



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:22 AM UTC

PDB ID : 6VGR / pdb_00006vgr
Title : Crystal Structure of Human Dipeptidase 3 in Complex with Fab of SC-003
Authors : Hayashi, K.; Longenecker, K.L.; Vivona, S.
Deposited on : 2020-01-08
Resolution : 2.84 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

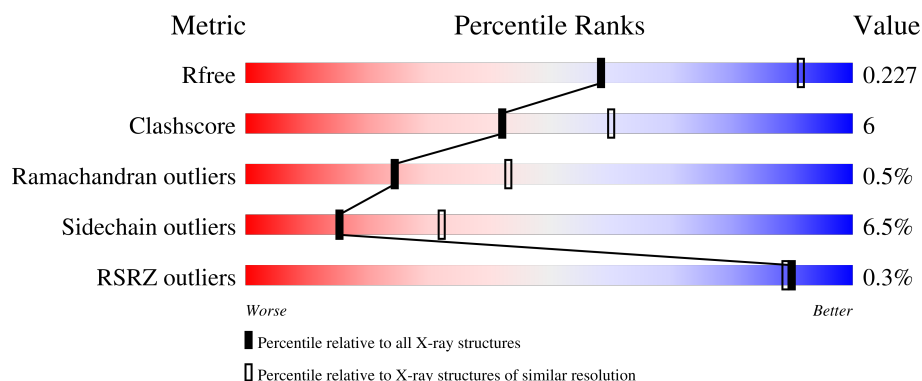
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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}	180053	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	488	59% 12% • 28%
1	B	488	60% 11% • 28%
2	C	226	% 66% 27% • •
2	H	226	81% 14% • •
3	D	215	71% 27% •

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Mol	Chain	Length	Quality of chain
3	L	215	80% 17% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12272 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 Dipeptidase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2732	1712	485	522	13			
1	B	350	Total	C	N	O	S	0	0	0
			2732	1712	485	522	13			

- Molecule 2 is a protein called SC-003 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	217	Total	C	N	O	S	0	0	0
			1642	1041	271	324	6			
2	H	217	Total	C	N	O	S	0	0	0
			1642	1041	271	324	6			

- Molecule 3 is a protein called SC-003 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	214	Total	C	N	O	S	0	0	0
			1661	1045	279	333	4			
3	L	214	Total	C	N	O	S	0	0	0
			1661	1045	279	333	4			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	58	Total	O	0	0
			58	58		
4	B	53	Total	O	0	0
			53	53		
4	C	14	Total	O	0	0
			14	14		
4	D	15	Total	O	0	0
			15	15		

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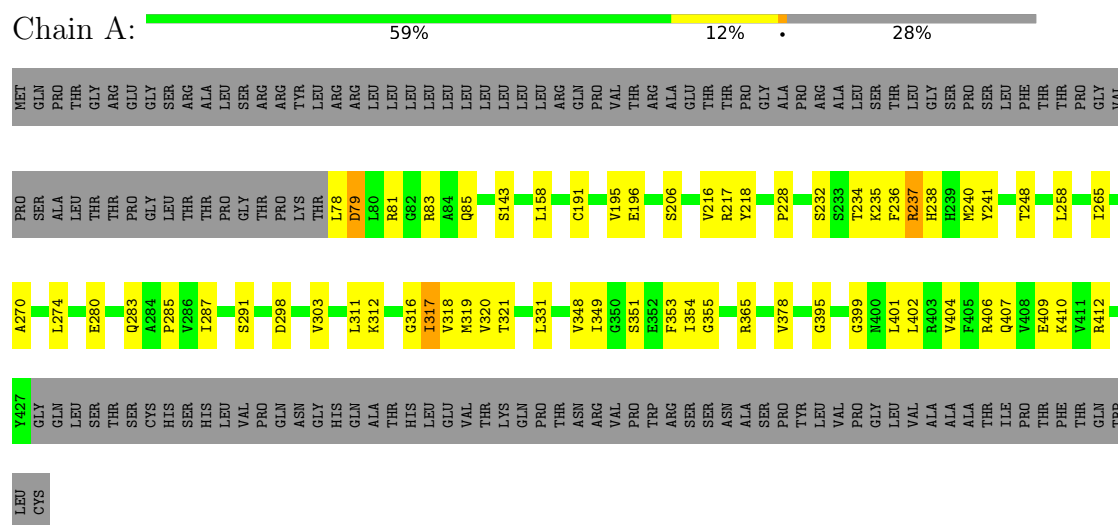
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	21	Total	O	0	0
			21	21		
4	L	41	Total	O	0	0
			41	41		

