Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:44 PM GMT

PDB ID	:	1C8G
Title	:	FELINE PANLEUKOPENIA VIRUS EMPTY CAPSID STRUCTURE
Authors	:	Rossmann, M.G.; Simpson, A.A.
Deposited on	:	2000-05-05
Resolution	:	3.00 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:

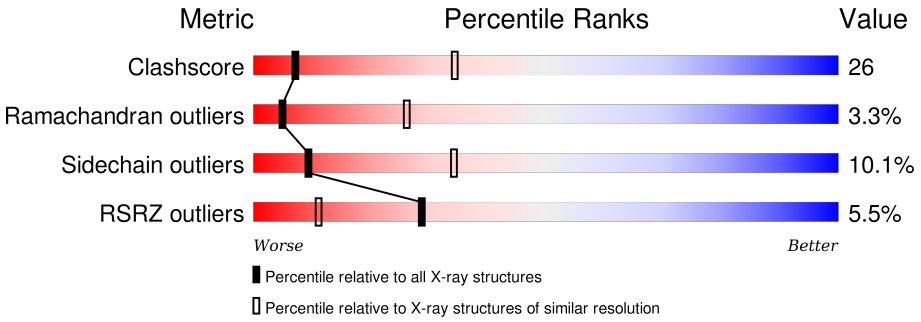
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.00 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	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	548	5%, 66%, 27%, 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4352 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 FELINE PANLEUKOPENIA VIRUS CAPSID.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	0	0
			4350	2766	739	829	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	ILE	THR	CONFLICT	UNP P24840
A	104	GLU	GLN	CONFLICT	UNP P24840
A	232	VAL	ILE	CONFLICT	UNP P24840
A	484	ILE	VAL	CONFLICT	UNP P24840
A	550	GLN	GLU	CONFLICT	UNP P24840
A	572	VAL	LEU	CONFLICT	UNP P24840

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

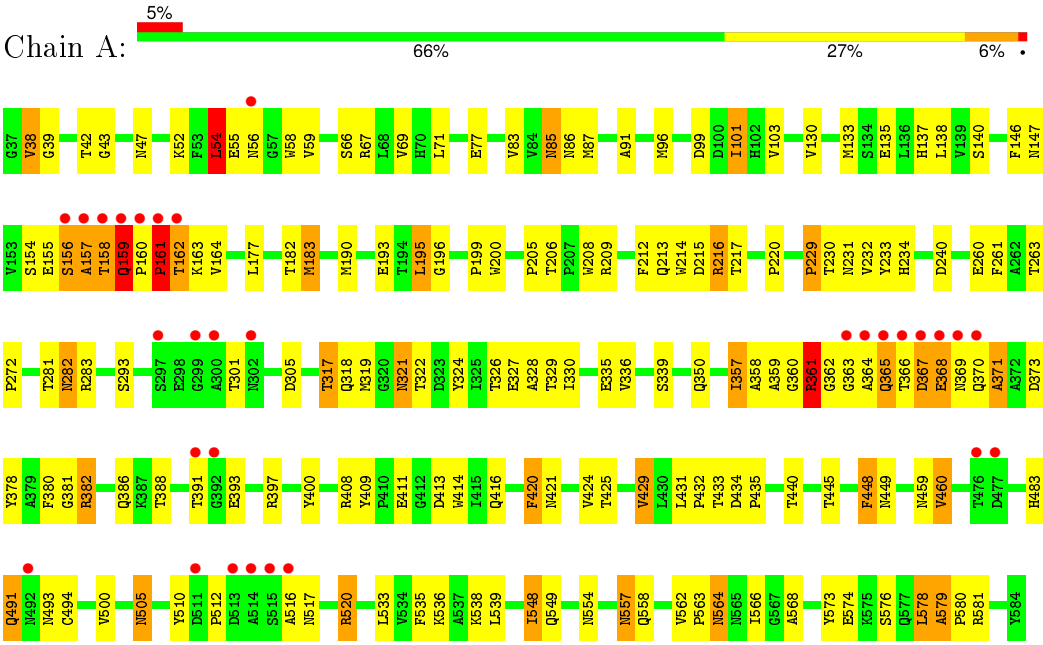
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

