Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:23 PM GMT

PDB ID	:	1K3V
Title	:	Porcine Parvovirus Capsid
Authors	:	Simpson, A.A.; Hebert, B.; Sullivan, G.M.; Parrish, C.R.; Zadori, Z.; Tijssen, P.; Rossmann, M.G.
Deposited on	:	2001-10-04
Resolution	:	3.50 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 (i)) were used in the production of this report:

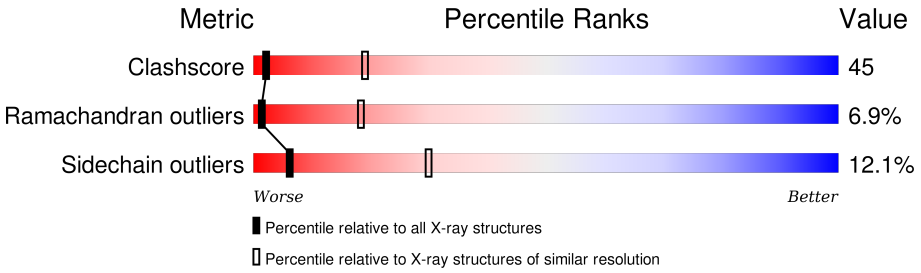
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.50 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	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	579	37% 46% 10% • 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4306 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 capsid protein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	542	4306	2727	735	828	16	0	0	0

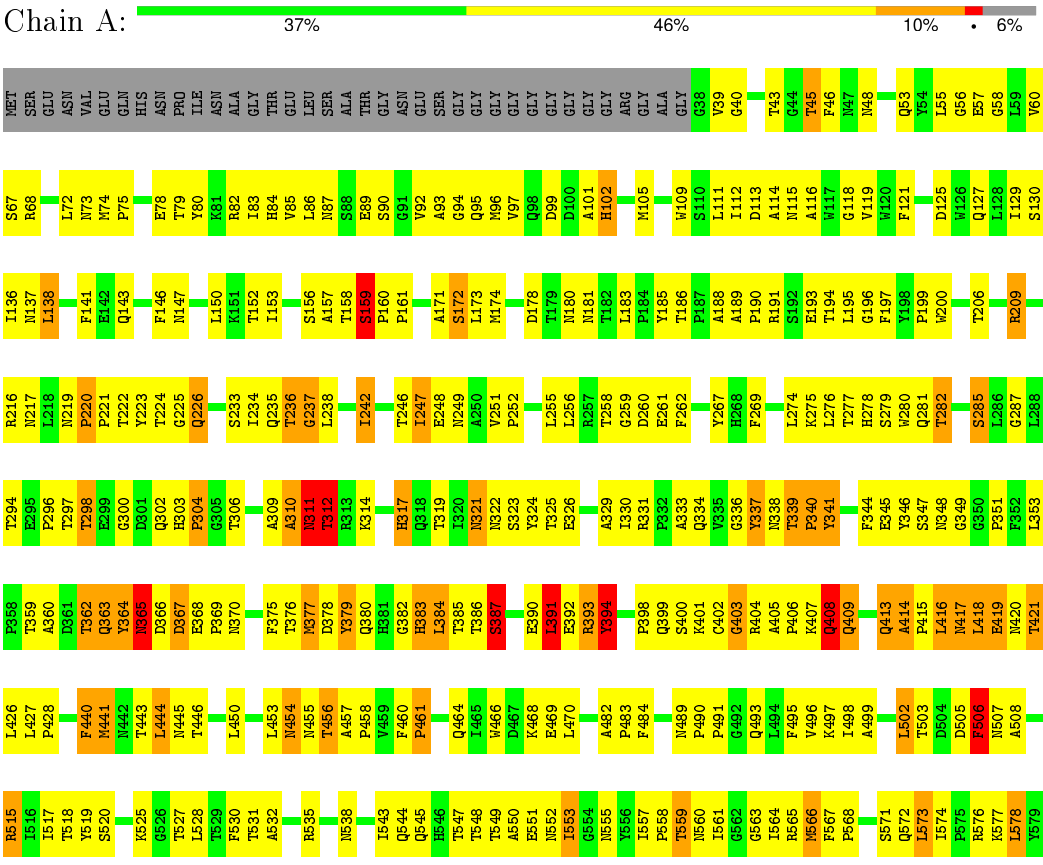
3 Residue-property plots (i)

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.

Note EDS was not executed.

- Molecule 1: capsid protein VP2

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	442.49Å 443.05Å 251.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50	Depositor
% Data completeness (in resolution range)	31.4 (50.00-3.50)	Depositor
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.286 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4306	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

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	0.49	0/4432	0.77	1/6067 (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	A	421	THR	N-CA-C	-5.04	97.38	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	4306	0	4137	377	0
All	All	4306	0	4137	377	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 45.

