



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:21 PM UTC

PDB ID : 1W52 / pdb_00001w52
Title : Crystal structure of a proteolyzed form of pancreatic lipase related protein 2 from horse
Authors : Mancheno, J.M.; Jayne, S.; Kerfelec, B.; Chapus, C.; Crenon, I.; Hermoso, J.A.
Deposited on : 2004-08-04
Resolution : 2.99 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
Mogul : 2022.3.0, CSD as543be (2022)
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

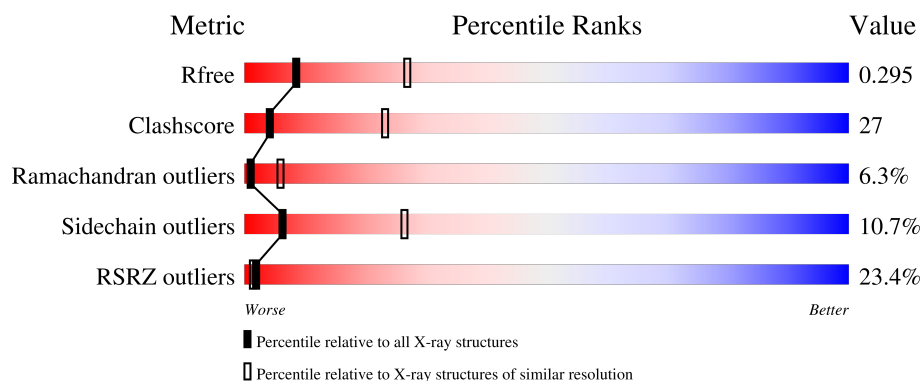
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 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	X	452	23% 50% 38% 10% ..

2 Entry composition [i](#)

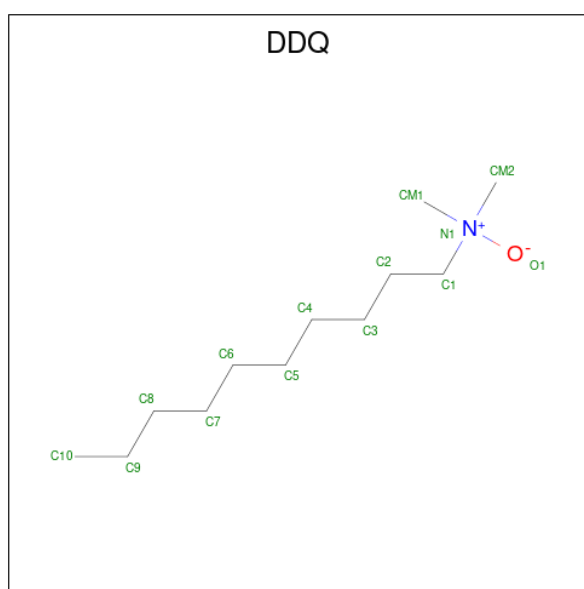
There are 3 unique types of molecules in this entry. The entry contains 3524 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PANCREATIC LIPASE RELATED PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	448	Total	C	N	O	S	0	0	0
			3494	2199	595	681	19			

- Molecule 2 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (CCD ID: DDQ) (formula: $C_{12}H_{27}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	X	1	Total	C	N	O	0	0
			14	12	1	1		
2	X	1	Total	C	N	O	0	0
			14	12	1	1		

