WORLDWIDE

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:05 pm GMT

PDB ID	:	1CJD
Title	:	THE BACTERIOPHAGE PRD1 COAT PROTEIN, P3, IS STRUCTURALLY SIMILAR TO HUMAN ADENOVIRUS HEXON
Authors	:	Benson, S.D.; Bamford, J.K.H.; Bamford, D.H.; Burnett, R.M.
Deposited on	:	1999-04-12
Resolution	:	1.85 Å(reported)

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

|		
MolProbity	:	4.02b-467
Xtriage (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 1.85 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.
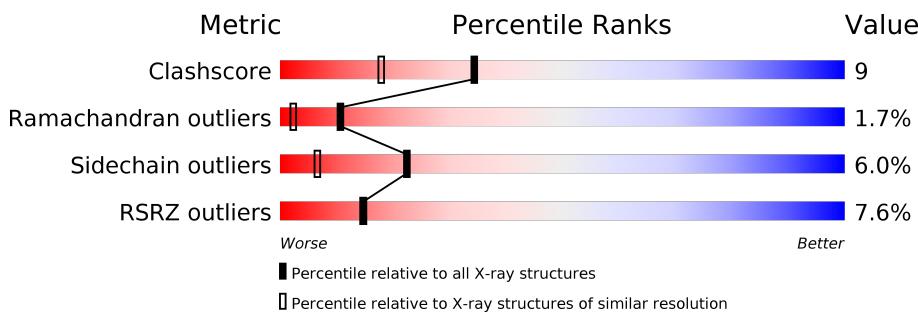
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2083 (1.86-1.86)
Ramachandran outliers	110173	2060 (1.86-1.86)
Sidechain outliers	110143	2060 (1.86-1.86)
RSRZ outliers	101464	1932 (1.86-1.86)

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	394	
1	B	394	
1	C	394	
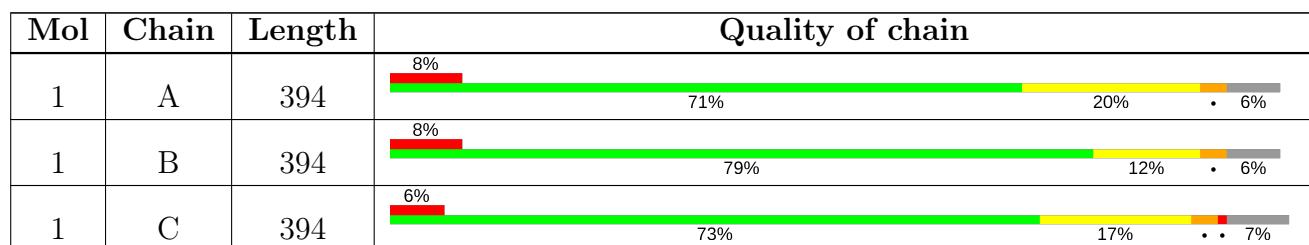
2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 8975 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 PROTEIN (MAJOR CAPSID PROTEIN (P3)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	0	0
			2825	1792	478	548	7			
1	B	372	Total	C	N	O	S	0	0	0
			2847	1805	483	552	7			
1	C	367	Total	C	N	O	S	0	0	0
			2830	1798	478	547	7			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	148	Total	O	0	0
			148	148		
2	B	186	Total	O	0	0
			186	186		
2	C	139	Total	O	0	0
			139	139		