All (377) 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:246:THR:HG22	1:A:249:ASN:H	1.22	1.05
1:A:82:ARG:HE	1:A:236:THR:HG21	1.17	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ALA:HB1	1:A:415:PRO:HD3	1.34	1.03
1:A:559:THR:HG22	1:A:561:ILE:H	1.24	1.02
1:A:193:GLU:HB3	1:A:206:THR:HG21	1.41	1.00
1:A:418:LEU:H	1:A:418:LEU:HD22	1.25	0.99
1:A:359:THR:HG21	1:A:402:CYS:HB2	1.47	0.95
1:A:406:PRO:HA	1:A:409:GLN:HG3	1.51	0.93
1:A:573:LEU:HD23	1:A:573:LEU:H	1.35	0.92
1:A:194:THR:HG22	1:A:195:LEU:H	1.34	0.92
1:A:453:LEU:HD12	1:A:454:ASN:H	1.34	0.91
1:A:544:GLN:O	1:A:545:GLN:HG2	1.71	0.91
1:A:101:ALA:HB3	1:A:216:ARG:NH1	1.85	0.91
1:A:79:THR:HG22	1:A:80:TYR:H	1.34	0.90
1:A:362:THR:HG21	1:A:405:ALA:HB2	1.55	0.88
1:A:174:MET:HE2	1:A:499:ALA:HA	1.55	0.87
1:A:441:MET:H	1:A:441:MET:HE3	1.39	0.86
1:A:48:ASN:HD22	1:A:67:SER:H	1.18	0.86
1:A:573:LEU:CD2	1:A:573:LEU:H	1.88	0.86
1:A:555:ASN:HA	1:A:565:ARG:HD2	1.58	0.85
1:A:261:GLU:HG2	1:A:262:PHE:N	1.92	0.85
1:A:321:ASN:H	1:A:321:ASN:HD22	1.21	0.85
1:A:159:SER:HB2	1:A:160:PRO:HD3	1.63	0.81
1:A:127:GLN:O	1:A:131:ASN:HB2	1.81	0.81
1:A:421:THR:HB	1:A:424:GLY:H	1.47	0.80
1:A:441:MET:H	1:A:441:MET:CE	1.93	0.80
1:A:414:ALA:HB1	1:A:415:PRO:CD	2.13	0.79
1:A:414:ALA:CB	1:A:415:PRO:HD3	2.11	0.79
1:A:212:LEU:HD23	1:A:213:SER:N	1.98	0.78
1:A:181:ASN:HD22	1:A:489:ASN:HD21	1.28	0.78
1:A:333:ALA:HB1	1:A:450:LEU:O	1.84	0.78
1:A:379:TYR:HE1	1:A:390:GLU:HA	1.49	0.76
1:A:292:LEU:HD12	1:A:292:LEU:H	1.51	0.76
1:A:159:SER:HB2	1:A:160:PRO:CD	2.15	0.75
1:A:559:THR:CG2	1:A:561:ILE:H	1.98	0.75
1:A:321:ASN:HD22	1:A:321:ASN:N	1.83	0.75
1:A:553:ILE:N	1:A:553:ILE:HD12	2.01	0.75
1:A:414:ALA:CB	1:A:415:PRO:CD	2.65	0.74
1:A:357:VAL:HG11	1:A:453:LEU:HD11	1.68	0.73
1:A:99:ASP:CG	1:A:216:ARG:HH12	1.91	0.73
1:A:215:ILE:HG13	1:A:237:GLY:HA2	1.71	0.73
1:A:183:LEU:HD12	1:A:495:PHE:CE2	2.24	0.72
1:A:82:ARG:NE	1:A:236:THR:HG21	2.00	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ASN:ND2	1:A:67:SER:H	1.88	0.72
1:A:82:ARG:HH11	1:A:82:ARG:HB3	1.54	0.71
1:A:413:GLN:CD	1:A:414:ALA:H	1.93	0.71
1:A:359:THR:HG21	1:A:403:GLY:H	1.55	0.71
1:A:359:THR:CG2	1:A:403:GLY:H	2.04	0.70
1:A:317:HIS:HB2	1:A:324:TYR:HE2	1.56	0.70
1:A:133:MET:HB2	1:A:276:LEU:HD12	1.72	0.70
1:A:559:THR:HG22	1:A:561:ILE:N	2.04	0.70
1:A:274:LEU:HD11	1:A:458:PRO:HG3	1.72	0.70
1:A:79:THR:HG22	1:A:80:TYR:N	2.07	0.69
1:A:111:LEU:HD23	1:A:112:ILE:N	2.06	0.69
1:A:43:THR:OG1	1:A:146:PHE:HB2	1.92	0.69
1:A:246:THR:HG22	1:A:249:ASN:N	2.03	0.69
1:A:129:ILE:O	1:A:133:MET:HG2	1.93	0.69
1:A:357:VAL:HG21	1:A:453:LEU:HD21	1.73	0.69
1:A:194:THR:HG22	1:A:195:LEU:N	2.08	0.69
1:A:390:GLU:HB3	1:A:391:LEU:HD23	1.73	0.68
1:A:440:PHE:CD2	1:A:441:MET:HE2	2.28	0.68