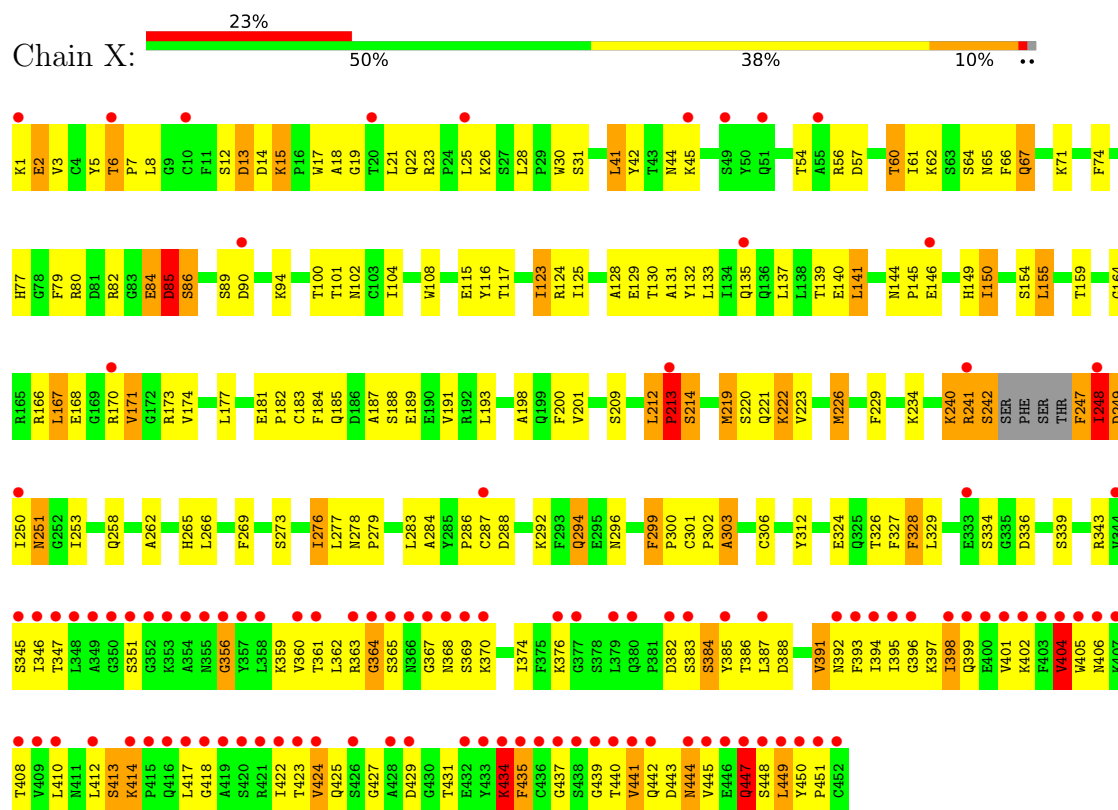
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	X	2	Total	Ca	0	0
			2	2		

3 Residue-property plots [i](#)

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: PANCREATIC LIPASE RELATED PROTEIN 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.43Å 128.43Å 85.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.17 – 2.99 26.17 – 2.99	Depositor EDS
% Data completeness (in resolution range)	100.0 (26.17-2.99) 99.8 (26.17-2.99)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.54 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.231 , 0.294 0.240 , 0.295	Depositor DCC
R_{free} test set	847 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	3524	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	X	1.20	13/3579 (0.4%)	1.28	11/4848 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	0	2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	404	VAL	C-N	-10.45	1.20	1.33
1	X	241	ARG	CA-C	6.75	1.61	1.52
1	X	248	ILE	CA-CB	6.30	1.63	1.54
1	X	328	PHE	C-O	-6.13	1.16	1.23
1	X	150	ILE	CA-CB	-5.87	1.47	1.54
1	X	391	VAL	CA-CB	5.80	1.60	1.53
1	X	299	PHE	CA-C	5.49	1.57	1.52
1	X	336	ASP	CA-C	5.46	1.59	1.52
1	X	226	MET	SD-CE	-5.38	1.66	1.79
1	X	219	MET	SD-CE	-5.35	1.66	1.79
1	X	276	ILE	CA-CB	-5.21	1.48	1.54
1	X	441	VAL	CA-CB	5.15	1.59	1.54
1	X	213	PRO	CB-CG	5.09	1.75	1.49

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	137	LEU	N-CA-C	-9.96	101.63	113.88
1	X	85	ASP	O-C-N	-8.75	110.95	122.59
1	X	334	SER	N-CA-C	8.36	120.84	108.14
1	X	356	GLY	N-CA-C	7.91	122.58	110.88
1	X	404	VAL	O-C-N	-7.65	113.01	122.57
1	X	189	GLU	N-CA-C	-6.28	104.88	112.54
1	X	213	PRO	CA-C-O	-6.25	109.23	120.60
1	X	253	ILE	N-CA-C	-5.50	107.44	111.90
1	X	132	TYR	N-CA-C	5.43	117.62	111.11
1	X	286	PRO	CA-C-O	-5.36	115.33	121.86
1	X	2	GLU	N-CA-C	5.06	116.47	110.19

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	212	LEU	Peptide
1	X	85	ASP	Mainchain

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	X	3494	0	3343	188	0
2	X	28	0	54	1	0
3	X	2	0	0	0	0
All	All	3524	0	3397	189	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 27.