3 Residue-property plots ⓘ

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: PROTEIN (MAJOR CAPSID PROTEIN (P3))
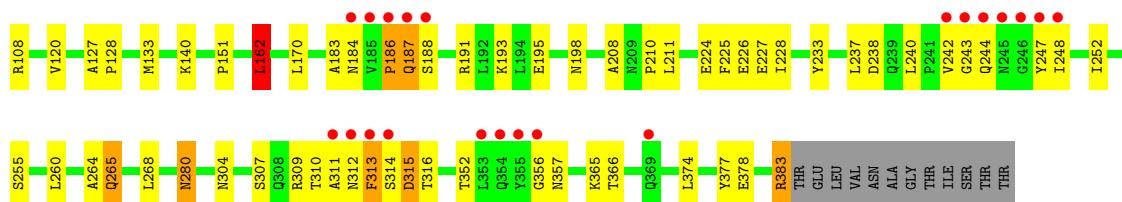
• Molecule 1: PROTEIN (MAJOR CAPSID PROTEIN (P3))
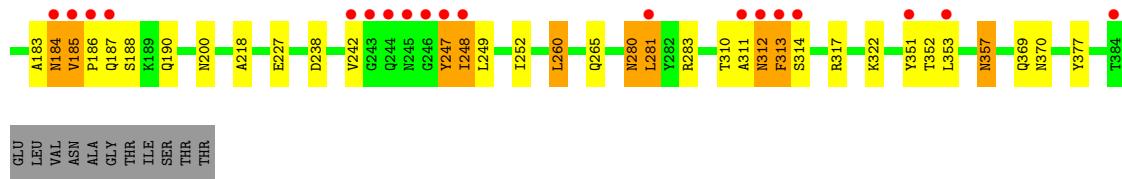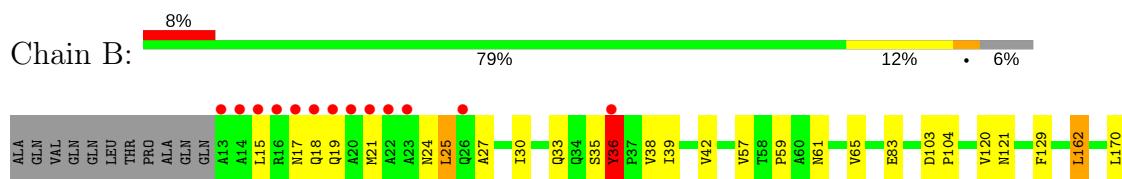
• Molecule 1: PROTEIN (MAJOR CAPSID PROTEIN (P3))

4 Data and refinement statistics (i)

| Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	117.96Å 121.30Å 126.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 1.85 40.10 – 1.84	Depositor EDS
% Data completeness (in resolution range)	78.3 (35.00-1.85) 90.2 (40.10-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 1.84Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.178 , 0.205 0.197 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	18.9	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 66.7	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.009 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8975	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.70	0/2889	0.82	2/3954 (0.1%)
1	B	0.73	1/2911 (0.0%)	0.85	2/3984 (0.1%)
1	C	0.66	0/2893	0.85	6/3956 (0.2%)
All	All	0.70	1/8693 (0.0%)	0.84	10/11894 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	357	ASN	CG-OD1	5.14	1.35	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	LEU	CA-CB-CG	7.45	132.43	115.30
1	B	162	LEU	CA-CB-CG	6.78	130.90	115.30
1	C	162	LEU	CA-CB-CG	6.41	130.03	115.30
1	C	281	LEU	N-CA-C	-6.15	94.39	111.00
1	C	260	LEU	CA-CB-CG	6.01	129.13	115.30
1	B	36	TYR	CA-CB-CG	5.94	124.69	113.40
1	A	170	LEU	N-CA-C	-5.32	96.64	111.00
1	C	312	ASN	N-CA-C	-5.20	96.96	111.00
1	C	170	LEU	N-CA-C	-5.18	97.01	111.00
1	C	108	ARG	NE-CZ-NH2	-5.17	117.71	120.30

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	2825	0	2697	61	0
1	B	2847	0	2718	48	0
1	C	2830	0	2726	53	0
2	A	148	0	0	2	0
2	B	186	0	0	1	0
2	C	139	0	0	1	0
All	All	8975	0	8141	158	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 9.