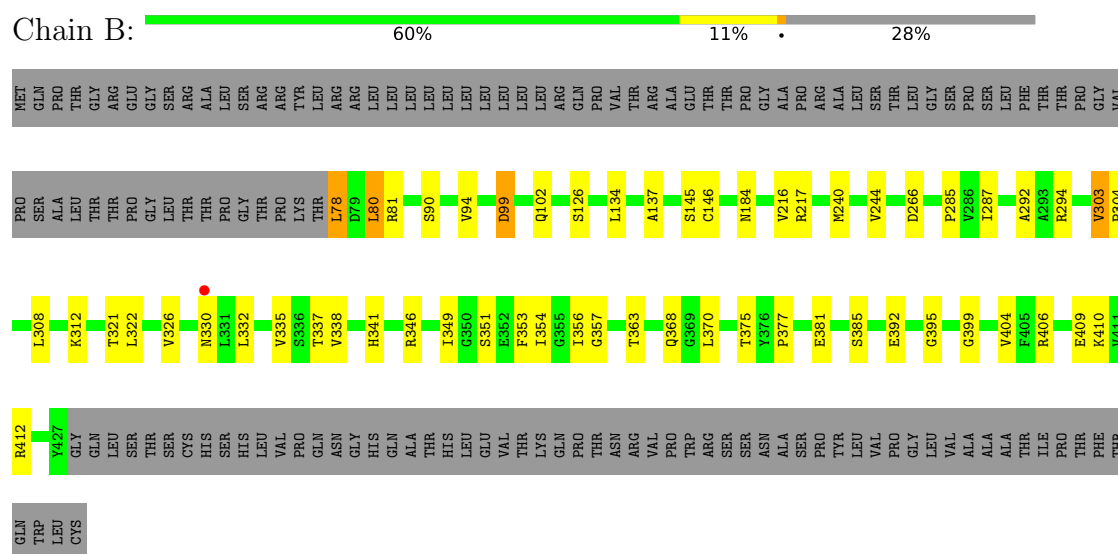
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

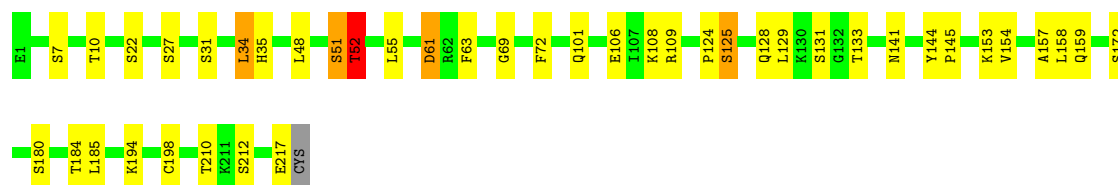
• Molecule 1: Dipeptidase 3



• Molecule 1: Dipeptidase 3



• Molecule 2: SC-003 Fab Heavy Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	167.03Å 167.03Å 116.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.12 – 2.84 40.12 – 2.84	Depositor EDS
% Data completeness (in resolution range)	96.2 (40.12-2.84) 96.2 (40.12-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.58 (at 2.82Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.190 , 0.248 (Not available) , 0.227	Depositor DCC
R_{free} test set	2073 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	71.0	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.024 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12272	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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