All (189) 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:X:213:PRO:CB	1:X:213:PRO:CG	1.75	1.49
1:X:84:GLU:O	1:X:85:ASP:HB2	1.34	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:423:THR:HG23	1:X:434:LYS:HD3	1.45	0.96
1:X:115:GLU:OE1	1:X:117:THR:HB	1.69	0.91
1:X:17:TRP:CE3	1:X:124:ARG:HD3	2.14	0.83
1:X:84:GLU:O	1:X:85:ASP:CB	2.17	0.79
1:X:345:SER:CB	1:X:386:THR:HG22	2.15	0.77
1:X:167:LEU:N	1:X:167:LEU:HD23	2.00	0.77
1:X:399:GLN:HA	1:X:435:PHE:HE1	1.48	0.76
1:X:361:THR:O	1:X:362:LEU:HD23	1.86	0.76
1:X:346:ILE:HG12	1:X:422:ILE:HG12	1.66	0.76
1:X:94:LYS:HE2	1:X:273:SER:OG	1.85	0.76
1:X:222:LYS:NZ	1:X:326:THR:HG21	2.02	0.74
1:X:6:THR:HB	1:X:7:PRO:HD3	1.69	0.74
1:X:144:ASN:ND2	1:X:146:GLU:HG2	2.04	0.73
1:X:345:SER:OG	1:X:386:THR:HG22	1.89	0.73
1:X:276:ILE:HG22	1:X:277:LEU:HD23	1.70	0.71
1:X:54:THR:HG22	1:X:56:ARG:H	1.56	0.71
1:X:212:LEU:HB3	1:X:213:PRO:HD2	1.71	0.70
1:X:398:ILE:HD12	1:X:424:VAL:HG11	1.73	0.70
1:X:447:GLN:HG2	1:X:447:GLN:O	1.91	0.69
1:X:294:GLN:NE2	1:X:294:GLN:HA	2.07	0.69
1:X:347:THR:HA	1:X:384:SER:HA	1.73	0.68
1:X:57:ASP:O	1:X:60:THR:OG1	2.11	0.68
1:X:423:THR:CG2	1:X:434:LYS:HD3	2.22	0.68
1:X:345:SER:CA	1:X:386:THR:HG22	2.23	0.68
1:X:181:GLU:HB3	1:X:182:PRO:HD3	1.78	0.66
1:X:17:TRP:CZ3	1:X:124:ARG:HD3	2.31	0.66
1:X:398:ILE:HD12	1:X:424:VAL:CG1	2.26	0.66
1:X:247:PHE:CD2	1:X:247:PHE:N	2.63	0.65
1:X:144:ASN:HD21	1:X:146:GLU:HG2	1.62	0.65
1:X:279:PRO:HB3	1:X:312:TYR:CD1	2.33	0.63
1:X:247:PHE:N	1:X:247:PHE:HD2	1.96	0.63
1:X:423:THR:HA	1:X:434:LYS:HB3	1.80	0.63
1:X:184:PHE:O	1:X:185:GLN:C	2.41	0.62
1:X:345:SER:HA	1:X:386:THR:HG22	1.80	0.62
1:X:149:HIS:CD2	1:X:173:ARG:HD3	2.35	0.61
1:X:79:PHE:HB2	1:X:155:LEU:HD22	1.83	0.61
1:X:30:TRP:O	1:X:125:ILE:HD11	2.01	0.61
1:X:362:LEU:O	1:X:368:ASN:HA	2.00	0.61
1:X:393:PHE:CZ	1:X:395:ILE:CG2	2.84	0.61
1:X:131:ALA:HB1	1:X:167:LEU:HD21	1.83	0.60
1:X:363:ARG:O	1:X:367:GLY:O	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:6:THR:CB	1:X:7:PRO:HD3	2.32	0.60
1:X:6:THR:CB	1:X:7:PRO:CD	2.79	0.60
1:X:213:PRO:O	1:X:214:SER:HB2	2.02	0.59