1:A:382:GLY:HA2	1:A:566:MET:HB2	1.76	0.68
1:A:132:ASN:HA	1:A:535:ARG:HD3	1.73	0.68
1:A:310:ALA:HB1	1:A:323:SER:HB2	1.75	0.68
1:A:121:PHE:HB3	1:A:125:ASP:HB2	1.76	0.67
1:A:418:LEU:O	1:A:419:GLU:HB2	1.93	0.67
1:A:427:LEU:HB3	1:A:428:PRO:HD2	1.77	0.66
1:A:456:THR:HG22	1:A:457:ALA:N	2.10	0.66
1:A:543:ILE:HG13	1:A:544:GLN:O	1.94	0.66
1:A:359:THR:HG21	1:A:402:CYS:CB	2.24	0.65
1:A:506:PHE:CD2	1:A:506:PHE:C	2.70	0.65
1:A:547:THR:OG1	1:A:548:THR:N	2.27	0.65
1:A:515:ARG:HG3	1:A:515:ARG:HH11	1.61	0.65
1:A:90:SER:OG	1:A:216:ARG:NH2	2.29	0.64
1:A:427:LEU:CB	1:A:428:PRO:HD2	2.27	0.64
1:A:453:LEU:CD1	1:A:454:ASN:H	2.09	0.64
1:A:216:ARG:HG2	1:A:216:ARG:HH11	1.62	0.63
1:A:48:ASN:ND2	1:A:66:ALA:HA	2.13	0.63
1:A:399:GLN:O	1:A:401:LYS:HD2	1.98	0.63
1:A:418:LEU:HD22	1:A:418:LEU:N	2.06	0.63
1:A:251:VAL:HG13	1:A:252:PRO:HD2	1.80	0.63
1:A:72:LEU:HD22	1:A:496:VAL:CG1	2.28	0.63
1:A:454:ASN:HD21	1:A:576:ARG:NH2	1.96	0.63
1:A:341:TYR:CD2	1:A:369:PRO:HB3	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:THR:HG23	1:A:515:ARG:HA	1.81	0.63
1:A:136:ILE:HG22	1:A:276:LEU:HD21	1.79	0.62
1:A:150:LEU:HD11	1:A:172:SER:C	2.19	0.62
1:A:216:ARG:HD2	1:A:217:ASN:H	1.65	0.62
1:A:310:ALA:O	1:A:312:THR:N	2.33	0.61
1:A:330:ILE:O	1:A:331:ARG:HD3	1.99	0.61
1:A:321:ASN:ND2	1:A:321:ASN:N	2.45	0.61
1:A:444:LEU:HD22	1:A:445:ASN:N	2.15	0.61
1:A:378:ASP:C	1:A:380:GLN:H	2.04	0.61
1:A:456:THR:HG22	1:A:457:ALA:H	1.66	0.61
1:A:153:ILE:CG2	1:A:517:ILE:HB	2.31	0.61
1:A:317:HIS:HB2	1:A:324:TYR:CE2	2.34	0.60
1:A:150:LEU:CD2	1:A:520:SER:HB2	2.31	0.60
1:A:377:MET:HG3	1:A:392:GLU:HB3	1.81	0.60
1:A:453:LEU:HD12	1:A:454:ASN:N	2.12	0.60
1:A:390:GLU:O	1:A:391:LEU:HG	2.02	0.60
1:A:553:ILE:H	1:A:553:ILE:HD12	1.66	0.60
1:A:277:THR:HG22	1:A:574:ILE:HB	1.83	0.60
1:A:571:SER:O	1:A:572:GLN:HB2	2.01	0.59
1:A:87:ASN:HB2	1:A:89:GLU:OE1	2.02	0.59
1:A:362:THR:OG1	1:A:363:GLN:N	2.34	0.59
1:A:191:ARG:O	1:A:193:GLU:HG3	2.03	0.59
1:A:515:ARG:N	1:A:515:ARG:HD3	2.18	0.59
1:A:96:MET:HE1	1:A:221:PRO:HB3	1.85	0.58
1:A:573:LEU:N	1:A:573:LEU:HD23	2.07	0.58
1:A:402:CYS:O	1:A:403:GLY:O	2.21	0.58
1:A:111:LEU:HD23	1:A:111:LEU:C	2.24	0.58
1:A:181:ASN:HD22	1:A:489:ASN:ND2	2.00	0.58
1:A:287:GLY:O	1:A:289:PRO:HD3	2.03	0.58
1:A:408:GLN:C	1:A:408:GLN:HE21	2.06	0.57
1:A:377:MET:CG	1:A:392:GLU:HB3	2.33	0.57
1:A:274:LEU:HD23	1:A:275:LYS:O	2.04	0.57
1:A:43:THR:H	1:A:147:ASN:ND2	2.02	0.57
1:A:72:LEU:HD22	1:A:496:VAL:HG12	1.87	0.57
1:A:364:TYR:N	1:A:364:TYR:HD1	2.03	0.57
1:A:336:GLY:O	1:A:337:TYR:HB3	2.05	0.57
1:A:469:GLU:OE1	1:A:470:LEU:N	2.37	0.56
1:A:550:ALA:O	1:A:553:ILE:HD11	2.06	0.56
1:A:359:THR:HG21	1:A:403:GLY:N	2.20	0.56
1:A:394:TYR:CZ	1:A:568:PRO:HG3	2.39	0.56
