	1.75	0.67
1:B:92:THR:HA	1:B:105:LYS:HD3	1.77	0.66
1:B:57:PHE:HB2	1:B:58:PRO:HD2	1.76	0.66
1:B:137:GLN:HB3	1:B:138:PRO:HD3	1.78	0.66
1:B:201:LEU:HD22	1:B:307:LEU:HD13	1.76	0.66
1:B:213:SER:O	1:B:217:ILE:HG12	1.96	0.66
1:A:338:GLU:HG2	1:A:343:VAL:HG21	1.77	0.66
1:B:119:LYS:HG2	1:B:149:ILE:HD13	1.78	0.65
1:B:225:ILE:HD11	1:B:275:LEU:CB	2.27	0.65
1:A:56:ILE:HG13	1:A:57:PHE:HD1	1.60	0.65
1:B:50:LEU:HD12	1:B:51:PRO:HD2	1.79	0.65
1:B:164:LYS:HD3	1:B:169:ASP:OD1	1.97	0.64
1:B:231:GLN:HE22	1:B:268:ASN:ND2	1.92	0.64
1:A:229:VAL:HG13	1:A:247:MET:O	1.98	0.63
1:A:190:PHE:HB3	1:A:325:LEU:HD22	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:SER:O	1:A:273:ARG:HG3	1.99	0.63
1:B:55:THR:HG22	1:B:56:ILE:N	2.13	0.63
1:A:245:VAL:HG21	1:B:245:VAL:CG2	2.29	0.63
1:B:98:ILE:HG22	1:B:99:GLN:N	2.14	0.63
1:B:351:THR:HG22	1:B:352:GLY:O	1.99	0.62
1:A:229:VAL:HG12	1:A:229:VAL:O	1.99	0.62
1:B:236:THR:HA	1:B:242:VAL:HA	1.82	0.62
1:B:225:ILE:HD11	1:B:275:LEU:HB3	1.81	0.62
1:A:83:ILE:O	1:A:86:PRO:HD2	2.00	0.62
1:A:119:LYS:HD2	1:A:346:PRO:HB3	1.81	0.61
1:A:274:VAL:HA	1:A:295:GLU:HG2	1.81	0.61
1:B:125:TYR:HA	1:B:128:MET:HG3	1.82	0.61
1:B:47:ILE:HG12	1:B:48:ASP:N	2.15	0.61
1:B:55:THR:HG22	1:B:56:ILE:H	1.66	0.60
1:A:245:VAL:HG22	1:A:246:SER:N	2.15	0.60
1:A:231:GLN:NE2	1:A:267:PRO:HB2	2.17	0.59
1:A:194:ASP:O	1:A:196:ASP:N	2.35	0.59
1:B:147:THR:O	1:B:346:PRO:HG3	2.02	0.59
1:A:232:ARG:HD3	1:B:248:PRO:CB	2.33	0.59
1:A:351:THR:HG22	1:A:352:GLY:O	2.02	0.59
1:B:299:ASP:HA	1:B:302:THR:CG2	2.34	0.58
1:A:271:GLN:H	1:A:271:GLN:CD	2.07	0.58
1:B:180:LYS:CD	1:B:315:ILE:HD11	2.33	0.57
1:A:112:ILE:HG23	1:A:153:MET:HE3	1.86	0.57
1:A:354:GLY:HA3	1:A:371:LEU:HD22	1.86	0.57
1:B:83:ILE:O	1:B:86:PRO:HD2	2.05	0.57
1:A:122:ARG:NH1	1:A:143:TYR:O	2.38	0.56
1:A:237:ASP:OD1	1:A:238:ALA:N	2.38	0.56
1:A:360:SER:HB2	1:A:383:SER:HB2	1.87	0.56
1:B:100:LEU:CD2	1:B:105:LYS:HA	2.33	0.56
1:A:85:LYS:HB3	1:A:86:PRO:HD3	1.86	0.56
1:A:273:ARG:HG2	1:A:273:ARG:HH11	1.71	0.56
1:A:237:ASP:HA	1:B:237:ASP:OD2	2.06	0.56
1:A:56:ILE:C	1:A:58:PRO:HD2	2.26	0.56
1:B:75:LEU:HD21	1:B:356:GLN:HG2	1.87	0.55