1:X:141:LEU:HD23	1:X:141:LEU:N	2.16	0.59
1:X:166:ARG:C	1:X:167:LEU:HD23	2.27	0.59
1:X:100:THR:C	1:X:101:THR:OG1	2.44	0.59
1:X:251:ASN:OD1	1:X:258:GLN:HB2	2.03	0.59
1:X:345:SER:HB2	1:X:423:THR:HB	1.86	0.58
1:X:77:HIS:C	1:X:77:HIS:CD2	2.81	0.58
1:X:222:LYS:HZ1	1:X:326:THR:HG21	1.67	0.58
1:X:45:LYS:HB2	1:X:65:ASN:HD22	1.69	0.58
1:X:384:SER:O	1:X:385:TYR:CD2	2.57	0.57
1:X:212:LEU:HB3	1:X:213:PRO:CD	2.34	0.57
1:X:45:LYS:CB	1:X:65:ASN:HD22	2.16	0.56
1:X:80:ARG:HD3	1:X:247:PHE:HB3	1.87	0.56
1:X:188:SER:O	1:X:191:VAL:HG22	2.05	0.56
1:X:437:GLY:CA	1:X:449:LEU:HG	2.35	0.56
1:X:284:ALA:HB1	1:X:327:PHE:HB3	1.86	0.56
1:X:294:GLN:HE21	1:X:294:GLN:CA	2.17	0.56
1:X:133:LEU:HD12	1:X:133:LEU:O	2.06	0.56
1:X:77:HIS:CE1	1:X:82:ARG:HA	2.41	0.55
1:X:402:LYS:NZ	1:X:448:SER:OG	2.26	0.55
1:X:345:SER:OG	1:X:386:THR:CG2	2.54	0.55
1:X:61:ILE:O	1:X:64:SER:OG	2.12	0.55
1:X:284:ALA:HB1	1:X:327:PHE:CB	2.36	0.55
1:X:14:ASP:O	1:X:15:LYS:O	2.25	0.54
1:X:391:VAL:C	1:X:393:PHE:H	2.16	0.54
1:X:300:PRO:HB2	1:X:427:GLY:O	2.08	0.54
1:X:405:TRP:NE1	1:X:443:ASP:HA	2.22	0.54
1:X:404:VAL:O	1:X:405:TRP:HB3	2.08	0.54
1:X:296:ASN:HA	1:X:388:ASP:OD2	2.07	0.54
1:X:123:ILE:HD12	1:X:155:LEU:HG	1.91	0.53
1:X:242:SER:O	1:X:242:SER:OG	2.20	0.53
1:X:435:PHE:N	1:X:435:PHE:CD2	2.76	0.53
1:X:391:VAL:O	1:X:393:PHE:N	2.42	0.53
1:X:361:THR:HG22	1:X:362:LEU:H	1.74	0.53
1:X:424:VAL:CG1	1:X:425:GLN:N	2.72	0.52
1:X:17:TRP:CD2	1:X:124:ARG:NH1	2.78	0.52
1:X:140:GLU:C	1:X:141:LEU:HD23	2.35	0.52
1:X:167:LEU:N	1:X:167:LEU:CD2	2.72	0.52
1:X:418:GLY:HA2	1:X:447:GLN:HE22	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:213:PRO:O	1:X:214:SER:CB	2.58	0.51
1:X:443:ASP:O	1:X:445:VAL:HG23	2.10	0.51
1:X:283:LEU:HD23	1:X:306:CYS:HB2	1.92	0.51
1:X:177:LEU:HD13	1:X:269:PHE:HA	1.92	0.51
1:X:398:ILE:HG22	1:X:399:GLN:N	2.26	0.51
1:X:150:ILE:O	1:X:174:VAL:HA	2.11	0.51
1:X:327:PHE:N	1:X:327:PHE:CD1	2.78	0.50
1:X:364:GLY:O	1:X:397:LYS:O	2.30	0.50
1:X:8:LEU:HD11	1:X:129:GLU:OE2	2.10	0.50
1:X:266:LEU:HD22	1:X:269:PHE:HE2	1.76	0.50
