



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:55 AM GMT

PDB ID : 2ERQ
Title : Crystal structure of vascular apoptosis-inducing protein-1(tetragonal crystal form)
Authors : Takeda, S.; Igarashi, T.; Araki, S.
Deposited on : 2005-10-25
Resolution : 2.50 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

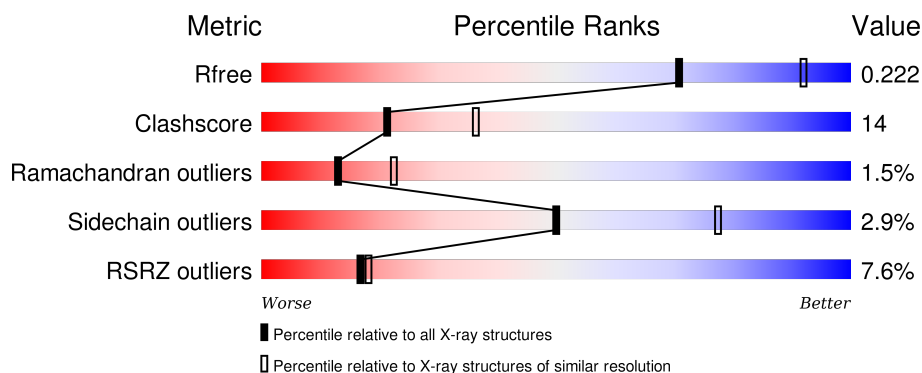
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 $\leq 5\%$. 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	427	<div> <div>8%</div> <div>75%</div> <div>21%</div> <div>• •</div> </div>
1	B	427	<div> <div>7%</div> <div>71%</div> <div>25%</div> <div>• • •</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6724 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.

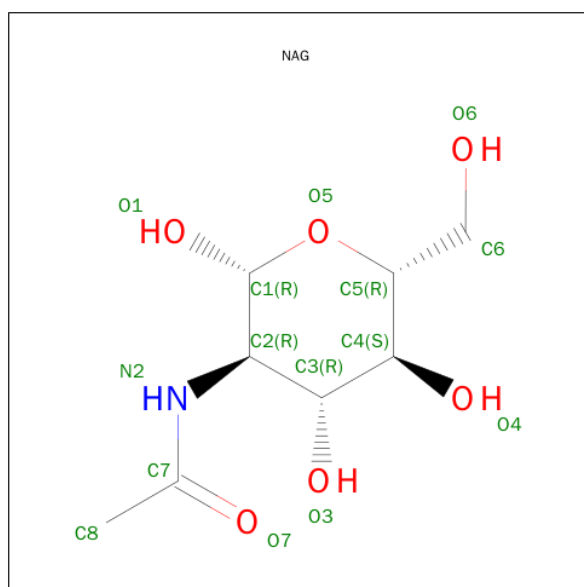
- Molecule 1 is a protein called vascular apoptosis-inducing protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3259	2008	582	622	47			
1	B	423	Total	C	N	O	S	0	0	0
			3252	2006	580	619	47			

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Zn 1	0	0
4	A	1	Total 1	Zn 1	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

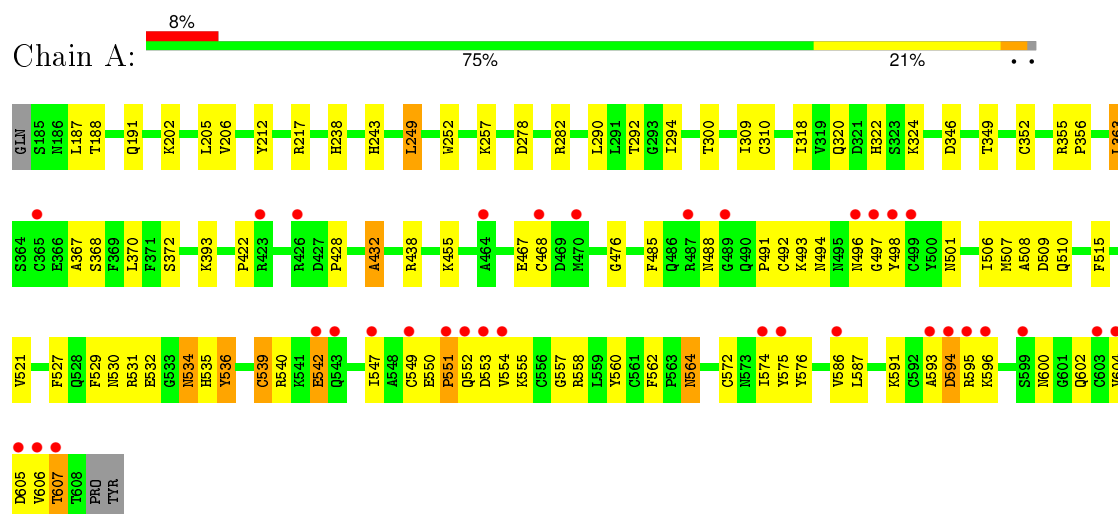
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	89	Total 89	O 89	0	0
6	B	76	Total 76	O 76	0	0