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	0.82	1/2777 (0.0%)	1.17	3/3760 (0.1%)
1	B	0.81	0/2777	1.17	2/3760 (0.1%)
2	C	0.75	0/1685	1.15	8/2299 (0.3%)
2	H	0.80	0/1685	1.08	6/2299 (0.3%)
3	D	0.75	0/1701	1.16	5/2313 (0.2%)
3	L	0.81	0/1701	1.09	4/2313 (0.2%)
All	All	0.79	1/12326 (0.0%)	1.14	28/16744 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	CYS	CA-C	-5.16	1.46	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	122	SER	CA-C-N	6.04	130.05	121.42
2	C	122	SER	C-N-CA	6.04	130.05	121.42
2	H	184	GLY	N-CA-C	-6.03	106.83	115.64
3	L	51	SER	CA-C-N	5.93	132.86	121.54
3	L	51	SER	C-N-CA	5.93	132.86	121.54
2	C	123	SER	CA-C-N	5.92	132.36	121.70
2	C	123	SER	C-N-CA	5.92	132.36	121.70
2	H	194	VAL	N-CA-CB	-5.87	107.78	111.83
1	B	330	ASN	CA-CB-CG	5.86	118.46	112.60
2	H	54	GLY	CA-C-N	5.76	128.79	120.38
2	H	54	GLY	C-N-CA	5.76	128.79	120.38
3	L	61	ASP	CA-CB-CG	5.59	118.19	112.60
2	C	182	SER	CA-C-N	5.48	128.38	120.38
2	C	182	SER	C-N-CA	5.48	128.38	120.38
1	B	303	VAL	N-CA-C	5.41	113.83	107.77
3	L	141	ASN	N-CA-C	5.29	117.59	109.07
1	A	79	ASP	N-CA-C	-5.26	106.70	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	221	VAL	N-CA-CB	5.22	118.92	111.82
2	H	181	GLN	CA-C-N	5.22	127.28	120.28
2	H	181	GLN	C-N-CA	5.22	127.28	120.28
3	D	130	LYS	CA-C-N	5.21	127.79	120.28
3	D	130	LYS	C-N-CA	5.21	127.79	120.28
2	C	90	ASP	CA-CB-CG	5.19	117.79	112.60
3	D	80	SER	N-CA-C	5.14	117.67	111.40
1	A	280	GLU	CA-C-N	5.10	127.66	120.42
1	A	280	GLU	C-N-CA	5.10	127.66	120.42
3	D	84	PRO	CA-C-N	5.09	127.61	120.28
3	D	84	PRO	C-N-CA	5.09	127.61	120.28

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	2732	0	2718	35	0
1	B	2732	0	2718	23	0
2	C	1642	0	1587	35	0
2	H	1642	0	1587	12	0
3	D	1661	0	1608	33	0
3	L	1661	0	1608	16	0
4	A	58	0	0	0	0
4	B	53	0	0	0	0
4	C	14	0	0	0	0
4	D	15	0	0	0	0
4	H	21	0	0	0	0
4	L	41	0	0	1	0
All	All	12272	0	11826	149	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 6.