1:A:199:TRP:CZ3	1:A:312:ALA:O	2.60	0.55
1:B:299:ASP:CA	1:B:302:THR:HG22	2.35	0.55
1:B:285:GLN:NE2	1:B:292:PRO:HG3	2.21	0.55
1:A:285:GLN:OE1	1:A:292:PRO:HD3	2.08	0.54
1:B:129:LEU:HB2	1:B:132:GLU:HG3	1.90	0.54
1:B:260:ASP:O	1:B:262:ILE:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ASP:CA	1:A:302:THR:HG22	2.36	0.53
1:A:180:LYS:HD3	1:A:315:ILE:HD11	1.91	0.53
1:B:107:ASN:HB3	1:B:193:ILE:HD12	1.90	0.53
1:A:164:LYS:O	1:A:164:LYS:HG3	2.09	0.53
1:A:194:ASP:C	1:A:196:ASP:H	2.12	0.52
1:B:251:THR:H	1:B:253:GLN:HE21	1.57	0.52
1:B:47:ILE:HG12	1:B:48:ASP:H	1.75	0.52
1:A:231:GLN:HE22	1:A:268:ASN:ND2	2.07	0.52
1:B:354:GLY:O	1:B:357:THR:HB	2.10	0.52
1:A:281:MET:HE2	1:A:300:LEU:HD21	1.92	0.52
1:A:47:ILE:HG12	1:A:48:ASP:N	2.25	0.52
1:A:245:VAL:HG21	1:B:245:VAL:HG21	1.91	0.52
1:A:299:ASP:HA	1:A:302:THR:CG2	2.39	0.52
1:B:278:ALA:HA	1:B:281:MET:CG	2.38	0.52
1:A:251:THR:N	1:A:253:GLN:HE22	2.09	0.51
1:B:282:SER:OG	1:B:285:GLN:HG3	2.09	0.51
1:B:225:ILE:HD11	1:B:275:LEU:HB2	1.92	0.51
1:B:119:LYS:HA	1:B:119:LYS:HE3	1.93	0.50
1:A:125:TYR:HA	1:A:128:MET:HG3	1.92	0.50
1:A:122:ARG:HE	1:A:348:ALA:HB2	1.77	0.50
1:A:122:ARG:NE	1:A:348:ALA:HB2	2.26	0.50
1:B:264:ASP:N	1:B:264:ASP:OD2	2.45	0.50
1:A:260:ASP:O	1:A:262:ILE:N	2.41	0.50
1:A:202:ASP:OD2	1:A:205:LYS:HE3	2.11	0.50
1:A:248:PRO:HB3	1:B:232:ARG:HD3	1.93	0.50
1:A:249:GLN:NE2	1:B:249:GLN:NE2	2.60	0.50
1:B:338:GLU:HG2	1:B:343:VAL:HG21	1.93	0.50
1:A:72:GLU:N	1:A:170:VAL:HG13	2.26	0.50
1:B:351:THR:HG22	1:B:352:GLY:N	2.26	0.50
1:A:111:SER:O	1:A:115:LEU:HB2	2.12	0.50
1:B:263:PRO:HG2	1:B:266:ALA:HB2	1.94	0.50
1:B:291:LEU:HD11	1:B:297:ARG:HA	1.94	0.50
1:A:231:GLN:HE21	1:A:267:PRO:HB2	1.77	0.49
1:A:131:HIS:O	1:A:134:ALA:HB3	2.11	0.49
1:B:360:SER:HB2	1:B:383:SER:HB2	1.94	0.49
1:B:255:LEU:HB2	1:B:256:PRO:HD3	1.93	0.49
1:A:382:PHE:O	1:A:383:SER:C	2.51	0.49
1:B:201:LEU:HD12	1:B:313:TYR:CE1	2.47	0.49
1:B:140:LYS:HG2	1:B:144:TYR:CE1	2.47	0.49
1:A:291:LEU:HD11	1:A:297:ARG:HA	1.94	0.49
1:B:260:ASP:C	1:B:262:ILE:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ILE:HA	1:B:356:GLN:OE1	2.13	0.48
