



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:22 am GMT

PDB ID : 1YUE
Title : Bacteriophage T4 capsid vertex protein gp24
Authors : Fokine, A.; Leiman, P.G.; Shneider, M.M.; Ahvazi, B.; Boeshans, K.M.;
Steven, A.C.; Black, L.W.; Mesyanzhinov, V.V.; Rossmann, M.G.
Deposited on : 2005-02-14
Resolution : 2.90 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtrriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

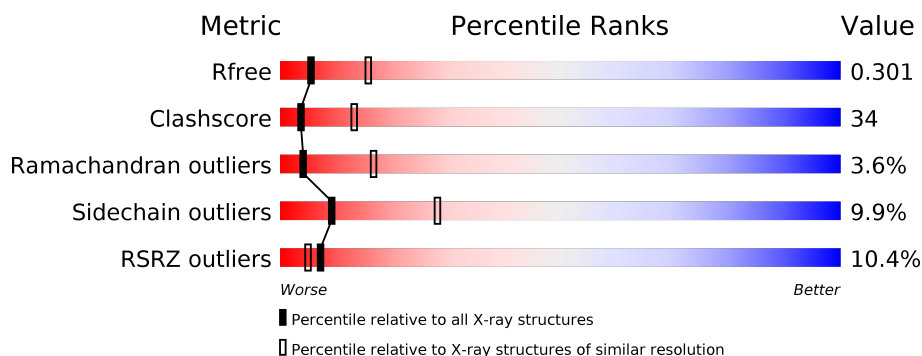
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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 $\leq 5\%$. 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	427	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3028 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 Head vertex protein Gp24.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	390	3028	1925	496	599	3	5	0	0	0

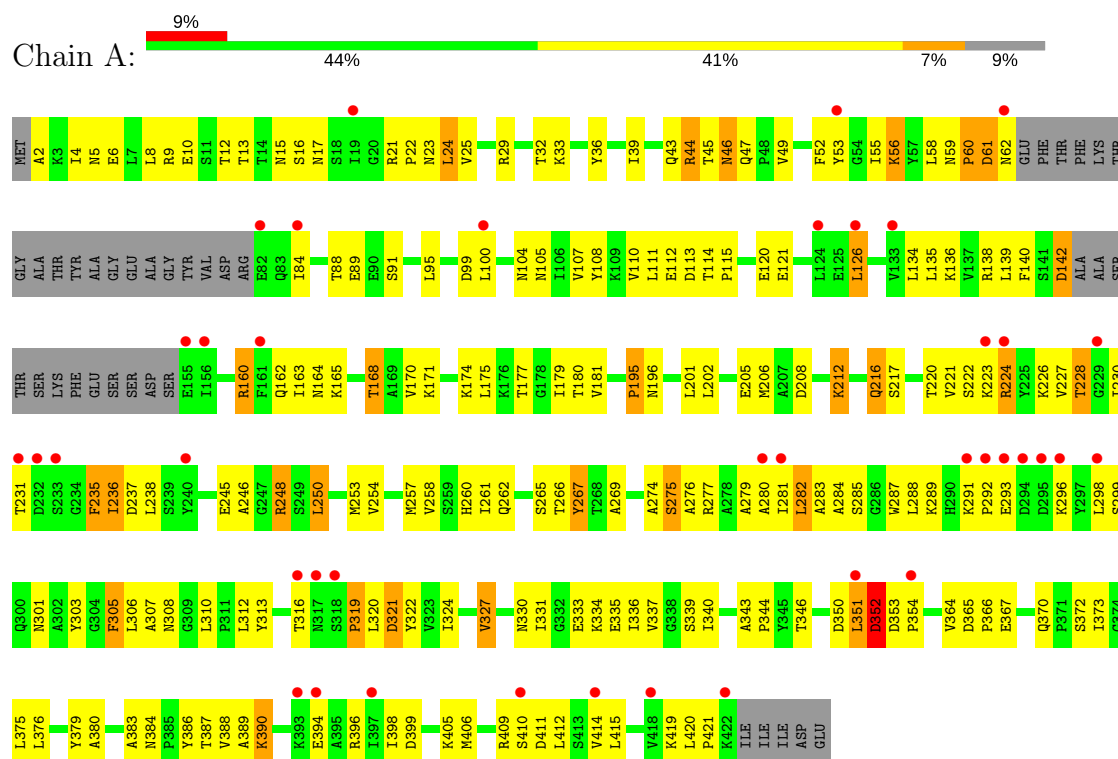
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	206	MSE	MET	MODIFIED RESIDUE	UNP P19896
A	253	MSE	MET	MODIFIED RESIDUE	UNP P19896
A	257	MSE	MET	MODIFIED RESIDUE	UNP P19896
A	403	MSE	MET	MODIFIED RESIDUE	UNP P19896
A	406	MSE	MET	MODIFIED RESIDUE	UNP P19896