All (149) 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)
3:D:124:PRO:HD3	3:D:136:VAL:HG12	1.52	0.90
2:C:191:VAL:HG11	3:D:139:LEU:HD11	1.57	0.84
3:D:4:LEU:HD21	3:D:92:CYS:SG	2.23	0.78
3:D:136:VAL:HG22	3:D:183:LEU:HB3	1.66	0.76
3:L:34:LEU:HB3	3:L:52:THR:HG22	1.72	0.71
1:A:283:GLN:HB3	3:D:97:ARG:HH12	1.56	0.71
3:D:153:LYS:NZ	3:D:199:GLU:HB2	2.07	0.68
3:L:31:SER:O	3:L:52:THR:HG23	1.93	0.68
3:D:187:LYS:HE2	3:D:191:GLU:HG3	1.75	0.68
2:H:203:THR:HG23	2:H:220:LYS:HE3	1.75	0.67
3:L:124:PRO:HB2	3:L:129:LEU:HD21	1.76	0.66
3:D:40:TYR:HD2	3:D:50:LEU:HA	1.61	0.65
2:C:36:TRP:CE2	2:C:81:MET:HB2	2.32	0.65
2:C:134:LEU:HB3	3:D:122:PHE:CD1	2.33	0.62
2:H:136:PRO:HG3	2:H:148:LEU:HB3	1.81	0.62
1:A:195:VAL:HG23	1:A:216:VAL:HG11	1.82	0.61
1:A:258:LEU:HD13	1:A:265:ILE:HG12	1.83	0.61
1:A:81:ARG:HE	1:A:85:GLN:NE2	1.99	0.61
2:C:199:LEU:HD12	2:C:223:PRO:HB3	1.82	0.60
1:A:283:GLN:HB3	3:D:97:ARG:NH1	2.17	0.60
1:B:395:GLY:HA2	1:B:399:GLY:HA3	1.84	0.60
3:D:198:CYS:O	3:D:210:THR:HA	2.02	0.59
2:C:156:PHE:HB2	2:C:185:LEU:HD23	1.84	0.59
3:D:40:TYR:CD2	3:D:50:LEU:HA	2.39	0.58
3:L:194:LYS:HG2	4:L:308:HOH:O	2.03	0.58
1:B:184:ASN:ND2	1:B:406:ARG:HH22	2.02	0.58
3:D:140:LEU:HD21	3:D:200:VAL:HG21	1.85	0.58
1:A:237:ARG:HH11	1:A:237:ARG:HA	1.68	0.58
2:C:194:VAL:HG22	2:C:195:PRO:HD2	1.87	0.57
1:B:78:LEU:HD22	1:B:80:LEU:HB2	1.87	0.57
2:C:149:GLY:HA2	2:C:191:VAL:HA	1.87	0.57
1:B:346:ARG:HD2	1:B:392:GLU:OE2	2.06	0.56
3:D:15:PRO:HD3	3:D:110:ILE:HG23	1.87	0.56
1:A:287:ILE:HG22	1:A:317:ILE:HG22	1.88	0.56
3:L:34:LEU:HD22	3:L:72:PHE:CG	2.41	0.56
1:B:322:LEU:HD22	1:B:338:VAL:HG11	1.89	0.55
1:B:335:VAL:HG23	1:B:370:LEU:HD11	1.88	0.55
2:C:10:GLU:HB2	2:C:119:VAL:HG22	1.87	0.55
2:C:210:HIS:CE1	2:C:212:PRO:HG2	2.42	0.55
3:L:144:TYR:CD1	3:L:145:PRO:HA	2.42	0.55
2:C:173:VAL:HG22	2:C:192:VAL:HG22	1.87	0.55
1:A:331:LEU:H	1:A:331:LEU:HD23	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:38:HIS:CE1	3:D:54:SER:H	2.25	0.54
2:H:173:VAL:HG22	2:H:192:VAL:HB	1.90	0.53
3:D:146:ARG:HD2	3:D:177:TYR:CE2	2.44	0.53
2:C:158:GLU:HG2	2:C:159:PRO:HA	1.89	0.53
3:L:154:VAL:HG12	3:L:159:GLN:NE2	2.23	0.53
3:L:35:HIS:CE1	3:L:51:SER:H	2.26	0.53
3:D:4:LEU:HD21	3:D:23:CYS:SG	2.48	0.52
3:D:153:LYS:HZ1	3:D:199:GLU:HB2	1.72	0.52
3:D:70:GLY:HA3	3:D:75:PHE:HA	1.92	0.52
2:C:13:LYS:HA	2:C:122:SER:HB2	1.90	0.52
1:A:238:HIS:HB3	1:A:240:MET:CE	2.39	0.52
1:A:395:GLY:HA2	1:A:399:GLY:HA3	1.92	0.51
3:D:189:ASP:HA	3:D:192:LYS:HE2	1.92	0.51
1:B:134:LEU:HD12	1:B:377:PRO:HG3	1.91	0.51
3:D:165:GLU:HG2	3:D:179:LEU:HD21	1.93	0.51
1:B:294:ARG:NH1	1:B:304:PRO:HG3	2.24	0.51
2:C:81:MET:HE1	2:C:83:LEU:HB2	1.93	0.51
1:B:94:VAL:HG22	1:B:137:ALA:HB3	1.92	0.50
2:C:36:TRP:CZ3	2:C:96:CYS:HB3	2.46	0.50
1:B:312:LYS:HG3	1:B:353:PHE:CZ	2.46	0.50
1:B:146:CYS:O	1:B:240:MET:HE1	2.12	0.50
2:C:129:PRO:HB2	2:C:152:VAL:CG1	2.42	0.50
1:A:79:ASP:O	1:A:83:ARG:HG3	2.12	0.50
3:D:87:PHE:CD1	3:D:110:ILE:HG13	2.46	0.49
2:C:61:ASN:HB3	2:C:64:PHE:HE2	1.77	0.49
1:B:285:PRO:HB2	1:B:404:VAL:HG13	1.94	0.49
3:D:155:ASP:HA	3:D:195:VAL:HG12	1.95	0.49
1:B:308:LEU:HB3	1:B:349:ILE:HD13	1.94	0.49
1:A:285:PRO:HB2	1:A:404:VAL:HG13	1.95	0.49
1:A:351:SER:HA	1:A:354:ILE:HD12	1.93	0.48
2:C:73:ASP:CG	2:C:76:THR:HG22	2.38	0.48
2:C:107:PRO:HG3	3:D:53:TYR:CZ	2.48	0.48
3:L:48:LEU:HD21	3:L:63:PHE:CD1	2.49	0.48
3:L:125:SER:O	3:L:129:LEU:HG	2.14	0.48
1:A:238:HIS:HB3	1:A:240:MET:HE2	1.95	0.48
1:A:234:THR:O	1:A:237:ARG:HB2	2.14	0.48
1:A:195:VAL:HG23	1:A:216:VAL:CG1	2.44	0.47
3:D:153:LYS:HZ3	3:D:199:GLU:HB2	1.78	0.47
1:B:351:SER:HA	1:B:354:ILE:HD12	1.96	0.47
2:C:162:VAL:HG12	2:C:208:VAL:HG22	1.95	0.47
2:C:194:VAL:CG2	2:C:195:PRO:HD2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:36:TRP:CE2	2:H:81:MET:HB2	2.49	0.47