All (158) 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:B:185:VAL:H	1:B:186:PRO:HD3	1.20	1.04
1:C:353:LEU:HD23	1:C:353:LEU:H	1.23	1.01
1:B:185:VAL:H	1:B:186:PRO:CD	1.76	0.97
1:A:106:ASN:ND2	1:A:191:ARG:HH22	1.63	0.96
1:A:106:ASN:ND2	1:A:191:ARG:NH2	2.20	0.88
1:B:185:VAL:N	1:B:186:PRO:HD3	1.90	0.87
1:A:106:ASN:HD22	1:A:191:ARG:NH2	1.74	0.86
1:C:280:ASN:O	1:C:281:LEU:HB2	1.80	0.82
1:A:80:HIS:HD2	1:A:82:THR:H	1.25	0.81
1:C:29:GLN:O	1:C:33:GLN:HG2	1.79	0.80
1:C:281:LEU:HA	1:C:353:LEU:HD21	1.63	0.80
1:A:80:HIS:CD2	1:A:83:GLU:H	2.01	0.79
1:B:280:ASN:O	1:B:281:LEU:HB2	1.85	0.76
1:B:30:ILE:HB	1:B:248:ILE:HD11	1.65	0.76
1:A:16:ARG:O	1:A:19:GLN:HG3	1.87	0.75
1:C:383:ARG:HG2	1:C:384:THR:N	2.03	0.73
1:B:310:THR:HG22	1:B:312:ASN:H	1.52	0.73
1:A:80:HIS:CD2	1:A:82:THR:H	2.08	0.72
1:A:106:ASN:HD21	1:A:191:ARG:HH22	1.38	0.71
1:A:280:ASN:HB3	1:A:352:THR:OG1	1.92	0.69
1:B:242:VAL:HG22	1:B:247:TYR:CE1	2.31	0.66
1:C:353:LEU:H	1:C:353:LEU:CD2	2.03	0.66
1:B:184:ASN:HB2	1:B:186:PRO:HD3	1.77	0.66
1:C:104:PRO:CB	1:C:185:VAL:HG21	2.26	0.65
1:A:39:ILE:CD1	1:A:233:TYR:HB3	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:LYS:HD3	1:C:163:THR:HG21	1.80	0.64
1:C:79:ASN:HB2	2:C:516:HOH:O	1.97	0.64
1:A:102:TYR:CE2	1:A:108:ARG:HG3	2.33	0.64
1:A:243:GLY:HA3	1:A:248:ILE:HD11	1.80	0.63
1:B:283:ARG:HG2	1:B:351:TYR:CD1	2.34	0.63
1:C:354:GLN:HG2	1:C:354:GLN:O	1.99	0.63
1:A:242:VAL:HG22	1:A:247:TYR:CD1	2.34	0.62
1:C:277:GLN:HE22	1:C:357:ASN:HB3	1.65	0.61
1:A:56:ASP:OD2	1:A:193:LYS:HE3	1.99	0.61
1:A:39:ILE:HD11	1:A:233:TYR:HB3	1.82	0.61
1:C:111:GLU:HG3	1:C:111:GLU:O	2.01	0.60
1:B:185:VAL:N	1:B:186:PRO:CD	2.50	0.60
1:B:27:ALA:HA	1:B:248:ILE:CD1	2.31	0.60
1:A:307:SER:OG	1:A:315:ASP:HB3	2.02	0.60
1:C:34:GLN:HG3	1:C:241:PRO:HB3	1.84	0.60
1:A:79:ASN:ND2	1:A:224:GLU:OE1	2.33	0.59
1:C:30:ILE:O	1:C:34:GLN:HG2	2.03	0.59
1:C:356:GLY:O	1:C:357:ASN:C	2.41	0.59
1:C:310:THR:HG23	1:C:358:VAL:HG22	1.85	0.58
1:A:120:VAL:HG21	1:A:260:LEU:HD13	1.85	0.58
1:C:260:LEU:HD22	1:C:378:GLU:HG3	1.85	0.58
1:A:309:ARG:HD3	1:A:315:ASP:OD2	2.04	0.58
1:C:383:ARG:CG	1:C:384:THR:N	2.67	0.57
1:A:184:ASN:O	1:A:186:PRO:HD3	2.04	0.57
1:A:312:ASN:O	1:A:313:PHE:O	2.23	0.57
1:B:311:ALA:C	1:B:313:PHE:H	2.09	0.57
1:B:27:ALA:HA	1:B:248:ILE:HD11	1.87	0.56
1:B:248:ILE:HG13	1:B:248:ILE:O	2.02	0.56