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 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: Head vertex protein Gp24



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	107.61Å 107.61Å 82.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.00 – 2.90 35.22 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (35.00-2.90) 97.7 (35.22-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.42 (at 2.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.270 , 0.300 0.270 , 0.301	Depositor DCC
R_{free} test set	586 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	100.7	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 71.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3028	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0/3071	0.71	2/4158 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	ASP	N-CA-C	-6.24	94.15	111.00
1	A	100	LEU	CA-CB-CG	5.37	127.65	115.30

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	3028	0	3046	208	0
All	All	3028	0	3046	208	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 34.

All (208) 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:389:ALA:HB2	1:A:398:ILE:HD11	1.27	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:MSE:HE2	1:A:414:VAL:HG23	1.24	1.09
1:A:16:SER:HB3	1:A:21:ARG:NH1	1.68	1.08
1:A:16:SER:HB3	1:A:21:ARG:HH11	1.04	1.07
1:A:160:ARG:HD3	1:A:160:ARG:H	1.22	1.02
1:A:276:ALA:HB2	1:A:316:THR:HA	1.45	0.98
1:A:227:VAL:HG23	1:A:231:THR:HA	1.51	0.90
1:A:390:LYS:HD2	1:A:390:LYS:H	1.37	0.89
1:A:330:ASN:HB3	1:A:335:GLU:HA	1.56	0.86
1:A:46:ASN:H	1:A:46:ASN:HD22	1.22	0.86
1:A:262:GLN:HG3	1:A:266:THR:HA	1.60	0.84
1:A:216:GLN:O	1:A:220:THR:HG22	1.79	0.83
1:A:139:LEU:H	1:A:139:LEU:HD12	1.43	0.83
1:A:224:ARG:HD3	1:A:224:ARG:H	1.43	0.83
1:A:202:LEU:HD22	1:A:375:LEU:HD21	1.61	0.82
1:A:248:ARG:HG2	1:A:248:ARG:HH11	1.45	0.82
1:A:330:ASN:HB2	1:A:334:LYS:O	1.79	0.81
1:A:88:THR:H	1:A:91:SER:HB3	1.46	0.80
1:A:10:GLU:HB2	1:A:24:LEU:HD23	1.63	0.79
1:A:257:MSE:CE	1:A:414:VAL:HG23	2.11	0.79
1:A:334:LYS:HG2	1:A:336:ILE:HG23	1.64	0.78
1:A:331:ILE:HG12	1:A:336:ILE:HD11	1.65	0.78
1:A:336:ILE:HD12	1:A:337:VAL:HG23	1.68	0.75
1:A:208:ASP:O	1:A:212:LYS:HD2	1.87	0.74
1:A:160:ARG:HD3	1:A:160:ARG:N	2.02	0.74
1:A:224:ARG:HB2	1:A:235:PHE:HE2	1.53	0.73
1:A:245:GLU:HB3	1:A:248:ARG:NH1	2.02	0.73
1:A:2:ALA:HB3	1:A:5:ASN:ND2	2.04	0.72
1:A:246:ALA:HB1	1:A:285:SER:O	1.90	0.71
1:A:84:ILE:H	1:A:84:ILE:HD12	1.54	0.71
1:A:10:GLU:CB	1:A:24:LEU:HD23	2.21	0.70