1:B:190:PHE:HB3	1:B:325:LEU:HD22	1.96	0.48
1:A:377:ASN:ND2	1:B:56:ILE:HD12	2.28	0.48
1:A:274:VAL:O	1:A:277:ALA:HB3	2.14	0.48
1:A:231:GLN:HE22	1:A:268:ASN:HD22	1.60	0.48
1:B:147:THR:HG21	1:B:329:TYR:CE2	2.49	0.48
1:B:86:PRO:O	1:B:90:THR:HG23	2.14	0.48
1:A:165:THR:C	1:A:167:VAL:H	2.17	0.48
1:B:163:MET:HE3	1:B:353:TYR:O	2.13	0.48
1:B:201:LEU:HD12	1:B:313:TYR:CD1	2.49	0.47
1:B:224:LYS:O	1:B:228:LEU:HG	2.14	0.47
1:A:281:MET:CE	1:A:300:LEU:HD21	2.44	0.47
1:A:63:PRO:HB3	1:B:367:TRP:HZ2	1.78	0.47
1:A:405:ALA:HB1	1:B:381:LEU:HD21	1.96	0.47
1:A:243:TYR:O	1:A:245:VAL:N	2.47	0.47
1:A:377:ASN:HD22	1:B:56:ILE:HD12	1.78	0.47
1:B:382:PHE:O	1:B:383:SER:C	2.53	0.47
1:B:199:TRP:CZ3	1:B:312:ALA:O	2.67	0.47
1:A:266:ALA:O	1:A:269:SER:HB2	2.15	0.47
1:B:137:GLN:O	1:B:140:LYS:HB2	2.14	0.47
1:A:112:ILE:HG23	1:A:153:MET:CE	2.44	0.47
1:B:391:PHE:N	1:B:392:PRO:HD3	2.29	0.47
1:B:263:PRO:HB2	1:B:265:VAL:HG12	1.97	0.47
1:A:174:ASP:OD1	1:A:219:ARG:NH2	2.48	0.47
1:A:352:GLY:HA3	1:A:356:GLN:NE2	2.30	0.47
1:B:66:GLU:HB2	1:B:395:VAL:HG23	1.97	0.47
1:B:259:TYR:CE1	1:B:273:ARG:HB3	2.50	0.47
1:B:280:GLN:HE22	1:B:293:HIS:CD2	2.33	0.47
1:B:85:LYS:CB	1:B:86:PRO:HD3	2.44	0.47
1:A:150:PRO:HB2	1:A:153:MET:HB3	1.95	0.47
1:A:278:ALA:O	1:A:281:MET:HG2	2.15	0.46
1:B:71:GLY:O	1:B:170:VAL:HA	2.14	0.46
1:A:243:TYR:O	1:A:244:SER:C	2.53	0.46
1:B:296:ASP:HB2	1:B:299:ASP:OD2	2.16	0.46
1:B:50:LEU:HD12	1:B:51:PRO:CD	2.44	0.46
1:A:351:THR:HG22	1:A:352:GLY:N	2.31	0.46
1:B:393:LYS:HE3	1:B:393:LYS:HB2	1.68	0.46
1:B:328:ARG:HG3	1:B:328:ARG:HH11	1.81	0.46
1:A:73:VAL:HG22	1:A:388:PHE:CD1	2.50	0.46
1:B:101:VAL:HG12	1:B:102:ASP:N	2.30	0.46
1:A:56:ILE:HG13	1:A:57:PHE:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:CYS:HA	1:A:206:LEU:HG	1.98	0.46
1:B:243:TYR:HB3	1:B:244:SER:H	1.60	0.45
1:B:79:LEU:N	1:B:80:PRO:HD2	2.31	0.45
1:A:54:ASP:HA	1:A:57:PHE:CD1	2.51	0.45
1:B:101:VAL:HG12	1:B:102:ASP:H	1.82	0.45
1:A:207:VAL:HG11	1:A:306:LEU:HD13	1.98	0.45
1:A:273:ARG:NH1	1:A:273:ARG:HG2	2.31	0.45
1:B:42:MET:O	1:B:166:LYS:NZ	2.49	0.45
1:A:225:ILE:HD11	1:A:275:LEU:HB3	1.99	0.45
1:B:122:ARG:NH1	1:B:348:ALA:HB2	2.32	0.45