1:C:103:ASP:HB2	1:C:104:PRO:CD	2.35	0.56
1:B:65:VAL:HG12	1:B:170:LEU:HD12	1.87	0.56
1:C:369:GLN:O	1:C:370:ASN:HB2	2.04	0.56
1:B:184:ASN:CB	1:B:186:PRO:HD3	2.37	0.55
1:C:275:VAL:HG22	1:C:361:VAL:HG22	1.88	0.55
1:C:353:LEU:N	1:C:353:LEU:HD23	2.07	0.55
1:C:35:SER:HB2	1:C:238:ASP:O	2.08	0.54
1:A:242:VAL:HG22	1:A:247:TYR:CE1	2.43	0.53
1:C:255:SER:O	1:C:383:ARG:HB3	2.09	0.52
1:A:25:LEU:O	1:A:25:LEU:HD12	2.09	0.52
1:C:104:PRO:HB3	1:C:185:VAL:HG21	1.93	0.51
1:C:310:THR:HG21	1:C:355:TYR:O	2.10	0.51
1:C:120:VAL:HG21	1:C:260:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:THR:O	1:C:356:GLY:N	2.42	0.51
1:B:184:ASN:HB2	1:B:186:PRO:CD	2.40	0.51
1:B:15:LEU:HA	1:B:18:GLN:OE1	2.11	0.50
1:A:140:LYS:HG3	1:C:89:ASP:HA	1.92	0.50
1:C:103:ASP:HB2	1:C:104:PRO:HD2	1.93	0.50
1:A:54:VAL:HG22	1:A:195:GLU:HG3	1.94	0.49
1:B:120:VAL:HG21	1:B:260:LEU:HD13	1.94	0.49
1:A:80:HIS:HD2	1:A:82:THR:N	2.01	0.49
1:A:304:ASN:OD1	1:A:365:LYS:HE2	2.12	0.49
1:A:280:ASN:HA	1:A:352:THR:OG1	2.13	0.49
1:C:312:ASN:O	1:C:314:SER:N	2.46	0.49
1:A:255:SER:O	1:A:383:ARG:HG3	2.13	0.49
1:B:184:ASN:HB2	1:B:186:PRO:HG3	1.94	0.49
1:A:80:HIS:HD2	1:A:83:GLU:H	1.60	0.48
1:B:280:ASN:HA	1:B:352:THR:OG1	2.13	0.48
1:A:198:ASN:HB2	2:A:481:HOH:O	2.14	0.48
1:A:52:ARG:HG3	1:A:55:PHE:CZ	2.49	0.48
1:A:186:PRO:O	1:A:187:GLN:C	2.53	0.47
1:A:49:PRO:HG2	1:A:225:PHE:CB	2.45	0.47
1:B:83:GLU:HB3	1:B:218:ALA:HB3	1.95	0.47
1:C:280:ASN:O	1:C:281:LEU:CB	2.58	0.46
1:A:106:ASN:HD22	1:A:191:ARG:HH21	1.57	0.46
1:B:59:PRO:HG2	1:B:190:GLN:HB2	1.97	0.46
1:B:103:ASP:HB2	1:B:104:PRO:CD	2.45	0.46
1:C:311:ALA:O	1:C:312:ASN:CB	2.63	0.46
1:B:184:ASN:HB2	1:B:186:PRO:CG	2.45	0.46
1:B:185:VAL:C	1:B:187:GLN:H	2.18	0.46
1:C:185:VAL:HG23	1:C:185:VAL:O	2.15	0.46
1:B:36:TYR:CD1	1:B:238:ASP:HB3	2.51	0.45
1:C:280:ASN:C	1:C:282:TYR:H	2.14	0.45
1:C:83:GLU:HB3	1:C:218:ALA:HB3	1.98	0.44
1:C:57:VAL:O	1:C:59:PRO:HD3	2.18	0.44
1:B:242:VAL:HG22	1:B:247:TYR:CD1	2.52	0.44
1:B:369:GLN:O	1:B:370:ASN:HB2	2.17	0.44
1:B:57:VAL:O	1:B:59:PRO:HD3	2.17	0.44
1:C:281:LEU:HA	1:C:353:LEU:CD2	2.43	0.44
1:C:284:TYR:HB2	1:C:350:ILE:HB	1.99	0.44
1:C:305:TYR:CE1	1:C:318:LYS:HD2	2.53	0.44
1:C:353:LEU:N	1:C:353:LEU:CD2	2.75	0.44
1:A:260:LEU:HA	1:A:377:TYR:O	2.18	0.44
1:B:260:LEU:HA	1:B:377:TYR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:SER:HB2	1:A:238:ASP:O	2.18	0.43