1:A:44:ARG:NH1	1:A:44:ARG:HB2	2.07	0.70
1:A:245:GLU:HB3	1:A:248:ARG:HH12	1.54	0.70
1:A:174:LYS:HE2	1:A:376:LEU:HD13	1.73	0.70
1:A:336:ILE:CD1	1:A:337:VAL:HG23	2.22	0.69
1:A:398:ILE:HA	1:A:405:LYS:HZ2	1.58	0.69
1:A:324:ILE:HD11	1:A:415:LEU:HD12	1.73	0.69
1:A:88:THR:HG22	1:A:89:GLU:H	1.58	0.69
1:A:257:MSE:HE2	1:A:414:VAL:CG2	2.13	0.69
1:A:250:LEU:CD2	1:A:283:ALA:HB2	2.24	0.68
1:A:248:ARG:CD	1:A:287:TRP:HE1	2.06	0.68
1:A:58:LEU:O	1:A:60:PRO:HD3	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ARG:HD2	1:A:287:TRP:HE1	1.59	0.67
1:A:289:LYS:NZ	1:A:292:PRO:HA	2.09	0.67
1:A:237:ASP:OD2	1:A:419:LYS:HD3	1.96	0.65
1:A:46:ASN:H	1:A:46:ASN:ND2	1.91	0.65
1:A:171:LYS:HG2	1:A:379:TYR:O	1.96	0.65
1:A:180:THR:HA	1:A:372:SER:HA	1.76	0.65
1:A:110:VAL:HG13	1:A:115:PRO:HG2	1.78	0.64
1:A:10:GLU:HB2	1:A:24:LEU:CD2	2.27	0.64
1:A:288:LEU:HD21	1:A:303:TYR:CD2	2.32	0.64
1:A:139:LEU:N	1:A:139:LEU:HD12	2.13	0.64
1:A:6:GLU:O	1:A:10:GLU:HG3	1.97	0.64
1:A:350:ASP:HB3	1:A:353:ASP:O	1.98	0.63
1:A:134:LEU:O	1:A:135:LEU:HG	1.99	0.63
1:A:112:GLU:HG2	1:A:113:ASP:N	2.13	0.63
1:A:212:LYS:O	1:A:216:GLN:HB2	1.99	0.63
1:A:4:ILE:O	1:A:8:LEU:HD23	1.99	0.63
1:A:298:LEU:HD13	1:A:305:PHE:CD1	2.34	0.62
1:A:56:LYS:HE3	1:A:162:GLN:NE2	2.15	0.62
1:A:181:VAL:HG22	1:A:373:ILE:HD11	1.82	0.61
1:A:224:ARG:HH21	1:A:226:LYS:HB3	1.66	0.61
1:A:372:SER:O	1:A:373:ILE:HD13	2.00	0.60
1:A:22:PRO:HA	1:A:25:VAL:CG1	2.31	0.60
1:A:276:ALA:O	1:A:280:ALA:HB3	2.01	0.60
1:A:267:TYR:CZ	1:A:337:VAL:HG21	2.37	0.60
1:A:217:SER:HA	1:A:220:THR:CG2	2.31	0.60
1:A:293:GLU:HB3	1:A:296:LYS:HB2	1.83	0.59
1:A:44:ARG:HH11	1:A:44:ARG:HB2	1.67	0.59
1:A:168:THR:HG23	1:A:399:ASP:OD1	2.02	0.59
1:A:52:PHE:CE2	1:A:343:ALA:HB2	2.38	0.59
1:A:343:ALA:HB3	1:A:380:ALA:HB3	1.85	0.59
1:A:104:ASN:O	1:A:105:ASN:HB2	2.02	0.59
1:A:287:TRP:O	1:A:306:LEU:HD23	2.02	0.58
1:A:248:ARG:HH11	1:A:248:ARG:CG	2.16	0.58
1:A:289:LYS:HZ2	1:A:292:PRO:HA	1.68	0.58
1:A:160:ARG:H	1:A:160:ARG:CD	2.03	0.57
1:A:2:ALA:HB3	1:A:5:ASN:HD22	1.68	0.57
1:A:262:GLN:HA	1:A:265:SER:O	2.04	0.57
1:A:324:ILE:HA	1:A:414:VAL:O	2.04	0.57
1:A:275:SER:CB	1:A:321:ASP:HA	2.35	0.57
1:A:246:ALA:HB3	1:A:248:ARG:NE	2.20	0.57
1:A:250:LEU:HD21	1:A:283:ALA:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:THR:O	1:A:346:THR:HG22	2.05	0.57
1:A:181:VAL:HG22	1:A:373:ILE:CD1	2.35	0.56
1:A:227:VAL:CG2	1:A:231:THR:HA	2.29	0.56
1:A:250:LEU:HD13	1:A:282:LEU:HD23	1.88	0.55
1:A:238:LEU:HD12	1:A:238:LEU:N	2.21	0.55
1:A:254:VAL:O	1:A:258:VAL:HG23	2.06	0.55
1:A:224:ARG:HB2	1:A:235:PHE:CE2	2.38	0.55