1:A:92:VAL:HG12	1:A:93:ALA:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:LEU:O	1:A:419:GLU:CB	2.53	0.56
1:A:573:LEU:N	1:A:573:LEU:CD2	2.62	0.56
1:A:68:ARG:NH1	1:A:196:GLY:O	2.37	0.56
1:A:394:TYR:CE2	1:A:568:PRO:HG3	2.40	0.56
1:A:341:TYR:HD1	1:A:341:TYR:H	1.54	0.56
1:A:246:THR:CG2	1:A:249:ASN:H	2.08	0.56
1:A:321:ASN:H	1:A:321:ASN:ND2	1.98	0.56
1:A:129:ILE:HG23	1:A:133:MET:HG3	1.88	0.55
1:A:364:TYR:N	1:A:364:TYR:CD1	2.75	0.55
1:A:200:TRP:CZ2	1:A:564:ILE:HD13	2.41	0.55
1:A:101:ALA:HB3	1:A:216:ARG:HH11	1.71	0.55
1:A:75:PRO:HG2	1:A:497:LYS:HG3	1.89	0.55
1:A:309:ALA:O	1:A:310:ALA:O	2.25	0.55
1:A:223:TYR:O	1:A:225:GLY:N	2.40	0.54
1:A:159:SER:CB	1:A:160:PRO:CD	2.83	0.54
1:A:246:THR:HB	1:A:249:ASN:HB2	1.88	0.54
1:A:298:THR:HB	1:A:303:HIS:ND1	2.23	0.54
1:A:39:VAL:HG13	1:A:40:GLY:H	1.72	0.54
1:A:274:LEU:HD23	1:A:275:LYS:N	2.23	0.54
1:A:150:LEU:HD23	1:A:520:SER:HB2	1.90	0.54
1:A:118:GLY:CA	1:A:461:PRO:HB2	2.38	0.54
1:A:421:THR:HB	1:A:424:GLY:N	2.21	0.53
1:A:506:PHE:CD2	1:A:507:ASN:N	2.75	0.53
1:A:404:ARG:HH11	1:A:404:ARG:HG3	1.72	0.53
1:A:553:ILE:N	1:A:553:ILE:CD1	2.66	0.53
1:A:353:LEU:HD23	1:A:354:THR:C	2.29	0.53
1:A:378:ASP:OD2	1:A:379:TYR:N	2.42	0.53
1:A:553:ILE:H	1:A:553:ILE:CD1	2.17	0.53
1:A:216:ARG:HD2	1:A:233:SER:O	2.09	0.53
1:A:97:VAL:HG13	1:A:344:PHE:CE2	2.44	0.53
1:A:506:PHE:CG	1:A:507:ASN:N	2.75	0.53
1:A:212:LEU:HD23	1:A:213:SER:H	1.70	0.52
1:A:426:LEU:HD23	1:A:440:PHE:CD2	2.44	0.52
1:A:413:GLN:OE1	1:A:414:ALA:N	2.36	0.52
1:A:153:ILE:HG23	1:A:153:ILE:O	2.10	0.52
1:A:296:PRO:HG3	1:A:304:PRO:O	2.10	0.52
1:A:48:ASN:ND2	1:A:68:ARG:HH21	2.07	0.52
1:A:375:PHE:HB2	1:A:394:TYR:CE2	2.44	0.52
1:A:185:TYR:HA	1:A:493:GLN:NE2	2.24	0.52
1:A:215:ILE:O	1:A:215:ILE:HG22	2.10	0.52
1:A:359:THR:HG22	1:A:360:ALA:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:PHE:CG	1:A:441:MET:HE2	2.44	0.52
1:A:255:LEU:O	1:A:256:LEU:HD23	2.10	0.52
1:A:544:GLN:NE2	1:A:573:LEU:HB2	2.25	0.52
1:A:454:ASN:HD21	1:A:576:ARG:HH22	1.57	0.52
1:A:518:THR:HG22	1:A:519:TYR:N	2.25	0.52
1:A:96:MET:HE1	1:A:221:PRO:CB	2.40	0.52
1:A:216:ARG:HD2	1:A:217:ASN:N	2.25	0.52
1:A:174:MET:HB2	1:A:497:LYS:O	2.11	0.51
1:A:60:VAL:HG22	1:A:532:ALA:O	2.10	0.51
1:A:130:SER:HB2	1:A:573:LEU:HD21	1.92	0.51
1:A:186:THR:H	1:A:493:GLN:HE22	1.57	0.51
1:A:339:THR:HB	1:A:356:ILE:HG23	1.93	0.51
1:A:115:ASN:ND2	1:A:464:GLN:CG	2.73	0.51
1:A:213:SER:OG	1:A:237:GLY:HA3	2.11	0.51
1:A:235:GLN:O	1:A:236:THR:C	2.50	0.51
1:A:236:THR:O	1:A:237:GLY:O	2.29	0.51
1:A:294:THR:HB	1:A:306:THR:H	1.75	0.51
1:A:406:PRO:O	1:A:408:GLN:N	2.44	0.50
1:A:489:ASN:HD22	1:A:490:PRO:HD2	1.76	0.50
1:A:74:MET:HE1	1:A:517:ILE:HA	1.92	0.50
1:A:416:LEU:O	1:A:417:ASN:CB	2.60	0.50
1:A:276:LEU:O	1:A:572:GLN:HA	2.11	0.50