1:C:255:SER:HA	1:C:383:ARG:HE	1.83	0.43
1:A:66:LYS:HE3	2:A:414:HOH:O	2.18	0.43
1:B:65:VAL:CG1	1:B:170:LEU:HD12	2.49	0.43
1:A:312:ASN:C	1:A:313:PHE:O	2.57	0.43
1:B:25:LEU:HA	1:B:25:LEU:HD13	1.84	0.43
1:C:242:VAL:HG22	1:C:247:TYR:CD1	2.54	0.43
1:B:61:ASN:HA	1:B:183:ALA:HB1	2.00	0.43
1:A:226:GLU:O	1:A:227:GLU:HB3	2.18	0.43
1:B:185:VAL:C	1:B:187:GLN:N	2.71	0.43
1:B:310:THR:C	1:B:312:ASN:N	2.71	0.43
1:A:102:TYR:HB2	1:A:191:ARG:HB2	2.01	0.42
1:A:64:ILE:HD12	1:A:240:LEU:CD2	2.49	0.42
1:A:208:ALA:O	1:A:210:PRO:HD3	2.19	0.42
1:C:31:VAL:HA	1:C:241:PRO:HG3	2.02	0.42
1:A:39:ILE:HD13	1:A:233:TYR:HB3	2.00	0.42
1:B:35:SER:HB2	1:B:238:ASP:O	2.19	0.42
1:B:39:ILE:HG23	1:B:39:ILE:O	2.19	0.42
1:A:66:LYS:HD2	1:A:237:LEU:HG	2.01	0.42
1:A:264:ALA:C	1:A:265:GLN:HG2	2.38	0.42
1:A:309:ARG:NH1	1:A:315:ASP:OD2	2.50	0.42
1:C:150:ALA:HB1	1:C:162:LEU:HD13	2.02	0.42
1:C:127:ALA:O	1:C:128:PRO:C	2.58	0.42
1:C:167:TRP:O	1:C:169:PRO:HD3	2.20	0.42
1:C:44:THR:HG22	1:C:45:GLN:N	2.34	0.42
1:A:24:ASN:CG	1:A:252:ILE:HB	2.41	0.42
1:C:312:ASN:C	1:C:314:SER:N	2.73	0.42
1:A:127:ALA:O	1:A:128:PRO:C	2.58	0.41
1:A:151:PRO:HD2	1:A:162:LEU:HD22	2.01	0.41
1:B:185:VAL:O	1:B:187:GLN:N	2.53	0.41
1:C:184:ASN:O	1:C:186:PRO:CD	2.68	0.41
1:A:61:ASN:HA	1:A:183:ALA:HB1	2.02	0.41
1:A:57:VAL:O	1:A:59:PRO:HD3	2.21	0.41
1:A:103:ASP:HB2	1:A:104:PRO:CD	2.50	0.41
1:C:66:LYS:HD2	1:C:237:LEU:HG	2.03	0.41
1:A:211:LEU:HD21	1:A:374:LEU:HD13	2.03	0.41
1:A:316:THR:HA	1:B:38:VAL:HG13	2.03	0.41
1:B:121:ASN:HB3	1:B:129:PHE:CD1	2.55	0.41
1:B:15:LEU:O	1:B:19:GLN:CG	2.68	0.41
1:B:17:ASN:O	1:B:21:MET:HG2	2.20	0.41
1:B:24:ASN:CG	1:B:252:ILE:HB	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:MET:SD	1:C:133:MET:HG3	2.61	0.41
1:A:39:ILE:CG2	1:A:39:ILE:O	2.69	0.41
1:A:260:LEU:HD22	1:A:378:GLU:HG3	2.03	0.40
1:B:186:PRO:C	1:B:188:SER:N	2.73	0.40
1:A:19:GLN:H	1:A:19:GLN:HG2	1.56	0.40
1:A:104:PRO:O	1:A:188:SER:HB3	2.22	0.40
1:A:49:PRO:HG3	1:A:228:ILE:HD12	2.04	0.40
1:B:200:ASN:C	2:B:480:HOH:O	2.60	0.40
1:C:186:PRO:O	1:C:187:GLN:CB	2.69	0.40
1:B:311:ALA:C	1:B:313:PHE:N	2.75	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	A	367/394 (93%)	346 (94%)	15 (4%)	6 (2%)	11	3
1	B	370/394 (94%)	346 (94%)	18 (5%)	6 (2%)	11	3
1	C	363/394 (92%)	339 (93%)	17 (5%)	7 (2%)	9	2
All	All	1100/1182 (93%)	1031 (94%)	50 (4%)	19 (2%)	11	2