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: FELINE PANLEUKOPENIA VIRUS CAPSID

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	266.17Å 250.12Å 379.10Å 90.00° 94.11° 90.00°	Depositor
Resolution (Å)	9.00 – 3.00 24.99 – 3.01	Depositor EDS
% Data completeness (in resolution range)	55.3 (9.00-3.00) 38.5 (24.99-3.01)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.87 (at 2.99Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.245 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å^2)	21.6	Xtriage
Anisotropy	1.109	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 46.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 375496 reflections	Xtriage
F_o,F_c correlation	0.10	EDS
Total number of atoms	4352	wwPDB-VP
Average B, all atoms (Å^2)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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

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

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	0.49	0/4479	0.75	0/6128

There are no bond length outliers.

There are no bond angle outliers.

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	4350	0	4153	223	0
2	A	2	0	0	0	0
All	All	4352	0	4153	223	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 26.

All (223) 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:157:ALA:C	1:A:161:PRO:HB2	1.72	1.08
1:A:156:SER:HB3	1:A:162:THR:HB	1.40	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:VAL:HG13	1:A:578:LEU:HD21	1.41	1.00
1:A:361:ARG:HD3	1:A:362:GLY:H	1.26	0.99
1:A:414:TRP:HE1	1:A:416:GLN:HE21	1.10	0.98
1:A:155:GLU:HG3	1:A:157:ALA:HB2	1.44	0.98
1:A:326:THR:HG22	1:A:328:ALA:H	1.27	0.97
1:A:360:GLY:O	1:A:361:ARG:HB2	1.69	0.93
1:A:193:GLU:HB3	1:A:206:THR:HG21	1.49	0.93
1:A:485:ASN:H	1:A:485:ASN:HD22	1.17	0.92
1:A:216:ARG:HD3	1:A:217:THR:N	1.84	0.92
1:A:154:SER:OG	1:A:164:VAL:HB	1.71	0.90
1:A:554:ASN:H	1:A:557:ASN:HD21	1.19	0.90
1:A:156:SER:CB	1:A:162:THR:HB	2.03	0.88
1:A:158:THR:O	1:A:161:PRO:HA	1.73	0.88
1:A:365:GLN:C	1:A:367:ASP:H	1.77	0.87
1:A:459:ASN:ND2	1:A:460:VAL:H	1.74	0.85
1:A:564:ASN:ND2	1:A:568:ALA:H	1.77	0.82
1:A:361:ARG:HD3	1:A:362:GLY:N	1.94	0.80