1:A:224:ARG:HD3	1:A:224:ARG:N	2.13	0.55
1:A:246:ALA:HA	1:A:285:SER:CB	2.36	0.55
1:A:257:MSE:O	1:A:261:ILE:HG12	2.06	0.55
1:A:330:ASN:CB	1:A:335:GLU:HA	2.33	0.55
1:A:412:LEU:N	1:A:412:LEU:HD22	2.22	0.55
1:A:221:VAL:HG12	1:A:410:SER:HB2	1.89	0.54
1:A:310:LEU:O	1:A:310:LEU:HD12	2.08	0.54
1:A:365:ASP:HB3	1:A:372:SER:HB2	1.88	0.54
1:A:46:ASN:N	1:A:46:ASN:ND2	2.51	0.54
1:A:281:ILE:HA	1:A:284:ALA:HB3	1.90	0.54
1:A:288:LEU:HD21	1:A:303:TYR:HD2	1.73	0.53
1:A:9:ARG:HB3	1:A:9:ARG:NH2	2.24	0.53
1:A:52:PHE:CZ	1:A:343:ALA:HB2	2.43	0.53
1:A:388:VAL:HG21	1:A:406:MSE:HE1	1.91	0.53
1:A:246:ALA:HA	1:A:285:SER:HB3	1.90	0.52
1:A:22:PRO:HA	1:A:25:VAL:HG12	1.91	0.52
1:A:231:THR:HB	1:A:235:PHE:HA	1.92	0.52
1:A:298:LEU:HD13	1:A:305:PHE:CE1	2.45	0.52
1:A:206:MSE:CG	1:A:375:LEU:HD13	2.40	0.52
1:A:390:LYS:HD3	1:A:394:GLU:OE1	2.10	0.52
1:A:88:THR:HG22	1:A:89:GLU:N	2.22	0.52
1:A:10:GLU:OE1	1:A:23:ASN:HB2	2.09	0.51
1:A:248:ARG:HD3	1:A:287:TRP:HE1	1.76	0.51
1:A:120:GLU:CD	1:A:120:GLU:H	2.14	0.51
1:A:179:ILE:O	1:A:373:ILE:HG12	2.11	0.51
1:A:55:ILE:HG22	1:A:163:ILE:HG13	1.92	0.51
1:A:275:SER:OG	1:A:321:ASP:HA	2.11	0.51
1:A:298:LEU:HD13	1:A:305:PHE:HD1	1.76	0.51
1:A:320:LEU:O	1:A:321:ASP:HB2	2.10	0.51
1:A:383:ALA:HB3	1:A:406:MSE:HG3	1.91	0.51
1:A:293:GLU:HB3	1:A:296:LYS:HD2	1.92	0.51
1:A:277:ARG:HH12	1:A:420:LEU:HB2	1.75	0.51
1:A:53:TYR:CE2	1:A:165:LYS:HG3	2.46	0.51
1:A:274:ALA:HB3	1:A:279:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:GLU:CB	1:A:296:LYS:HD2	2.41	0.50
1:A:384:ASN:HB3	1:A:387:THR:HG23	1.93	0.50
1:A:364:VAL:O	1:A:366:PRO:HD3	2.11	0.50
1:A:367:GLU:OE2	1:A:367:GLU:N	2.46	0.49
1:A:95:LEU:O	1:A:114:THR:HA	2.13	0.49
1:A:236:ILE:O	1:A:236:ILE:HG23	2.11	0.49
1:A:230:ILE:O	1:A:230:ILE:HG22	2.13	0.49
1:A:4:ILE:O	1:A:8:LEU:CD2	2.61	0.48
1:A:299:SER:C	1:A:301:ASN:H	2.15	0.48
1:A:23:ASN:H	1:A:23:ASN:HD22	1.60	0.48
1:A:246:ALA:HB3	1:A:248:ARG:CZ	2.44	0.48
1:A:221:VAL:HG21	1:A:340:ILE:HD11	1.95	0.48
1:A:248:ARG:CG	1:A:248:ARG:NH1	2.74	0.48
1:A:275:SER:OG	1:A:321:ASP:CA	2.62	0.48
1:A:280:ALA:HA	1:A:303:TYR:CE2	2.49	0.48
1:A:84:ILE:HD12	1:A:84:ILE:N	2.26	0.48
1:A:292:PRO:HD3	1:A:305:PHE:HB2	1.96	0.48
1:A:312:LEU:C	1:A:312:LEU:HD23	2.34	0.48
1:A:231:THR:HG22	1:A:231:THR:O	2.14	0.47
1:A:280:ALA:HA	1:A:303:TYR:CZ	2.50	0.47
1:A:4:ILE:HG23	1:A:5:ASN:N	2.30	0.47
1:A:111:LEU:HD11	1:A:138:ARG:HD3	1.95	0.47
1:A:140:PHE:CZ	1:A:142:ASP:HB2	2.49	0.47
1:A:246:ALA:O	1:A:285:SER:HB2	2.15	0.47
1:A:84:ILE:H	1:A:84:ILE:CD1	2.27	0.47
1:A:99:ASP:O	1:A:110:VAL:HG23	2.15	0.47