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	PRO
1	A	311	ALA
1	A	313	PHE
1	B	184	ASN
1	B	185	VAL
1	C	280	ASN
1	C	312	ASN

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Mol	Chain	Res	Type
1	A	244	GLN
1	B	312	ASN
1	B	313	PHE
1	B	353	LEU
1	C	313	PHE
1	A	187	GLN
1	C	357	ASN
1	B	317	ARG
1	C	185	VAL
1	C	281	LEU
1	C	354	GLN
1	A	356	GLY

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	292/325 (90%)	276 (94%)	16 (6%)	25	9
1	B	293/325 (90%)	278 (95%)	15 (5%)	28	10
1	C	296/325 (91%)	274 (93%)	22 (7%)	16	4
All	All	881/975 (90%)	828 (94%)	53 (6%)	22	6

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	21	MET
1	A	26	GLN
1	A	36	TYR
1	A	39	ILE
1	A	52	ARG
1	A	162	LEU
1	A	265	GLN
1	A	268	LEU
1	A	280	ASN

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Mol	Chain	Res	Type
1	A	310	THR
1	A	314	SER
1	A	315	ASP
1	A	357	ASN
1	A	366	THR
1	A	383	ARG
1	B	25	LEU
1	B	33	GLN
1	B	36	TYR
1	B	42	VAL
1	B	162	LEU
1	B	227	GLU
1	B	247	TYR
1	B	248	ILE
1	B	249	LEU
1	B	260	LEU
1	B	265	GLN
1	B	280	ASN
1	B	281	LEU
1	B	314	SER
1	B	357	ASN
1	C	17	ASN
1	C	42	VAL
1	C	111	GLU
1	C	162	LEU
1	C	182	LEU
1	C	188	SER
1	C	189	LYS
1	C	191	ARG
1	C	193	LYS
1	C	227	GLU
1	C	229	SER
1	C	244	GLN
1	C	247	TYR
1	C	296	SER
1	C	310	THR
1	C	314	SER
1	C	322	LYS
1	C	353	LEU
1	C	354	GLN
1	C	366	THR
1	C	369	GLN