1:A:85:ASN:C	1:A:85:ASN:HD22	1.84	0.80
1:A:156:SER:O	1:A:158:THR:HG22	1.81	0.80
1:A:293:SER:HB3	1:A:305:ASP:HB3	1.64	0.80
1:A:491:GLN:C	1:A:491:GLN:HE21	1.85	0.80
1:A:281:THR:HG22	1:A:283:ARG:H	1.45	0.79
1:A:557:ASN:HD22	1:A:558:GLN:N	1.80	0.79
1:A:554:ASN:H	1:A:557:ASN:ND2	1.82	0.77
1:A:157:ALA:CA	1:A:161:PRO:HB2	2.15	0.75
1:A:317:THR:CG2	1:A:319:MET:H	2.00	0.75
1:A:263:THR:HG22	1:A:264:GLY:O	1.87	0.74
1:A:156:SER:O	1:A:158:THR:N	2.17	0.74
1:A:155:GLU:CG	1:A:157:ALA:HB2	2.18	0.74
1:A:366:THR:N	1:A:370:GLN:OE1	2.21	0.74
1:A:557:ASN:HD22	1:A:557:ASN:C	1.93	0.72
1:A:158:THR:N	1:A:161:PRO:HB2	2.05	0.72
1:A:564:ASN:HD21	1:A:568:ALA:H	1.37	0.70
1:A:368:GLU:HG2	1:A:369:ASN:N	2.07	0.70
1:A:159:GLN:HB2	1:A:160:PRO:CD	2.20	0.69
1:A:578:LEU:CD2	1:A:578:LEU:H	2.05	0.69
1:A:365:GLN:HA	1:A:370:GLN:OE1	1.91	0.69
1:A:321:ASN:H	1:A:321:ASN:HD22	1.39	0.69
1:A:367:ASP:HA	1:A:370:GLN:HB3	1.74	0.69
1:A:368:GLU:HG2	1:A:369:ASN:HD22	1.56	0.69
1:A:52:LYS:O	1:A:54:LEU:HD13	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:THR:HG22	1:A:301:THR:O	1.94	0.67
1:A:155:GLU:C	1:A:157:ALA:H	1.98	0.67
1:A:85:ASN:ND2	1:A:87:MET:H	1.93	0.67
1:A:368:GLU:C	1:A:370:GLN:N	2.47	0.67
1:A:578:LEU:H	1:A:578:LEU:HD23	1.60	0.67
1:A:282:ASN:HD21	1:A:336:VAL:H	1.42	0.67
1:A:420:PHE:O	1:A:421:ASN:HB2	1.95	0.67
1:A:357:ILE:HD13	1:A:358:ALA:H	1.60	0.66
1:A:162:THR:HG22	1:A:163:LYS:H	1.59	0.66
1:A:157:ALA:HA	1:A:161:PRO:HB2	1.76	0.66
1:A:158:THR:O	1:A:160:PRO:HD2	1.96	0.65
1:A:366:THR:C	1:A:370:GLN:HB2	2.17	0.65
1:A:414:TRP:HE1	1:A:416:GLN:NE2	1.87	0.65
1:A:99:ASP:CG	1:A:216:ARG:HH12	1.99	0.65
1:A:361:ARG:CD	1:A:362:GLY:H	2.04	0.64
1:A:155:GLU:OE2	1:A:155:GLU:HA	1.97	0.64
1:A:564:ASN:ND2	1:A:566:ILE:H	1.94	0.64
1:A:155:GLU:HG3	1:A:157:ALA:CB	2.23	0.64
1:A:317:THR:HG22	1:A:319:MET:H	1.63	0.64
1:A:459:ASN:ND2	1:A:460:VAL:N	2.46	0.63
1:A:322:THR:HG21	1:A:420:PHE:HD2	1.63	0.63
1:A:156:SER:HB2	1:A:164:VAL:CG2	2.29	0.62
1:A:367:ASP:N	1:A:370:GLN:HB2	2.13	0.62
1:A:431:LEU:C	1:A:433:THR:H	2.03	0.62
1:A:42:THR:H	1:A:147:ASN:ND2	1.97	0.62
1:A:269:ASP:OD1	1:A:490:CYS:HB3	2.00	0.62
1:A:365:GLN:C	1:A:367:ASP:N	2.51	0.61
1:A:367:ASP:HA	1:A:370:GLN:CB	2.29	0.61