1:A:348:VAL:HG12	1:A:349:ILE:HG23	1.96	0.47
2:C:219:LYS:HD3	2:C:220:LYS:N	2.30	0.47
3:L:198:CYS:O	3:L:210:THR:HA	2.15	0.47
3:D:150:VAL:HG22	3:D:200:VAL:HG22	1.97	0.47
2:C:86:LEU:HD22	2:C:121:VAL:HG21	1.98	0.46
2:H:91:THR:HG23	2:H:120:THR:HA	1.98	0.46
1:A:401:LEU:C	1:A:401:LEU:HD13	2.41	0.46
2:H:164:TRP:CH2	2:H:206:CYS:HB3	2.51	0.46
1:A:237:ARG:HG3	1:A:237:ARG:NH1	2.31	0.45
3:D:136:VAL:CG2	3:D:183:LEU:HB3	2.40	0.45
1:A:217:ARG:HD3	1:A:217:ARG:HA	1.78	0.45
2:C:64:PHE:CD2	2:C:64:PHE:N	2.85	0.45
1:B:81:ARG:HD2	1:B:381:GLU:OE1	2.16	0.45
3:D:2:ILE:HD13	3:D:29:VAL:HG22	1.99	0.45
1:A:311:LEU:HD11	1:A:316:GLY:HA3	1.98	0.44
1:A:402:LEU:O	1:A:406:ARG:HG3	2.18	0.44
1:A:409:GLU:O	1:A:412:ARG:HB3	2.17	0.44
2:C:213:SER:C	2:C:215:THR:H	2.26	0.44
2:H:164:TRP:CZ3	2:H:206:CYS:HB3	2.52	0.44
1:A:237:ARG:HB3	1:A:238:HIS:ND1	2.32	0.44
1:A:407:GLN:OE1	1:A:410:LYS:HD3	2.18	0.44
1:B:321:THR:HA	1:B:357:GLY:O	2.17	0.44
2:H:60:TYR:HE1	2:H:70:ILE:HG13	1.83	0.44
1:A:235:LYS:HE3	1:A:236:PHE:CE2	2.52	0.44
3:L:128:GLN:HG2	3:L:133:THR:O	2.18	0.43
1:B:370:LEU:HA	1:B:375:THR:OG1	2.18	0.43
2:C:121:VAL:HG12	2:C:122:SER:HB3	2.00	0.43
2:C:194:VAL:HG11	2:C:204:TYR:CE2	2.53	0.43
1:B:216:VAL:O	1:B:217:ARG:HD3	2.18	0.43
1:A:270:ALA:HB1	1:A:274:LEU:HD23	1.99	0.43
2:H:6:GLN:HA	2:H:21:SER:O	2.18	0.43
2:C:134:LEU:HB2	2:C:148:LEU:O	2.19	0.43
2:C:6:GLN:HA	2:C:21:SER:O	2.19	0.43
2:H:158:GLU:HG2	2:H:159:PRO:HA	2.01	0.43
2:H:196:SER:HA	2:H:199:LEU:CD1	2.49	0.43
3:D:124:PRO:HD3	3:D:136:VAL:CG1	2.37	0.42
3:L:55:LEU:HD11	3:L:61:ASP:HA	2.00	0.42
1:A:143:SER:HA	1:A:196:GLU:HB3	2.00	0.42
1:A:158:LEU:HD23	1:A:158:LEU:HA	1.87	0.42
1:B:99:ASP:CG	1:B:102:GLN:HE21	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:88:SER:HA	2:C:121:VAL:O	2.19	0.42
2:C:129:PRO:HB2	2:C:152:VAL:HG13	2.01	0.42
3:D:24:THR:HA	3:D:73:THR:O	2.19	0.42
2:C:148:LEU:HD21	2:C:194:VAL:HG12	2.02	0.42
1:B:409:GLU:O	1:B:412:ARG:HB3	2.20	0.42
1:A:237:ARG:HH11	1:A:237:ARG:HG3	1.85	0.41
1:A:291:SER:O	1:A:320:VAL:HA	2.20	0.41
1:A:317:ILE:HG12	1:A:318:VAL:N	2.35	0.41
2:C:126:THR:HA	2:C:156:PHE:O	2.19	0.41
3:L:108:LYS:HA	3:L:144:TYR:OH	2.19	0.41
2:C:178:ALA:HB2	2:C:188:LEU:HD23	2.02	0.41
3:D:128:GLN:HG2	3:D:133:THR:O	2.20	0.41
1:A:319:MET:HA	1:A:355:GLY:C	2.45	0.41
1:B:266:ASP:HA	1:B:287:ILE:HG13	2.01	0.41
1:B:292:ALA:HB1	1:B:341:HIS:ND1	2.35	0.41
2:C:126:THR:HG22	2:C:157:PRO:HD3	2.03	0.41
3:L:153:LYS:HA	3:L:157:ALA:O	2.20	0.41
1:A:228:PRO:HG3	1:A:241:TYR:CZ	2.56	0.41
1:A:312:LYS:HG3	1:A:353:PHE:CZ	2.56	0.41
3:D:37:LEU:HA	3:D:93:HIS:O	2.20	0.41
3:L:109:ARG:HG3	3:L:144:TYR:CD2	2.56	0.41
1:B:78:LEU:HD22	1:B:80:LEU:H	1.86	0.40
2:C:91:THR:HA	2:C:119:VAL:O	2.22	0.40
3:D:21:LEU:HG	3:D:106:THR:HG21	2.04	0.40
2:H:64:PHE:CD1	2:H:64:PHE:N	2.89	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	348/488 (71%)	326 (94%)	21 (6%)	1 (0%)	36 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	348/488 (71%)	330 (95%)	18 (5%)	0	100	100
2	C	213/226 (94%)	198 (93%)	14 (7%)	1 (0%)	24	43
2	H	213/226 (94%)	205 (96%)	7 (3%)	1 (0%)	24	43
3	D	212/215 (99%)	198 (93%)	12 (6%)	2 (1%)	14	27
3	L	212/215 (99%)	204 (96%)	6 (3%)	2 (1%)	14	27
All	All	1546/1858 (83%)	1461 (94%)	78 (5%)	7 (0%)	24	43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	154	ASP
3	L	52	THR
3	D	170	GLN
2	H	66	ASP
1	A	298	ASP
3	D	72	GLY
3	L	69	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	305/423 (72%)	294 (96%)	11 (4%)	31	56
1	B	305/423 (72%)	289 (95%)	16 (5%)	21	43
2	C	181/190 (95%)	162 (90%)	19 (10%)	6	14
2	H	181/190 (95%)	170 (94%)	11 (6%)	17	35
3	D	189/190 (100%)	175 (93%)	14 (7%)	13	27
3	L	189/190 (100%)	172 (91%)	17 (9%)	9	20
All	All	1350/1606 (84%)	1262 (94%)	88 (6%)	15	32