1:A:121:GLU:HG2	1:A:126:LEU:HD12	1.96	0.46
1:A:313:TYR:N	1:A:313:TYR:CD1	2.83	0.46
1:A:36:TYR:O	1:A:39:ILE:HG12	2.15	0.46
1:A:126:LEU:HD13	1:A:126:LEU:O	2.15	0.46
1:A:275:SER:OG	1:A:321:ASP:N	2.49	0.46
1:A:230:ILE:N	1:A:230:ILE:HD12	2.30	0.46
1:A:282:LEU:HD22	1:A:420:LEU:HD13	1.96	0.46
1:A:389:ALA:CB	1:A:398:ILE:HD11	2.20	0.46
1:A:398:ILE:HG22	1:A:405:LYS:NZ	2.31	0.46
1:A:281:ILE:HG23	1:A:282:LEU:N	2.31	0.45
1:A:139:LEU:CD1	1:A:139:LEU:H	2.22	0.45
1:A:287:TRP:HA	1:A:307:ALA:HB2	1.98	0.45
1:A:388:VAL:HG23	1:A:389:ALA:H	1.82	0.45
1:A:322:TYR:CE1	1:A:324:ILE:HG13	2.52	0.44
1:A:250:LEU:HD22	1:A:283:ALA:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ASN:ND2	1:A:351:LEU:HD23	2.32	0.44
1:A:366:PRO:HG2	1:A:367:GLU:OE2	2.16	0.44
1:A:43:GLN:HE22	1:A:53:TYR:H	1.66	0.44
1:A:312:LEU:O	1:A:312:LEU:HD23	2.17	0.44
1:A:248:ARG:HG2	1:A:248:ARG:NH1	2.19	0.44
1:A:282:LEU:HD22	1:A:420:LEU:CD1	2.48	0.44
1:A:387:THR:O	1:A:409:ARG:HD3	2.17	0.44
1:A:108:TYR:CD1	1:A:108:TYR:N	2.86	0.43
1:A:223:LYS:HG3	1:A:411:ASP:H	1.82	0.43
1:A:10:GLU:HB3	1:A:24:LEU:HD23	2.00	0.43
1:A:250:LEU:O	1:A:253:MSE:HB2	2.19	0.43
1:A:55:ILE:HD11	1:A:267:TYR:CE1	2.53	0.43
1:A:177:THR:OG1	1:A:373:ILE:HB	2.19	0.43
1:A:299:SER:C	1:A:301:ASN:N	2.71	0.43
1:A:248:ARG:HD2	1:A:287:TRP:NE1	2.32	0.43
1:A:308:ASN:HD22	1:A:310:LEU:HG	1.82	0.43
1:A:284:ALA:HA	1:A:288:LEU:HB3	2.01	0.43
1:A:288:LEU:HD21	1:A:303:TYR:CE2	2.54	0.43
1:A:350:ASP:OD2	1:A:352:ASP:HB3	2.18	0.43
1:A:398:ILE:HG22	1:A:405:LYS:HZ3	1.84	0.43
1:A:217:SER:HA	1:A:220:THR:HG22	2.01	0.42
1:A:289:LYS:HZ1	1:A:292:PRO:HA	1.81	0.42
1:A:319:PRO:C	1:A:320:LEU:HD22	2.40	0.42
1:A:344:PRO:HA	1:A:379:TYR:CB	2.50	0.42
1:A:228:THR:O	1:A:228:THR:HG22	2.19	0.42
1:A:47:GLN:HB2	1:A:49:VAL:O	2.20	0.42
1:A:196:ASN:OD1	1:A:196:ASN:O	2.37	0.42
1:A:351:LEU:O	1:A:352:ASP:HB2	2.20	0.42
1:A:59:ASN:ND2	1:A:105:ASN:OD1	2.53	0.42
1:A:162:GLN:NE2	1:A:164:ASN:HD21	2.18	0.42
1:A:282:LEU:HD12	1:A:282:LEU:HA	1.83	0.42
1:A:61:ASP:O	1:A:62:ASN:HB3	2.20	0.42
1:A:269:ALA:HA	1:A:327:VAL:HB	2.02	0.41
1:A:406:MSE:HE2	1:A:406:MSE:N	2.36	0.41
1:A:301:ASN:HD22	1:A:301:ASN:HA	1.69	0.41
1:A:201:LEU:O	1:A:205:GLU:HG3	2.21	0.41
1:A:388:VAL:HG23	1:A:389:ALA:N	2.35	0.41
1:A:299:SER:O	1:A:301:ASN:N	2.54	0.41
1:A:275:SER:HB2	1:A:321:ASP:HA	2.03	0.41
1:A:322:TYR:CD1	1:A:324:ILE:HG13	2.56	0.40
1:A:29:ARG:O	1:A:33:LYS:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:HIS:ND1	1:A:260:HIS:O	2.54	0.40
1:A:276:ALA:O	1:A:280:ALA:CB	2.67	0.40