1:A:322:THR:HG21	1:A:420:PHE:CD2	2.36	0.61
1:A:554:ASN:N	1:A:557:ASN:HD21	1.95	0.61
1:A:424:VAL:HG22	1:A:429:VAL:HG22	1.81	0.61
1:A:382:ARG:HG2	1:A:382:ARG:HH11	1.65	0.61
1:A:362:GLY:HA3	1:A:370:GLN:NE2	2.16	0.61
1:A:137:HIS:CE1	1:A:272:PRO:HB3	2.35	0.60
1:A:216:ARG:C	1:A:216:ARG:HD3	2.22	0.60
1:A:47:ASN:HD21	1:A:67:ARG:HH21	1.49	0.60
1:A:562:VAL:HG13	1:A:563:PRO:HD2	1.83	0.60
1:A:158:THR:O	1:A:160:PRO:CD	2.49	0.59
1:A:357:ILE:HD13	1:A:358:ALA:N	2.18	0.59
1:A:54:LEU:N	1:A:54:LEU:CD1	2.65	0.59
1:A:282:ASN:ND2	1:A:336:VAL:H	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:LEU:O	1:A:579:ALA:HB2	2.02	0.59
1:A:548:ILE:HG12	1:A:580:PRO:HD2	1.85	0.59
1:A:564:ASN:C	1:A:564:ASN:HD22	2.06	0.59
1:A:459:ASN:HD22	1:A:460:VAL:H	1.50	0.58
1:A:54:LEU:N	1:A:54:LEU:HD13	2.18	0.58
1:A:510:TYR:CE2	1:A:512:PRO:HG3	2.39	0.57
1:A:260:GLU:HG2	1:A:261:PHE:N	2.19	0.57
1:A:213:GLN:HG3	1:A:240:ASP:CB	2.34	0.57
1:A:358:ALA:O	1:A:359:ALA:HB3	2.05	0.56
1:A:367:ASP:O	1:A:368:GLU:HB3	2.04	0.56
1:A:160:PRO:N	1:A:161:PRO:HA	2.19	0.56
1:A:413:ASP:O	1:A:432:PRO:HD3	2.05	0.56
1:A:157:ALA:HA	1:A:161:PRO:CB	2.36	0.56
1:A:159:GLN:C	1:A:161:PRO:HA	2.27	0.55
1:A:193:GLU:CB	1:A:206:THR:HG21	2.30	0.55
1:A:317:THR:HG23	1:A:319:MET:H	1.70	0.55
1:A:382:ARG:HG3	1:A:388:THR:HA	1.87	0.55
1:A:156:SER:O	1:A:162:THR:N	2.40	0.55
1:A:159:GLN:CB	1:A:160:PRO:CD	2.85	0.55
1:A:160:PRO:HB2	1:A:161:PRO:O	2.06	0.55
1:A:101:ILE:CD1	1:A:233:TYR:HB2	2.37	0.54
1:A:183:MET:HE2	1:A:183:MET:HA	1.90	0.54
1:A:156:SER:N	1:A:162:THR:O	2.41	0.54
1:A:578:LEU:O	1:A:579:ALA:CB	2.56	0.53
1:A:85:ASN:C	1:A:85:ASN:ND2	2.57	0.53
1:A:336:VAL:O	1:A:408:ARG:NH2	2.42	0.52
1:A:157:ALA:HA	1:A:161:PRO:CG	2.38	0.52
1:A:159:GLN:CB	1:A:160:PRO:HD2	2.40	0.52
1:A:376:PRO:HG2	1:A:400:TYR:HB3	1.92	0.52
1:A:69:VAL:CG1	1:A:205:PRO:HD3	2.39	0.52
1:A:429:VAL:HB	1:A:431:LEU:CD1	2.39	0.52
1:A:160:PRO:HG2	1:A:161:PRO:C	2.30	0.51
1:A:491:GLN:HE21	1:A:491:GLN:CA	2.20	0.51
1:A:282:ASN:HD21	1:A:335:GLU:HA	1.75	0.51
1:A:158:THR:C	1:A:161:PRO:HA	2.31	0.51
1:A:156:SER:OG	1:A:162:THR:HB	2.10	0.51
1:A:326:THR:CG2	1:A:327:GLU:N	2.74	0.51
1:A:321:ASN:H	1:A:321:ASN:ND2	2.08	0.51
1:A:566:ILE:O	1:A:566:ILE:HG22	2.11	0.50