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LEU
1	A	206	SER
1	A	218	TYR
1	A	232	SER
1	A	237	ARG
1	A	248	THR
1	A	303	VAL
1	A	317	ILE
1	A	321	THR
1	A	365	ARG
1	A	378	VAL
1	B	78	LEU
1	B	80	LEU
1	B	90	SER
1	B	99	ASP
1	B	126	SER
1	B	145	SER
1	B	244	VAL
1	B	303	VAL
1	B	326	VAL
1	B	332	LEU
1	B	337	THR
1	B	356	ILE
1	B	363	THR
1	B	368	GLN
1	B	385	SER
1	B	410	LYS
2	C	62	GLU
2	C	63	ARG
2	C	64	PHE
2	C	65	LYS
2	C	67	ARG
2	C	81	MET
2	C	88	SER
2	C	93	VAL
2	C	98	ARG
2	C	99	ARG
2	C	130	SER
2	C	148	LEU
2	C	150	CYS
2	C	166	SER
2	C	169	LEU
2	C	201	THR

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Mol	Chain	Res	Type
2	C	203	THR
2	C	218	ASP
2	C	220	LYS
3	D	12	SER
3	D	18	ARG
3	D	60	SER
3	D	67	SER
3	D	78	THR
3	D	79	ILE
3	D	86	ASP
3	D	97	ARG
3	D	119	VAL
3	D	130	LYS
3	D	198	CYS
3	D	203	GLN
3	D	206	SER
3	D	207	SER
2	H	28	THR
2	H	62	GLU
2	H	64	PHE
2	H	84	SER
2	H	99	ARG
2	H	105	SER
2	H	120	THR
2	H	158	GLU
2	H	183	SER
2	H	197	SER
2	H	202	GLN
3	L	7	SER
3	L	10	THR
3	L	22	SER
3	L	27	SER
3	L	34	LEU
3	L	52	THR
3	L	101	GLN
3	L	106	GLU
3	L	125	SER
3	L	131	SER
3	L	158	LEU
3	L	172	SER
3	L	180	SER
3	L	184	THR