1:A:229:VAL:CG1	1:A:229:VAL:O	2.63	0.45
1:A:128:MET:HB3	1:A:132:GLU:HB2	1.99	0.45
1:A:370:PRO:O	1:B:46:TRP:CZ3	2.69	0.45
1:B:115:LEU:HD11	1:B:329:TYR:CZ	2.51	0.45
1:B:65:VAL:HG22	1:B:394:MET:HE1	1.99	0.45
1:A:165:THR:HG22	1:B:47:ILE:HG13	1.98	0.45
1:A:199:TRP:CE2	1:A:321:GLN:HG2	2.52	0.45
1:B:259:TYR:CE2	1:B:293:HIS:HB3	2.51	0.45
1:B:69:PRO:HB3	1:B:171:LEU:CD1	2.47	0.45
1:B:258:TYR:O	1:B:262:ILE:HG13	2.16	0.44
1:A:128:MET:HA	1:A:162:HIS:CD2	2.52	0.44
1:B:358:VAL:HG12	1:B:359:SER:N	2.31	0.44
1:B:128:MET:HB3	1:B:132:GLU:HB2	1.98	0.44
1:A:405:ALA:CB	1:B:381:LEU:HD21	2.47	0.44
1:B:225:ILE:C	1:B:227:GLN:H	2.21	0.44
1:B:161:GLY:N	1:B:356:GLN:OE1	2.48	0.44
1:A:278:ALA:CB	1:A:281:MET:HE2	2.47	0.44
1:B:269:SER:O	1:B:273:ARG:HG3	2.18	0.44
1:A:249:GLN:NE2	1:B:249:GLN:HE21	2.16	0.44
1:A:221:ALA:HA	1:A:275:LEU:HD22	1.99	0.44
1:B:57:PHE:CB	1:B:58:PRO:HD2	2.46	0.44
1:B:240:GLY:O	1:B:241:HIS:O	2.35	0.44
1:B:50:LEU:O	1:B:52:GLN:N	2.48	0.44
1:A:281:MET:HE2	1:A:300:LEU:CD2	2.48	0.43
1:B:181:ARG:HH22	1:B:216:MET:HE1	1.83	0.43
1:B:140:LYS:HG2	1:B:144:TYR:HE1	1.84	0.43
1:B:328:ARG:HG3	1:B:328:ARG:NH1	2.34	0.43
1:B:183:THR:O	1:B:187:VAL:HG23	2.18	0.43
1:A:271:GLN:N	1:A:271:GLN:CD	2.72	0.43
1:A:187:VAL:HG13	1:A:321:GLN:HG3	2.01	0.43
1:B:214:LEU:HD11	1:B:281:MET:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:THR:CG2	1:B:56:ILE:H	2.26	0.42
1:B:262:ILE:HA	1:B:263:PRO:HD2	1.87	0.42
1:B:96:ASP:O	1:B:98:ILE:O	2.37	0.42
1:A:119:LYS:HD2	1:A:346:PRO:CB	2.47	0.42
1:A:278:ALA:HB1	1:A:281:MET:HE2	2.01	0.42
1:A:56:ILE:HG13	1:A:57:PHE:N	2.34	0.42
1:B:354:GLY:HA3	1:B:371:LEU:HD22	2.00	0.42
1:B:360:SER:OG	1:B:380:TYR:HA	2.19	0.42
1:A:228:LEU:C	1:A:230:LYS:H	2.22	0.42
1:B:65:VAL:HG22	1:B:394:MET:CE	2.49	0.42
1:B:224:LYS:HB3	1:B:275:LEU:HD13	2.01	0.42
1:A:101:VAL:HG12	1:A:102:ASP:N	2.34	0.42
1:B:378:ILE:HD13	1:B:378:ILE:HA	1.85	0.42
1:A:346:PRO:HA	1:A:347:PRO:HD3	1.94	0.42
1:A:221:ALA:O	1:A:225:ILE:HG12	2.20	0.42
1:A:301:LEU:CD1	1:A:308:TYR:HB2	2.50	0.42
1:A:85:LYS:CB	1:A:86:PRO:HD3	2.49	0.42
1:A:162:HIS:CE1	1:A:172:VAL:H	2.38	0.42