1:A:178:ASP:OD2	1:A:181:ASN:HA	2.11	0.50
1:A:505:ASP:O	1:A:506:PHE:O	2.30	0.50
1:A:83:ILE:HG22	1:A:84:HIS:O	2.11	0.50
1:A:364:TYR:O	1:A:365:ASN:C	2.49	0.50
1:A:115:ASN:HD21	1:A:464:GLN:HG2	1.77	0.50
1:A:565:ARG:HD3	1:A:567:PHE:CE1	2.47	0.50
1:A:94:GLY:N	1:A:222:THR:OG1	2.39	0.50
1:A:39:VAL:HG13	1:A:40:GLY:N	2.27	0.50
1:A:158:THR:HG23	1:A:158:THR:O	2.11	0.49
1:A:121:PHE:HB3	1:A:125:ASP:CB	2.42	0.49
1:A:379:TYR:CE1	1:A:390:GLU:HG2	2.48	0.49
1:A:55:LEU:HD12	1:A:55:LEU:N	2.27	0.49
1:A:113:ASP:O	1:A:195:LEU:HD13	2.11	0.49
1:A:515:ARG:HG3	1:A:515:ARG:NH1	2.27	0.49
1:A:82:ARG:HD2	1:A:212:LEU:HD13	1.95	0.49
1:A:407:LYS:O	1:A:408:GLN:HB2	2.13	0.49
1:A:216:ARG:NH1	1:A:216:ARG:HG2	2.27	0.49
1:A:440:PHE:C	1:A:440:PHE:CD1	2.85	0.49
1:A:43:THR:HB	1:A:261:GLU:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ASN:N	1:A:180:ASN:HD22	2.09	0.49
1:A:79:THR:CG2	1:A:80:TYR:H	2.15	0.49
1:A:346:TYR:HD1	1:A:351:PRO:HB3	1.76	0.49
1:A:297:THR:HG22	1:A:297:THR:O	2.12	0.49
1:A:310:ALA:O	1:A:311:ASN:C	2.51	0.49
1:A:111:LEU:HD21	1:A:113:ASP:HB2	1.95	0.49
1:A:392:GLU:HG2	1:A:567:PHE:HE2	1.78	0.48
1:A:62:ILE:HD11	1:A:133:MET:CE	2.43	0.48
1:A:158:THR:O	1:A:160:PRO:HD2	2.13	0.48
1:A:303:HIS:N	1:A:303:HIS:CD2	2.78	0.48
1:A:378:ASP:C	1:A:380:GLN:N	2.67	0.48
1:A:153:ILE:HG22	1:A:517:ILE:HB	1.96	0.48
1:A:130:SER:HB2	1:A:573:LEU:CD2	2.43	0.48
1:A:325:THR:HG22	1:A:326:GLU:N	2.28	0.48
1:A:102:HIS:HA	1:A:214:CYS:SG	2.53	0.48
1:A:115:ASN:ND2	1:A:464:GLN:HG3	2.29	0.48
1:A:85:VAL:O	1:A:101:ALA:HA	2.13	0.48
1:A:197:PHE:HB3	1:A:566:MET:CE	2.44	0.48
1:A:416:LEU:HB3	1:A:417:ASN:H	1.50	0.48
1:A:528:LEU:HG	1:A:530:PHE:CE2	2.49	0.48
1:A:559:THR:HB	1:A:563:GLY:H	1.78	0.48
1:A:392:GLU:HG3	1:A:393:ARG:N	2.29	0.48
1:A:549:THR:C	1:A:551:GLU:H	2.17	0.48
1:A:353:LEU:C	1:A:353:LEU:HD23	2.35	0.47
1:A:53:GLN:HB2	1:A:61:ARG:HB3	1.96	0.47
1:A:456:THR:CG2	1:A:457:ALA:N	2.76	0.47
1:A:360:ALA:HB2	1:A:398:PRO:O	2.14	0.47
1:A:212:LEU:HD21	1:A:242:ILE:HG13	1.97	0.47
1:A:48:ASN:HD21	1:A:68:ARG:HH21	1.60	0.47
1:A:384:LEU:HG	1:A:565:ARG:HG2	1.97	0.47
1:A:256:LEU:HD22	1:A:260:ASP:HB3	1.96	0.47
1:A:298:THR:HB	1:A:303:HIS:CE1	2.49	0.47
1:A:557:ILE:HG22	1:A:558:PRO:O	2.15	0.47
1:A:87:ASN:OD1	1:A:90:SER:HB2	2.15	0.47
1:A:468:LYS:HA	1:A:490:PRO:HG2	1.96	0.47
1:A:347:SER:O	1:A:349:GLY:N	2.48	0.47
1:A:223:TYR:CZ	1:A:226:GLN:HB3	2.50	0.46
1:A:209:ARG:HG2	1:A:209:ARG:O	2.15	0.46
1:A:274:LEU:CD1	1:A:483:PRO:HB2	2.44	0.46
1:A:506:PHE:HD2	1:A:506:PHE:C	2.19	0.46
1:A:200:TRP:HZ2	1:A:564:ILE:HD13	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:PHE:HA	1:A:461:PRO:HA	1.75	0.46
1:A:418:LEU:N	1:A:418:LEU:HD13	2.29	0.46
1:A:48:ASN:HD21	1:A:68:ARG:NH2	2.13	0.46