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Mol	Chain	Res	Type
3	L	185	LEU
3	L	212	SER
3	L	217	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	138	GLN
1	A	239	HIS
1	A	400	ASN
1	B	116	ASN
1	B	138	GLN
1	B	151	GLN
1	B	239	HIS
1	B	407	GLN
2	C	181	GLN
2	C	209	ASN
3	D	104	GLN
3	D	159	GLN
2	H	39	GLN
3	L	39	GLN
3	L	54	ASN
3	L	151	GLN
3	L	164	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 oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	350/488 (71%)	-0.57	0 100 100	47, 67, 86, 113	0
1	B	350/488 (71%)	-0.61	1 (0%) 90 89	47, 67, 91, 112	0
2	C	217/226 (96%)	0.08	2 (0%) 81 76	67, 107, 155, 170	0
2	H	217/226 (96%)	-0.48	1 (0%) 87 85	49, 75, 100, 111	0
3	D	214/215 (99%)	0.10	0 100 100	74, 103, 131, 153	0
3	L	214/215 (99%)	-0.57	0 100 100	49, 68, 96, 127	0
All	All	1562/1858 (84%)	-0.38	4 (0%) 90 89	47, 75, 130, 170	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	137	SER	3.2
2	C	137	SER	2.8
2	C	79	ALA	2.8
1	B	330	ASN	2.6

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 oligosaccharides 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.