There are no symmetry-related clashes.

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	384/427 (90%)	306 (80%)	64 (17%)	14 (4%)	4	17

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	PHE
1	A	236	ILE
1	A	352	ASP
1	A	421	PRO
1	A	60	PRO
1	A	195	PRO
1	A	15	ASN
1	A	61	ASP
1	A	282	LEU
1	A	291	LYS
1	A	354	PRO
1	A	222	SER
1	A	228	THR
1	A	386	TYR

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	332/356 (93%)	299 (90%)	33 (10%)	9 28

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	13	THR
1	A	24	LEU
1	A	32	THR
1	A	44	ARG
1	A	46	ASN
1	A	56	LYS
1	A	107	VAL
1	A	126	LEU
1	A	136	LYS
1	A	142	ASP
1	A	160	ARG
1	A	168	THR
1	A	170	VAL
1	A	175	LEU
1	A	195	PRO
1	A	212	LYS
1	A	216	GLN
1	A	224	ARG
1	A	248	ARG
1	A	250	LEU
1	A	267	TYR
1	A	275	SER
1	A	305	PHE
1	A	319	PRO
1	A	321	ASP
1	A	327	VAL
1	A	333	GLU
1	A	339	SER
1	A	351	LEU

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Mol	Chain	Res	Type
1	A	370	GLN
1	A	390	LYS
1	A	396	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	17	ASN
1	A	43	GLN
1	A	46	ASN
1	A	59	ASN
1	A	96	ASN
1	A	162	GLN
1	A	196	ASN
1	A	262	GLN
1	A	301	ASN
1	A	308	ASN
1	A	317	ASN
1	A	370	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 [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	385/427 (90%)	0.48	40 (10%) 7 5	64, 107, 156, 167	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	156	ILE	6.7
1	A	233	SER	5.5
1	A	293	GLU	5.2
1	A	292	PRO	5.1
1	A	62	ASN	4.8
1	A	280	ALA	4.8
1	A	161	PHE	4.3
1	A	231	THR	4.2
1	A	155	GLU	3.8
1	A	295	ASP	3.7
1	A	82	GLU	3.5
1	A	224	ARG	3.5
1	A	294	ASP	3.5
1	A	393	LYS	3.4
1	A	397	ILE	3.3
1	A	317	ASN	3.3
1	A	414	VAL	3.2
1	A	240	TYR	3.2
1	A	298	LEU	3.1
1	A	410	SER	3.1
1	A	422	LYS	3.1
1	A	318	SER	3.0
1	A	418	VAL	3.0
1	A	394	GLU	2.5
1	A	19	ILE	2.4
1	A	281	ILE	2.3
1	A	291	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	84	ILE	2.2
1	A	296	LYS	2.2
1	A	223	LYS	2.2
1	A	229	GLY	2.2
1	A	354	PRO	2.2
1	A	53	TYR	2.2
1	A	133	VAL	2.2
1	A	351	LEU	2.2
1	A	316	THR	2.1
1	A	232	ASP	2.1
1	A	126	LEU	2.1
1	A	100	LEU	2.0
1	A	124	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 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.