1:A:85:ASN:HD22	1:A:87:MET:H	1.60	0.50
1:A:358:ALA:HA	1:A:484:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:VAL:HB	1:A:431:LEU:HD12	1.94	0.50
1:A:213:GLN:HG3	1:A:240:ASP:HB2	1.93	0.50
1:A:155:GLU:C	1:A:157:ALA:N	2.65	0.49
1:A:505:ASN:O	1:A:520:ARG:HB2	2.12	0.49
1:A:58:TRP:CE2	1:A:538:LYS:HD3	2.47	0.49
1:A:156:SER:HB3	1:A:162:THR:C	2.33	0.49
1:A:368:GLU:C	1:A:370:GLN:H	2.16	0.49
1:A:85:ASN:HD22	1:A:86:ASN:N	2.11	0.49
1:A:71:LEU:CD2	1:A:500:VAL:HG12	2.43	0.49
1:A:42:THR:H	1:A:147:ASN:HD21	1.61	0.49
1:A:212:PHE:O	1:A:214:TRP:HE3	1.96	0.49
1:A:485:ASN:ND2	1:A:485:ASN:H	1.98	0.48
1:A:365:GLN:HB3	1:A:367:ASP:HB2	1.95	0.48
1:A:133:MET:SD	1:A:539:LEU:HD23	2.53	0.48
1:A:564:ASN:ND2	1:A:564:ASN:C	2.67	0.48
1:A:156:SER:HB3	1:A:162:THR:CB	2.28	0.48
1:A:130:VAL:CG2	1:A:576:SER:HA	2.43	0.48
1:A:367:ASP:CA	1:A:370:GLN:CB	2.92	0.48
1:A:183:MET:CE	1:A:183:MET:HA	2.43	0.48
1:A:156:SER:HB3	1:A:163:LYS:N	2.29	0.48
1:A:339:SER:O	1:A:449:ASN:HA	2.13	0.48
1:A:156:SER:HB2	1:A:164:VAL:HG22	1.96	0.48
1:A:130:VAL:CG1	1:A:578:LEU:HD21	2.29	0.48
1:A:158:THR:C	1:A:159:GLN:HG2	2.33	0.47
1:A:217:THR:OG1	1:A:234:HIS:HE1	1.97	0.47
1:A:368:GLU:O	1:A:369:ASN:C	2.53	0.47
1:A:183:MET:HG3	1:A:208:TRP:HH2	1.80	0.47
1:A:411:GLU:OE1	1:A:411:GLU:N	2.41	0.47
1:A:138:LEU:HD13	1:A:535:PHE:CE1	2.50	0.47
1:A:137:HIS:HB2	1:A:536:LYS:HB3	1.96	0.47
1:A:324:TYR:O	1:A:329:THR:HG21	2.15	0.46
1:A:269:ASP:N	1:A:269:ASP:OD1	2.48	0.46
1:A:505:ASN:HA	1:A:505:ASN:HD22	1.57	0.46
1:A:281:THR:CG2	1:A:282:ASN:N	2.79	0.46
1:A:321:ASN:HD22	1:A:321:ASN:N	2.02	0.46
1:A:485:ASN:N	1:A:485:ASN:HD22	1.93	0.46
1:A:424:VAL:HG21	1:A:429:VAL:HG13	1.97	0.46
1:A:157:ALA:HA	1:A:161:PRO:HG2	1.97	0.46
1:A:382:ARG:HG2	1:A:382:ARG:NH1	2.31	0.46
1:A:213:GLN:HG3	1:A:240:ASP:HB3	1.96	0.46
1:A:135:GLU:HG2	1:A:538:LYS:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:VAL:HG13	1:A:578:LEU:CD2	2.29	0.46
1:A:301:THR:CG2	1:A:301:THR:O	2.62	0.45
1:A:182:THR:HG22	1:A:183:MET:HE3	1.97	0.45
1:A:159:GLN:CG	1:A:160:PRO:HD2	2.46	0.45
1:A:55:GLU:O	1:A:56:ASN:HB2	2.16	0.45
1:A:83:VAL:HG22	1:A:103:VAL:HG22	1.98	0.45
1:A:130:VAL:HG21	1:A:576:SER:HA	1.97	0.45