1:X:14:ASP:O	1:X:15:LYS:C	2.55	0.50
1:X:74:PHE:CE2	1:X:104:ILE:HD12	2.46	0.49
1:X:140:GLU:CB	1:X:141:LEU:HD23	2.43	0.49
1:X:424:VAL:HG13	1:X:425:GLN:N	2.26	0.49
1:X:249:ASP:OD1	1:X:251:ASN:HB2	2.13	0.49
1:X:383:SER:O	1:X:384:SER:HB3	2.11	0.49
1:X:67:GLN:HG2	1:X:102:ASN:OD1	2.13	0.49
1:X:441:VAL:HG21	1:X:445:VAL:HG11	1.94	0.49
1:X:41:LEU:HD21	1:X:66:PHE:HB2	1.95	0.48
1:X:294:GLN:HA	1:X:294:GLN:HE21	1.72	0.48
1:X:1:LYS:O	1:X:28:LEU:HD11	2.14	0.48
1:X:262:ALA:O	1:X:266:LEU:HG	2.13	0.48
1:X:422:ILE:HG13	1:X:449:LEU:HD22	1.95	0.48
1:X:435:PHE:HB2	1:X:449:LEU:HB3	1.94	0.48
1:X:22:GLN:C	1:X:23:ARG:HG3	2.39	0.48
1:X:406:ASN:ND2	1:X:444:ASN:HD21	2.12	0.48
1:X:77:HIS:CD2	1:X:108:TRP:NE1	2.82	0.48
1:X:324:GLU:O	1:X:326:THR:HG23	2.14	0.48
1:X:13:ASP:HB3	1:X:28:LEU:HD21	1.96	0.47
1:X:443:ASP:OD1	1:X:444:ASN:HB2	2.14	0.47
1:X:300:PRO:O	1:X:301:CYS:C	2.57	0.47
1:X:413:SER:O	1:X:414:LYS:HB2	2.14	0.47
1:X:17:TRP:CG	1:X:124:ARG:NH1	2.83	0.47
1:X:30:TRP:O	1:X:125:ILE:CD1	2.63	0.47
1:X:71:LYS:O	1:X:101:THR:CG2	2.62	0.47
1:X:277:LEU:HD23	1:X:277:LEU:N	2.30	0.47
1:X:2:GLU:HB3	1:X:12:SER:HA	1.96	0.47
1:X:164:GLY:HA2	1:X:171:VAL:HG11	1.97	0.47
1:X:329:LEU:N	1:X:329:LEU:HD23	2.29	0.47
1:X:22:GLN:O	1:X:183:CYS:HA	2.14	0.47
1:X:402:LYS:HD3	1:X:402:LYS:HA	1.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:229:PHE:HB2	1:X:328:PHE:CD2	2.50	0.46
1:X:41:LEU:HD12	1:X:42:TYR:N	2.30	0.46
1:X:149:HIS:HA	1:X:173:ARG:O	2.15	0.46
1:X:182:PRO:O	1:X:183:CYS:HB2	2.15	0.46
1:X:345:SER:CB	1:X:386:THR:CG2	2.91	0.46
1:X:247:PHE:N	1:X:250:ILE:HG13	2.30	0.46
1:X:395:ILE:HG13	1:X:396:GLY:H	1.82	0.45
1:X:5:TYR:CZ	1:X:31:SER:HA	2.52	0.45
1:X:6:THR:OG1	1:X:7:PRO:HD2	2.16	0.45
1:X:374:ILE:HG23	1:X:387:LEU:HB3	1.97	0.45
1:X:240:LYS:HE2	1:X:240:LYS:HB3	1.81	0.45
1:X:404:VAL:HG12	1:X:405:TRP:N	2.31	0.45
1:X:441:VAL:CG2	1:X:445:VAL:HG21	2.47	0.45
1:X:181:GLU:HG3	1:X:185:GLN:HB2	2.00	0.44
1:X:299:PHE:HB3	1:X:343:ARG:NH2	2.32	0.44
1:X:356:GLY:O	1:X:376:LYS:HA	2.17	0.44
1:X:65:ASN:O	1:X:66:PHE:C	2.60	0.44
1:X:399:GLN:HA	1:X:435:PHE:CE1	2.39	0.44