1:A:135:VAL:HG23	1:A:136:ASN:N	2.35	0.42
1:B:332:ASP:N	1:B:332:ASP:OD1	2.51	0.42
1:A:47:ILE:HG13	1:B:165:THR:HG22	2.02	0.41
1:A:147:THR:HG21	1:A:329:TYR:CE2	2.55	0.41
1:B:156:ALA:O	1:B:159:ILE:HG12	2.19	0.41
1:A:296:ASP:HB2	1:A:299:ASP:OD2	2.20	0.41
1:A:249:GLN:HE21	1:B:249:GLN:HE21	1.68	0.41
1:A:255:LEU:HD23	1:A:255:LEU:HA	1.89	0.41
1:A:119:LYS:HA	1:A:119:LYS:HD3	1.62	0.41
1:A:174:ASP:OD2	1:A:216:MET:HB2	2.20	0.41
1:A:225:ILE:HD11	1:A:275:LEU:CB	2.50	0.41
1:B:319:ARG:HD3	1:B:323:GLU:OE2	2.20	0.41
1:A:56:ILE:O	1:A:58:PRO:HD2	2.20	0.41
1:A:82:THR:HG22	1:A:382:PHE:HD2	1.86	0.41
1:A:235:VAL:O	1:A:235:VAL:HG12	2.20	0.41
1:A:386:LYS:HA	1:A:386:LYS:HD3	1.84	0.41
1:A:245:VAL:CG2	1:A:246:SER:H	2.26	0.41
1:A:242:VAL:O	1:A:242:VAL:HG23	2.20	0.41
1:A:66:GLU:OE2	1:B:366:ARG:NH1	2.54	0.41
1:A:134:ALA:O	1:A:137:GLN:HB2	2.21	0.41
1:A:209:ALA:O	1:A:283:LEU:HD11	2.21	0.41
1:B:273:ARG:HG2	1:B:273:ARG:HH11	1.86	0.41
1:B:91:VAL:HG21	1:B:112:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:ASP:C	1:B:196:ASP:H	2.23	0.41
1:A:86:PRO:HB2	1:B:410:ALA:HB2	2.04	0.40
1:B:149:ILE:O	1:B:150:PRO:C	2.59	0.40
1:A:248:PRO:CB	1:B:232:ARG:HD3	2.51	0.40
1:B:274:VAL:O	1:B:277:ALA:HB3	2.21	0.40
1:B:249:GLN:O	1:B:253:GLN:NE2	2.54	0.40
1:A:137:GLN:N	1:A:138:PRO:CD	2.84	0.40
1:A:287:ARG:O	1:A:297:ARG:NH2	2.53	0.40
1:B:102:ASP:O	1:B:103:ASP:C	2.59	0.40

All (3) 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:B:236:THR:CG2	1:B:239:GLN:CG[32_555]	2.01	0.19
1:A:238:ALA:CB	1:A:238:ALA:CB[32_555]	2.10	0.10
1:B:236:THR:C	1:B:238:ALA:CB[32_555]	2.14	0.06

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	377/420 (90%)	321 (85%)	47 (12%)	9 (2%)	7 38
1	B	376/420 (90%)	327 (87%)	39 (10%)	10 (3%)	6 35
All	All	753/840 (90%)	648 (86%)	86 (11%)	19 (2%)	7 37

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	PHE
1	A	195	ASN

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Mol	Chain	Res	Type
1	A	261	SER
1	A	292	PRO
1	A	315	ILE
1	B	54	ASP
1	B	56	ILE
1	B	241	HIS
1	B	261	SER
1	A	61	LEU
1	A	244	SER
1	A	348	ALA
1	B	166	LYS
1	B	315	ILE
1	B	418	TYR
1	A	240	GLY
1	B	281	MET