1:A:409:TYR:CZ	1:A:411:GLU:HB2	2.52	0.45
1:A:381:GLY:HA2	1:A:386:GLN:HE21	1.82	0.45
1:A:326:THR:HG22	1:A:327:GLU:N	2.31	0.45
1:A:483:HIS:HB3	1:A:485:ASN:ND2	2.32	0.44
1:A:96:MET:HG2	1:A:220:PRO:HA	2.00	0.44
1:A:77:GLU:OE2	1:A:520:ARG:NH1	2.51	0.44
1:A:155:GLU:O	1:A:157:ALA:N	2.47	0.44
1:A:367:ASP:CA	1:A:370:GLN:HB2	2.48	0.44
1:A:159:GLN:HG2	1:A:160:PRO:HD2	2.00	0.44
1:A:431:LEU:C	1:A:433:THR:N	2.70	0.44
1:A:71:LEU:HD22	1:A:500:VAL:HG12	1.98	0.44
1:A:215:ASP:HB2	1:A:234:HIS:HB2	2.00	0.44
1:A:47:ASN:ND2	1:A:66:SER:H	2.15	0.44
1:A:445:THR:HA	1:A:448:PHE:HB2	1.99	0.44
1:A:159:GLN:O	1:A:160:PRO:C	2.56	0.43
1:A:43:GLY:HA3	1:A:146:PHE:CD2	2.53	0.43
1:A:157:ALA:HA	1:A:162:THR:H	1.83	0.43
1:A:190:MET:HG2	1:A:190:MET:O	2.19	0.43
1:A:321:ASN:ND2	1:A:321:ASN:N	2.66	0.43
1:A:87:MET:HG2	1:A:231:ASN:ND2	2.34	0.43
1:A:369:ASN:HD22	1:A:369:ASN:N	2.16	0.43
1:A:566:ILE:O	1:A:566:ILE:CG2	2.67	0.43
1:A:536:LYS:HB2	1:A:536:LYS:HE3	1.73	0.43
1:A:368:GLU:O	1:A:371:ALA:N	2.53	0.42
1:A:317:THR:CG2	1:A:318:GLN:N	2.82	0.42
1:A:562:VAL:CG1	1:A:563:PRO:HD2	2.49	0.42
1:A:548:ILE:HG23	1:A:549:GLN:N	2.34	0.42
1:A:380:PHE:N	1:A:380:PHE:CD1	2.87	0.42
1:A:87:MET:O	1:A:91:ALA:HB2	2.20	0.42
1:A:38:VAL:CG2	1:A:39:GLY:N	2.82	0.42
1:A:366:THR:O	1:A:367:ASP:O	2.38	0.42
1:A:362:GLY:CA	1:A:370:GLN:NE2	2.82	0.42
1:A:326:THR:H	1:A:329:THR:HB	1.85	0.42
1:A:378:TYR:O	1:A:397:ARG:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:THR:HG22	1:A:282:ASN:N	2.35	0.41
1:A:67:ARG:NH1	1:A:196:GLY:O	2.50	0.41
1:A:434:ASP:HA	1:A:435:PRO:HD3	1.85	0.41
1:A:578:LEU:N	1:A:578:LEU:HD23	2.31	0.41
1:A:54:LEU:HB3	1:A:55:GLU:H	1.64	0.41
1:A:158:THR:HG23	1:A:162:THR:OG1	2.21	0.41
1:A:159:GLN:C	1:A:161:PRO:CA	2.89	0.41
1:A:484:ILE:HA	1:A:484:ILE:HD12	1.84	0.41
1:A:420:PHE:HB3	1:A:421:ASN:H	1.73	0.41
1:A:183:MET:CG	1:A:208:TRP:CH2	3.04	0.41
1:A:199:PRO:HD2	1:A:200:TRP:CZ3	2.54	0.41
1:A:293:SER:O	1:A:305:ASP:N	2.51	0.41
1:A:490:CYS:HB3	1:A:493:ASN:O	2.21	0.41
1:A:140:SER:O	1:A:533:LEU:HD12	2.21	0.40
1:A:357:ILE:CG2	1:A:374:GLY:HA3	2.52	0.40
1:A:195:LEU:HD12	1:A:195:LEU:HA	1.90	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	546/548 (100%)	498 (91%)	30 (6%)	18 (3%)	5 26