1:A:383:HIS:O	1:A:384:LEU:C	2.54	0.46
1:A:416:LEU:O	1:A:417:ASN:HB3	2.16	0.46
1:A:141:PHE:CZ	1:A:143:GLN:CG	2.99	0.46
1:A:466:TRP:HA	1:A:484:PHE:HB2	1.97	0.46
1:A:443:THR:O	1:A:443:THR:CG2	2.64	0.46
1:A:274:LEU:C	1:A:274:LEU:HD23	2.36	0.46
1:A:197:PHE:HB3	1:A:566:MET:HE2	1.97	0.46
1:A:136:ILE:HG12	1:A:137:ASN:N	2.29	0.46
1:A:173:LEU:HD12	1:A:174:MET:N	2.31	0.46
1:A:428:PRO:HA	1:A:441:MET:HE1	1.97	0.46
1:A:74:MET:CE	1:A:517:ILE:HA	2.44	0.46
1:A:74:MET:HB2	1:A:518:THR:O	2.16	0.46
1:A:440:PHE:N	1:A:441:MET:HE3	2.31	0.46
1:A:68:ARG:NH2	1:A:199:PRO:HG3	2.30	0.46
1:A:94:GLY:C	1:A:96:MET:H	2.19	0.46
1:A:334:GLN:HE22	1:A:446:THR:HB	1.80	0.46
1:A:359:THR:CG2	1:A:360:ALA:N	2.78	0.45
1:A:150:LEU:HD12	1:A:171:ALA:C	2.36	0.45
1:A:329:ALA:HB3	1:A:331:ARG:NH1	2.32	0.45
1:A:94:GLY:O	1:A:96:MET:N	2.49	0.45
1:A:489:ASN:HD22	1:A:490:PRO:CD	2.29	0.45
1:A:92:VAL:CG1	1:A:93:ALA:N	2.80	0.45
1:A:274:LEU:HD12	1:A:483:PRO:HB2	1.98	0.45
1:A:93:ALA:HA	1:A:222:THR:OG1	2.17	0.45
1:A:82:ARG:NH1	1:A:82:ARG:HB3	2.28	0.45
1:A:200:TRP:HE1	1:A:564:ILE:HD11	1.80	0.45
1:A:379:TYR:CE1	1:A:390:GLU:HA	2.40	0.45
1:A:339:THR:O	1:A:340:PRO:C	2.55	0.45
1:A:56:GLY:O	1:A:58:GLY:N	2.50	0.45
1:A:82:ARG:HH11	1:A:82:ARG:CB	2.28	0.44
1:A:280:TRP:CG	1:A:281:GLN:N	2.85	0.44
1:A:576:ARG:HG2	1:A:577:LYS:O	2.17	0.44
1:A:378:ASP:O	1:A:380:GLN:N	2.50	0.44
1:A:367:ASP:O	1:A:370:ASN:N	2.44	0.44
1:A:368:GLU:N	1:A:369:PRO:HD2	2.32	0.44
1:A:310:ALA:HB1	1:A:323:SER:CB	2.45	0.44
1:A:302:GLN:HB2	1:A:303:HIS:CD2	2.52	0.44
1:A:409:GLN:HB3	1:A:409:GLN:HE21	1.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ALA:C	1:A:190:PRO:HD2	2.38	0.44
1:A:138:LEU:HA	1:A:138:LEU:HD12	1.81	0.44
1:A:274:LEU:CD2	1:A:275:LYS:O	2.66	0.44
1:A:48:ASN:ND2	1:A:67:SER:N	2.62	0.44
1:A:393:ARG:CG	1:A:394:TYR:H	2.31	0.44
1:A:114:ALA:HB1	1:A:119:VAL:HG11	2.00	0.44
1:A:97:VAL:HG13	1:A:344:PHE:CZ	2.52	0.43
1:A:367:ASP:C	1:A:369:PRO:HD2	2.39	0.43
1:A:279:SER:HB2	1:A:578:LEU:HD12	2.00	0.43
1:A:405:ALA:O	1:A:408:GLN:HB2	2.18	0.43
1:A:68:ARG:HD3	1:A:196:GLY:O	2.18	0.43
1:A:392:GLU:HG3	1:A:393:ARG:H	1.84	0.43
1:A:300:GLY:C	1:A:302:GLN:H	2.22	0.43
1:A:101:ALA:HB1	1:A:234:ILE:HD12	1.99	0.43
1:A:390:GLU:C	1:A:391:LEU:HG	2.38	0.43
1:A:559:THR:C	1:A:561:ILE:H	2.21	0.43
1:A:558:PRO:HA	1:A:563:GLY:O	2.18	0.43
1:A:550:ALA:C	1:A:553:ILE:HD11	2.38	0.43
1:A:141:PHE:CZ	1:A:143:GLN:HG2	2.53	0.43
1:A:565:ARG:HD3	1:A:567:PHE:HE1	1.83	0.43
1:A:261:GLU:HG2	1:A:262:PHE:H	1.77	0.43
1:A:353:LEU:HD23	1:A:354:THR:N	2.33	0.43
1:A:56:GLY:C	1:A:58:GLY:H	2.22	0.43
1:A:384:LEU:HD21	1:A:565:ARG:NH1	2.34	0.43
1:A:455:ASN:OD1	1:A:456:THR:N	2.51	0.43
1:A:180:ASN:N	1:A:180:ASN:ND2	2.66	0.43
1:A:267:TYR:CD2	1:A:491:PRO:HB3	2.54	0.43