1:X:450:TYR:HB3	1:X:451:PRO:HD2	2.00	0.44
1:X:170:ARG:HA	1:X:170:ARG:HD3	1.81	0.44
1:X:302:PRO:O	1:X:303:ALA:C	2.61	0.44
1:X:278:ASN:N	1:X:279:PRO:CD	2.81	0.43
1:X:328:PHE:O	1:X:329:LEU:HB3	2.17	0.43
1:X:89:SER:O	1:X:90:ASP:C	2.60	0.43
1:X:200:PHE:HZ	1:X:226:MET:CE	2.31	0.43
1:X:44:ASN:HD21	1:X:100:THR:HA	1.83	0.43
1:X:128:ALA:O	1:X:129:GLU:C	2.60	0.43
1:X:22:GLN:HG2	1:X:187:ALA:HB2	2.00	0.43
1:X:94:LYS:CE	1:X:273:SER:OG	2.60	0.43
1:X:173:ARG:HA	1:X:200:PHE:O	2.18	0.43
1:X:219:MET:HE2	1:X:221:GLN:HB3	1.99	0.43
1:X:77:HIS:NE2	1:X:108:TRP:CD1	2.87	0.43
1:X:71:LYS:O	1:X:101:THR:HG22	2.19	0.43
1:X:294:GLN:NE2	1:X:294:GLN:CA	2.71	0.43
1:X:54:THR:HG22	1:X:56:ARG:HG3	2.00	0.43
1:X:397:LYS:O	1:X:397:LYS:HG3	2.19	0.43
1:X:359:LYS:C	1:X:360:VAL:HG23	2.44	0.42
1:X:363:ARG:NH2	1:X:402:LYS:HE3	2.34	0.42
1:X:391:VAL:C	1:X:393:PHE:N	2.77	0.42
1:X:123:ILE:HG12	1:X:159:THR:OG1	2.19	0.42
1:X:181:GLU:HB3	1:X:182:PRO:CD	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:3:VAL:O	1:X:3:VAL:HG23	2.20	0.42
1:X:393:PHE:CZ	1:X:395:ILE:HG23	2.55	0.42
1:X:19:GLY:HA3	1:X:26:LYS:HE2	2.02	0.42
1:X:154:SER:HB2	1:X:265:HIS:NE2	2.35	0.42
2:X:502:DDQ:HM22	2:X:502:DDQ:H22	1.81	0.42
1:X:18:ALA:HB1	1:X:26:LYS:HA	2.01	0.42
1:X:248:ILE:HG23	1:X:248:ILE:O	2.20	0.42
1:X:130:THR:O	1:X:131:ALA:C	2.63	0.42
1:X:174:VAL:HG12	1:X:198:ALA:CB	2.49	0.42
1:X:185:GLN:NE2	1:X:220:SER:OG	2.49	0.42
1:X:288:ASP:OD2	1:X:292:LYS:NZ	2.36	0.42
1:X:174:VAL:O	1:X:201:VAL:HA	2.20	0.41
1:X:135:GLN:O	1:X:139:THR:HG23	2.21	0.41
1:X:174:VAL:HG12	1:X:198:ALA:HB2	2.03	0.41
1:X:185:GLN:HA	1:X:219:MET:HE3	2.02	0.41
1:X:402:LYS:HZ2	1:X:448:SER:CB	2.29	0.41
1:X:123:ILE:HD11	1:X:155:LEU:C	2.46	0.41
1:X:269:PHE:CD1	1:X:269:PHE:C	2.98	0.41
1:X:393:PHE:CZ	1:X:395:ILE:HG22	2.55	0.41
1:X:44:ASN:ND2	1:X:100:THR:HA	2.36	0.41
1:X:193:LEU:O	1:X:223:VAL:HB	2.21	0.40
1:X:418:GLY:HA3	1:X:440:THR:HB	2.03	0.40
1:X:115:GLU:O	1:X:116:TYR:C	2.64	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	X	444/452 (98%)	338 (76%)	78 (18%)	28 (6%)	1 6