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Mol	Chain	Res	Type
1	C	372	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	A	106	ASN
1	A	277	GLN
1	B	17	ASN
1	B	41	GLN
1	B	51	ASN
1	B	357	ASN
1	C	200	ASN
1	C	277	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, 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	369/394 (93%)	0.05	30 (8%)	13	13	10, 23, 58, 71	0
1	B	372/394 (94%)	-0.01	32 (8%)	11	11	11, 21, 56, 74	0
1	C	367/394 (93%)	-0.07	22 (5%)	23	22	10, 23, 55, 67	0
All	All	1108/1182 (93%)	-0.01	84 (7%)	15	15	10, 22, 57, 74	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	313	PHE	7.1
1	A	185	VAL	6.8
1	B	384	THR	6.6
1	A	15	LEU	6.0
1	B	15	LEU	5.8
1	A	355	TYR	5.7
1	A	353	LEU	5.7
1	B	311	ALA	5.6
1	B	186	PRO	5.4
1	B	14	ALA	5.4
1	A	311	ALA	5.3
1	A	186	PRO	4.8
1	B	313	PHE	4.8
1	B	36	TYR	4.7
1	B	185	VAL	4.7
1	C	384	THR	4.6
1	A	313	PHE	4.5
1	B	245	ASN	4.5
1	A	19	GLN	4.5
1	B	246	GLY	4.4
1	C	244	GLN	4.4
1	C	185	VAL	4.4
1	A	356	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	187	GLN	4.3
1	C	355	TYR	4.3
1	A	245	ASN	4.3
1	A	242	VAL	4.2
1	B	353	LEU	4.2
1	B	243	GLY	4.1
1	C	247	TYR	4.1
1	C	311	ALA	4.1
1	A	243	GLY	4.0
1	A	312	ASN	4.0
1	C	242	VAL	4.0
1	A	354	GLN	4.0
1	A	246	GLY	3.9
1	B	184	ASN	3.8
1	B	244	GLN	3.8
1	A	16	ARG	3.8
1	B	13	ALA	3.8
1	A	36	TYR	3.7
1	C	243	GLY	3.6
1	A	247	TYR	3.5
1	B	312	ASN	3.5
1	B	187	GLN	3.5
1	B	17	ASN	3.3
1	B	19	GLN	3.3
1	C	17	ASN	3.3
1	B	18	GLN	3.2
1	C	248	ILE	3.2
1	C	353	LEU	3.1
1	A	25	LEU	3.1
1	C	36	TYR	3.0
1	B	314	SER	3.0
1	A	188	SER	3.0
1	A	20	ALA	3.0
1	B	23	ALA	3.0
1	A	21	MET	2.9
1	B	22	ALA	2.7
1	C	281	LEU	2.7
1	C	184	ASN	2.7
1	C	20	ALA	2.6
1	C	354	GLN	2.6
1	A	184	ASN	2.6
1	B	281	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	186	PRO	2.6
1	A	314	SER	2.4
1	A	22	ALA	2.4
1	B	16	ARG	2.4
1	C	314	SER	2.4
1	A	369	GLN	2.4
1	B	242	VAL	2.4
1	B	247	TYR	2.3
1	A	244	GLN	2.3
1	C	312	ASN	2.3
1	B	351	TYR	2.3
1	A	248	ILE	2.3
1	B	20	ALA	2.3
1	B	248	ILE	2.3
1	A	17	ASN	2.2
1	C	279	ALA	2.2
1	B	26	GLN	2.1
1	C	62	VAL	2.1
1	B	21	MET	2.1

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 ⓘ

There are no ligands in this entry.

6.5   Other polymers ⓘ

There are no such residues in this entry.