1:A:360:ALA:N	1:A:398:PRO:HG2	2.34	0.42
1:A:200:TRP:HE1	1:A:564:ILE:CD1	2.32	0.42
1:A:274:LEU:HD22	1:A:276:LEU:HD23	2.01	0.42
1:A:505:ASP:O	1:A:506:PHE:HD2	2.02	0.42
1:A:517:ILE:HG13	1:A:517:ILE:H	1.69	0.42
1:A:282:THR:O	1:A:285:SER:N	2.50	0.42
1:A:101:ALA:O	1:A:102:HIS:HB3	2.19	0.42
1:A:549:THR:HG23	1:A:552:ASN:ND2	2.34	0.42
1:A:258:THR:HG23	1:A:259:GLY:N	2.34	0.42
1:A:386:THR:O	1:A:387:SER:C	2.58	0.42
1:A:46:PHE:C	1:A:46:PHE:CD1	2.92	0.42
1:A:418:LEU:H	1:A:418:LEU:CD2	2.01	0.42
1:A:456:THR:CG2	1:A:457:ALA:H	2.31	0.42
1:A:391:LEU:N	1:A:391:LEU:HD23	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:THR:HG22	1:A:525:LYS:NZ	2.35	0.42
1:A:48:ASN:HD22	1:A:67:SER:N	1.99	0.42
1:A:502:LEU:HD13	1:A:507:ASN:ND2	2.35	0.42
1:A:278:HIS:HB2	1:A:400:SER:HA	2.01	0.42
1:A:116:ALA:HB3	1:A:194:THR:HG21	2.02	0.42
1:A:482:ALA:HB1	1:A:483:PRO:HD2	2.01	0.42
1:A:425:THR:HG22	1:A:427:LEU:CD1	2.50	0.42
1:A:338:ASN:HB2	1:A:444:LEU:HD13	2.02	0.42
1:A:267:TYR:CE2	1:A:491:PRO:HD3	2.55	0.42
1:A:345:GLU:O	1:A:351:PRO:HA	2.21	0.41
1:A:111:LEU:CD2	1:A:113:ASP:HB2	2.50	0.41
1:A:156:SER:C	1:A:158:THR:H	2.23	0.41
1:A:138:LEU:HD13	1:A:530:PHE:CE1	2.55	0.41
1:A:280:TRP:O	1:A:281:GLN:C	2.58	0.41
1:A:109:TRP:CD1	1:A:247:ILE:HG13	2.55	0.41
1:A:559:THR:HG23	1:A:560:ASN:N	2.34	0.41
1:A:86:LEU:HA	1:A:86:LEU:HD23	1.90	0.41
1:A:453:LEU:CG	1:A:454:ASN:N	2.84	0.41
1:A:96:MET:H	1:A:96:MET:HG3	1.69	0.41
1:A:394:TYR:CD2	1:A:568:PRO:HG3	2.56	0.41
1:A:489:ASN:ND2	1:A:490:PRO:HD2	2.36	0.41
1:A:346:TYR:CE1	1:A:351:PRO:HD3	2.55	0.41
1:A:138:LEU:HG	1:A:269:PHE:CD1	2.56	0.41
1:A:549:THR:C	1:A:551:GLU:N	2.72	0.41
1:A:498:ILE:CD1	1:A:519:TYR:HA	2.50	0.41
1:A:246:THR:CG2	1:A:248:GLU:HB2	2.51	0.41
1:A:394:TYR:CE1	1:A:568:PRO:HG3	2.55	0.41
1:A:43:THR:HG21	1:A:260:ASP:O	2.21	0.41
1:A:421:THR:O	1:A:422:ASN:C	2.57	0.41
1:A:300:GLY:C	1:A:302:GLN:N	2.74	0.41
1:A:115:ASN:HD21	1:A:464:GLN:CG	2.33	0.41
1:A:138:LEU:HG	1:A:269:PHE:CE1	2.56	0.41
1:A:189:ALA:N	1:A:190:PRO:HD2	2.36	0.41
1:A:238:LEU:HA	1:A:238:LEU:HD23	1.95	0.41
1:A:275:LYS:HD2	1:A:576:ARG:NH1	2.36	0.41
1:A:317:HIS:CD2	1:A:319:THR:OG1	2.74	0.41
1:A:382:GLY:O	1:A:383:HIS:HB3	2.21	0.40
1:A:219:ASN:HA	1:A:220:PRO:HA	1.72	0.40
1:A:359:THR:HG22	1:A:403:GLY:H	1.82	0.40
1:A:366:ASP:HB3	1:A:369:PRO:CG	2.51	0.40
1:A:513:GLN:HG3	1:A:513:GLN:H	1.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:LYS:HE3	1:A:577:LYS:HB2	1.68	0.40
1:A:427:LEU:CB	1:A:428:PRO:CD	2.99	0.40
1:A:183:LEU:HD12	1:A:495:PHE:CZ	2.54	0.40
1:A:141:PHE:HA	1:A:527:THR:O	2.21	0.40
1:A:468:LYS:HA	1:A:490:PRO:CG	2.51	0.40
1:A:364:TYR:O	1:A:366:ASP:N	2.54	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	540/579 (93%)	425 (79%)	78 (14%)	37 (7%)	1 18