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	6	THR
1	X	15	LYS
1	X	213	PRO
1	X	214	SER
1	X	248	ILE
1	X	398	ILE
1	X	404	VAL
1	X	414	LYS
1	X	431	THR
1	X	434	LYS
1	X	442	GLN
1	X	447	GLN
1	X	85	ASP
1	X	86	SER
1	X	241	ARG
1	X	249	ASP
1	X	365	SER
1	X	369	SER
1	X	392	ASN
1	X	413	SER
1	X	303	ALA
1	X	364	GLY
1	X	384	SER
1	X	168	GLU
1	X	382	ASP
1	X	412	LEU
1	X	251	ASN
1	X	439	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	X	383/387 (99%)	342 (89%)	41 (11%)	6	26

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	13	ASP
1	X	21	LEU
1	X	25	LEU
1	X	41	LEU
1	X	60	THR
1	X	62	LYS
1	X	67	GLN
1	X	84	GLU
1	X	85	ASP
1	X	86	SER
1	X	123	ILE
1	X	141	LEU
1	X	145	PRO
1	X	155	LEU
1	X	167	LEU
1	X	171	VAL
1	X	209	SER
1	X	213	PRO
1	X	222	LYS
1	X	234	LYS
1	X	240	LYS
1	X	242	SER
1	X	247	PHE
1	X	248	ILE
1	X	287	CYS
1	X	294	GLN
1	X	339	SER
1	X	351	SER
1	X	370	LYS
1	X	394	ILE
1	X	401	VAL
1	X	408	THR
1	X	410	LEU
1	X	417	LEU
1	X	424	VAL
1	X	429	ASP
1	X	434	LYS
1	X	435	PHE
1	X	444	ASN
1	X	447	GLN
1	X	449	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	36	ASN
1	X	65	ASN
1	X	67	GLN
1	X	144	ASN
1	X	294	GLN
1	X	315	GLN
1	X	325	GLN
1	X	355	ASN
1	X	380	GLN
1	X	392	ASN
1	X	399	GLN
1	X	406	ASN
1	X	411	ASN
1	X	425	GLN
1	X	444	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DDQ	X	502	-	11,13,13	2.06	1 (9%)	12,15,15	1.13	1 (8%)
2	DDQ	X	501	-	11,13,13	1.70	1 (9%)	12,15,15	1.66	2 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DDQ	X	502	-	-	8/11/11/11	-
2	DDQ	X	501	-	-	5/11/11/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	502	DDQ	O1-N1	-6.60	1.26	1.42
2	X	501	DDQ	O1-N1	-5.42	1.28	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	501	DDQ	O1-N1-C1	-4.28	98.79	109.27
2	X	501	DDQ	CM2-N1-C1	2.99	116.51	110.23
2	X	502	DDQ	O1-N1-C1	-2.75	102.52	109.27