1	B	52	GLN
1	B	51	PRO

5.3.2 Protein sidechains

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	323/359 (90%)	311 (96%)	12 (4%)	41	76
1	B	322/359 (90%)	304 (94%)	18 (6%)	26	65
All	All	645/718 (90%)	615 (95%)	30 (5%)	32	70

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	TRP
1	A	94	VAL
1	A	115	LEU
1	A	153	MET
1	A	234	ARG
1	A	247	MET

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Mol	Chain	Res	Type
1	A	253	GLN
1	A	288	ASN
1	A	292	PRO
1	A	359	SER
1	A	361	THR
1	A	391	PHE
1	B	46	TRP
1	B	54	ASP
1	B	57	PHE
1	B	62	GLU
1	B	100	LEU
1	B	119	LYS
1	B	232	ARG
1	B	239	GLN
1	B	247	MET
1	B	264	ASP
1	B	316	SER
1	B	319	ARG
1	B	328	ARG
1	B	357	THR
1	B	361	THR
1	B	389	SER
1	B	391	PHE
1	B	393	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	137	GLN
1	A	231	GLN
1	A	249	GLN
1	A	253	GLN
1	A	268	ASN
1	A	288	ASN
1	A	377	ASN
1	B	231	GLN
1	B	239	GLN
1	B	249	GLN
1	B	253	GLN
1	B	271	GLN
1	B	280	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	379/420 (90%)	0.36	27 (7%)	19	15	25, 45, 90, 121	0
1	B	378/420 (90%)	0.30	23 (6%)	25	20	27, 44, 85, 113	0
All	All	757/840 (90%)	0.33	50 (6%)	22	17	25, 44, 87, 121	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	235	VAL	10.6
1	B	241	HIS	7.3
1	B	242	VAL	5.4
1	A	266	ALA	5.3
1	B	234	ARG	4.8
1	B	243	TYR	4.6
1	A	238	ALA	4.5
1	B	419	ALA	4.4
1	B	244	SER	4.4
1	A	243	TYR	4.3
1	B	235	VAL	4.2
1	B	238	ALA	4.0
1	A	269	SER	3.9
1	A	233	TYR	3.9
1	A	237	ASP	3.8
1	B	233	TYR	3.5
1	A	54	ASP	3.4
1	B	237	ASP	3.4
1	B	240	GLY	3.3
1	B	267	PRO	3.3
1	A	292	PRO	3.3
1	B	247	MET	3.0
1	A	236	THR	3.0
1	B	265	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	261	SER	2.6
1	B	236	THR	2.6
1	B	260	ASP	2.5
1	A	267	PRO	2.5
1	A	245	VAL	2.5
1	A	265	VAL	2.5
1	A	42	MET	2.5
1	B	55	THR	2.4
1	A	294	ASP	2.4
1	A	241	HIS	2.4
1	A	263	PRO	2.3
1	A	309	ALA	2.2
1	B	286	PHE	2.2
1	A	258	TYR	2.2
1	A	257	ASP	2.2
1	A	231	GLN	2.1
1	B	293	HIS	2.1
1	B	294	ASP	2.1
1	B	232	ARG	2.1
1	B	292	PRO	2.1
1	A	248	PRO	2.1
1	A	234	ARG	2.0
1	A	295	GLU	2.0
1	A	264	ASP	2.0
1	B	228	LEU	2.0
1	A	246	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.