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	ALA
1	A	159	GLN
1	A	230	THR
1	A	361	ARG
1	A	367	ASP

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Mol	Chain	Res	Type
1	A	371	ALA
1	A	373	ASP
1	A	516	ALA
1	A	517	ASN
1	A	579	ALA
1	A	54	LEU
1	A	363	GLY
1	A	365	GLN
1	A	364	ALA
1	A	368	GLU
1	A	229	PRO
1	A	156	SER
1	A	161	PRO

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	477/477 (100%)	429 (90%)	48 (10%)	9 34

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	VAL
1	A	54	LEU
1	A	59	VAL
1	A	85	ASN
1	A	101	ILE
1	A	150	LEU
1	A	152	THR
1	A	158	THR
1	A	159	GLN
1	A	161	PRO
1	A	162	THR
1	A	177	LEU
1	A	183	MET

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Mol	Chain	Res	Type
1	A	195	LEU
1	A	209	ARG
1	A	216	ARG
1	A	229	PRO
1	A	232	VAL
1	A	282	ASN
1	A	317	THR
1	A	321	ASN
1	A	330	ILE
1	A	350	GLN
1	A	357	ILE
1	A	361	ARG
1	A	377	ARG
1	A	382	ARG
1	A	391	THR
1	A	393	GLU
1	A	420	PHE
1	A	425	THR
1	A	429	VAL
1	A	440	THR
1	A	448	PHE
1	A	460	VAL
1	A	485	ASN
1	A	490	CYS
1	A	491	GLN
1	A	494	CYS
1	A	505	ASN
1	A	520	ARG
1	A	548	ILE
1	A	557	ASN
1	A	564	ASN
1	A	573	TYR
1	A	574	GLU
1	A	578	LEU
1	A	581	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	64	ASN
1	A	70	HIS

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Mol	Chain	Res	Type
1	A	78	ASN
1	A	85	ASN
1	A	147	ASN
1	A	180	ASN
1	A	234	HIS
1	A	282	ASN
1	A	292	ASN
1	A	302	ASN
1	A	310	GLN
1	A	321	ASN
1	A	369	ASN
1	A	383	GLN
1	A	384	HIS
1	A	386	GLN
1	A	416	GLN
1	A	459	ASN
1	A	466	ASN
1	A	468	GLN
1	A	485	ASN
1	A	491	GLN
1	A	505	ASN
1	A	546	ASN
1	A	557	ASN
1	A	560	ASN
1	A	564	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

Of 2 ligands modelled in this entry, 2 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	548/548 (100%)	0.20	30 (5%) 29 11	2, 8, 33, 54	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	162	THR	4.4
1	A	158	THR	4.3
1	A	160	PRO	4.3
1	A	159	GLN	4.2
1	A	366	THR	3.9
1	A	369	ASN	3.9
1	A	156	SER	3.9
1	A	161	PRO	3.8
1	A	157	ALA	3.4
1	A	515	SER	3.1
1	A	364	ALA	3.1
1	A	367	ASP	3.0
1	A	513	ASP	3.0
1	A	368	GLU	2.9
1	A	365	GLN	2.8
1	A	391	THR	2.7
1	A	300	ALA	2.7
1	A	299	GLY	2.6
1	A	302	ASN	2.5
1	A	516	ALA	2.4
1	A	514	ALA	2.4
1	A	370	GLN	2.4
1	A	363	GLY	2.3
1	A	511	ASP	2.3
1	A	56	ASN	2.2
1	A	297	SER	2.1
1	A	476	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	392	GLY	2.1
1	A	477	ASP	2.1
1	A	492	ASN	2.1

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)

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
2	CA	A	585	1/1	0.97	0.24	-	9,9,9,9	0
2	CA	A	586	1/1	0.94	0.23	-	9,9,9,9	0

6.5 Other polymers (i)

There are no such residues in this entry.