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	X	501	DDQ	N1-C1-C2-C3
2	X	502	DDQ	C2-C1-N1-O1
2	X	502	DDQ	C2-C1-N1-CM1
2	X	502	DDQ	C2-C1-N1-CM2
2	X	502	DDQ	N1-C1-C2-C3
2	X	502	DDQ	C5-C6-C7-C8
2	X	502	DDQ	C2-C3-C4-C5
2	X	501	DDQ	C6-C7-C8-C9
2	X	501	DDQ	C1-C2-C3-C4
2	X	502	DDQ	C1-C2-C3-C4
2	X	501	DDQ	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	X	502	DDQ	C7-C8-C9-C10
2	X	501	DDQ	C7-C8-C9-C10

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	X	502	DDQ	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	X	448/452 (99%)	1.09	105 (23%) 2 1	12, 47, 100, 100	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	399	GLN	7.7
1	X	438	SER	7.1
1	X	441	VAL	6.5
1	X	354	ALA	6.4
1	X	248	ILE	6.4
1	X	409	VAL	6.2
1	X	418	GLY	5.9
1	X	422	ILE	5.8
1	X	434	LYS	5.8
1	X	436	CYS	5.6
1	X	445	VAL	5.6
1	X	403	PHE	5.5
1	X	417	LEU	5.4
1	X	437	GLY	5.3
1	X	348	LEU	5.2
1	X	424	VAL	5.1
1	X	412	LEU	4.9
1	X	420	SER	4.7
1	X	396	GLY	4.7
1	X	442	GLN	4.7
1	X	433	TYR	4.6
1	X	350	GLY	4.6
1	X	213	PRO	4.5
1	X	379	LEU	4.4
1	X	366	ASN	4.3
1	X	408	THR	4.3
1	X	346	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	X	357	TYR	4.3
1	X	448	SER	4.2
1	X	349	ALA	4.2
1	X	352	GLY	4.1
1	X	447	GLN	4.1
1	X	405	TRP	4.0
1	X	435	PHE	3.9
1	X	449	LEU	3.9
1	X	444	ASN	3.9
1	X	419	ALA	3.9
1	X	440	THR	3.9
1	X	401	VAL	3.8
1	X	439	GLY	3.8
1	X	451	PRO	3.8
1	X	385	TYR	3.8
1	X	410	LEU	3.7
1	X	423	THR	3.7
1	X	415	PRO	3.7
1	X	345	SER	3.6
1	X	376	LYS	3.6
1	X	416	GLN	3.5
1	X	398	ILE	3.5
1	X	365	SER	3.5
1	X	450	TYR	3.5
1	X	347	THR	3.4
1	X	361	THR	3.4
1	X	400	GLU	3.4
1	X	351	SER	3.4
1	X	404	VAL	3.3
1	X	446	GLU	3.3
1	X	452	CYS	3.3
1	X	428	ALA	3.2
1	X	383	SER	3.2
1	X	394	ILE	3.2
1	X	369	SER	3.2
1	X	135	GLN	3.1
1	X	367	GLY	3.0
1	X	407	LYS	3.0
1	X	90	ASP	3.0
1	X	355	ASN	2.9
1	X	333	GLU	2.9
1	X	250	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	X	353	LYS	2.8
1	X	402	LYS	2.8
1	X	432	GLU	2.8
1	X	25	LEU	2.8
1	X	414	LYS	2.7
1	X	406	ASN	2.7
1	X	392	ASN	2.7
1	X	241	ARG	2.7
1	X	377	GLY	2.7
1	X	380	GLN	2.6
1	X	363	ARG	2.6
1	X	429	ASP	2.6
1	X	344	VAL	2.6
1	X	356	GLY	2.6
1	X	6	THR	2.6
1	X	395	ILE	2.6
1	X	393	PHE	2.6
1	X	387	LEU	2.5
1	X	51	GLN	2.5
1	X	49	SER	2.5
1	X	360	VAL	2.5
1	X	426	SER	2.4
1	X	358	LEU	2.4
1	X	146	GLU	2.4
1	X	368	ASN	2.3
1	X	20	THR	2.3
1	X	287	CYS	2.2
1	X	421	ARG	2.2
1	X	382	ASP	2.2
1	X	10	CYS	2.1
1	X	55	ALA	2.1
1	X	45	LYS	2.1
1	X	370	LYS	2.1
1	X	170	ARG	2.1
1	X	1	LYS	2.0
1	X	364	GLY	2.0

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 [i](#)

There are no oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	X	601	1/1	0.89	0.09	50,50,50,50	0
2	DDQ	X	501	14/14	0.90	0.16	20,28,35,41	0
2	DDQ	X	502	14/14	0.95	0.11	21,26,36,37	0
3	CA	X	602	1/1	0.97	0.08	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.