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	SER
1	A	224	THR
1	A	226	GLN
1	A	237	GLY
1	A	310	ALA
1	A	311	ASN
1	A	348	ASN
1	A	387	SER
1	A	403	GLY
1	A	408	GLN
1	A	414	ALA
1	A	419	GLU
1	A	420	ASN
1	A	506	PHE
1	A	511	PRO

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Mol	Chain	Res	Type
1	A	57	GLU
1	A	78	GLU
1	A	95	GLN
1	A	365	ASN
1	A	391	LEU
1	A	157	ALA
1	A	379	TYR
1	A	383	HIS
1	A	384	LEU
1	A	417	ASN
1	A	456	THR
1	A	322	ASN
1	A	337	TYR
1	A	367	ASP
1	A	394	TYR
1	A	502	LEU
1	A	102	HIS
1	A	161	PRO
1	A	312	THR
1	A	340	PRO
1	A	508	ALA
1	A	377	MET

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	480/501 (96%)	422 (88%)	58 (12%)	6 30

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	THR
1	A	73	ASN
1	A	105	MET
1	A	131	ASN

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Mol	Chain	Res	Type
1	A	138	LEU
1	A	152	THR
1	A	159	SER
1	A	172	SER
1	A	209	ARG
1	A	220	PRO
1	A	236	THR
1	A	242	ILE
1	A	247	ILE
1	A	282	THR
1	A	285	SER
1	A	292	LEU
1	A	293	LEU
1	A	298	THR
1	A	304	PRO
1	A	311	ASN
1	A	312	THR
1	A	314	LYS
1	A	317	HIS
1	A	321	ASN
1	A	339	THR
1	A	341	TYR
1	A	356	ILE
1	A	362	THR
1	A	363	GLN
1	A	364	TYR
1	A	365	ASN
1	A	376	THR
1	A	385	THR
1	A	387	SER
1	A	391	LEU
1	A	393	ARG
1	A	394	TYR
1	A	408	GLN
1	A	409	GLN
1	A	413	GLN
1	A	416	LEU
1	A	418	LEU
1	A	440	PHE
1	A	441	MET
1	A	444	LEU
1	A	454	ASN

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Mol	Chain	Res	Type
1	A	461	PRO
1	A	506	PHE
1	A	512	GLN
1	A	513	GLN
1	A	515	ARG
1	A	531	THR
1	A	538	ASN
1	A	553	ILE
1	A	559	THR
1	A	566	MET
1	A	573	LEU
1	A	578	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	49	GLN
1	A	73	ASN
1	A	147	ASN
1	A	180	ASN
1	A	303	HIS
1	A	317	HIS
1	A	321	ASN
1	A	380	GLN
1	A	408	GLN
1	A	409	GLN
1	A	412	GLN
1	A	454	ASN
1	A	462	ASN
1	A	489	ASN
1	A	493	GLN
1	A	513	GLN
1	A	541	ASN
1	A	544	GLN
1	A	555	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

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.