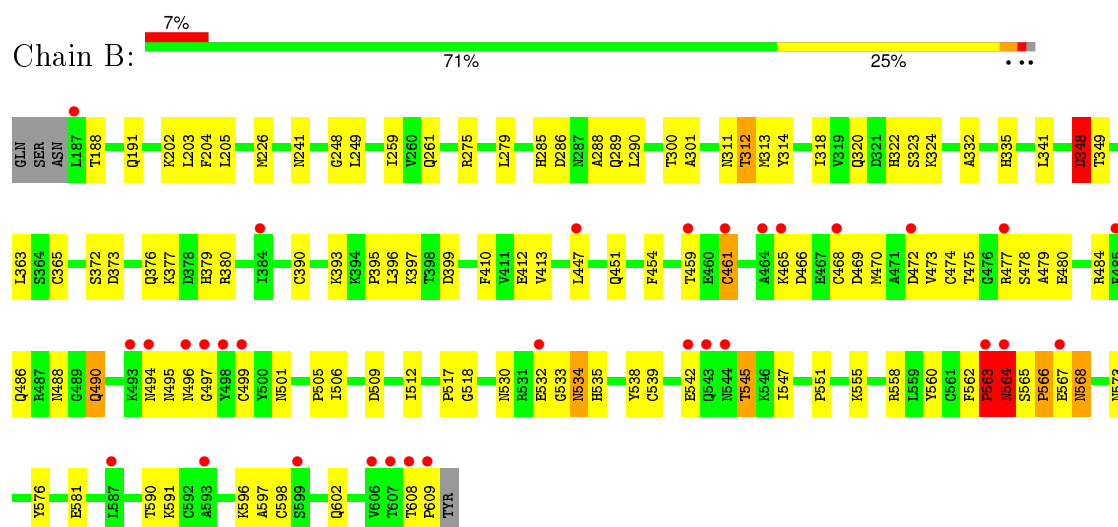
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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: vascular apoptosis-inducing protein 1



- Molecule 1: vascular apoptosis-inducing protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	93.94Å 93.94Å 244.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 46.13 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.50) 99.8 (46.13-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.84 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.229 , 0.269 0.234 , 0.222	Depositor DCC
R_{free} test set	1943 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 38786 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6724	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, CA, NAG

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	0.41	0/3321	0.66	0/4487
1	B	0.41	0/3315	0.66	1/4480 (0.0%)
All	All	0.41	0/6636	0.66	1/8967 (0.0%)

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	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	564	ASN	N-CA-C	6.55	128.68	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	536	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	3259	0	3124	92	0
1	B	3252	0	3120	93	0
2	A	28	0	25	0	0
3	B	14	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	89	0	0	2	0
6	B	76	0	0	4	0
All	All	6724	0	6282	182	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 14.

All (182) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:THR:HG23	1:B:191:GLN:HE21	1.12	1.14
1:B:488:ASN:ND2	1:B:501:ASN:H	1.65	0.93
1:B:188:THR:HG23	1:B:191:GLN:NE2	1.88	0.88
1:A:542:GLU:HB2	1:A:547:ILE:HD11	1.56	0.87
1:A:496:ASN:HB3	1:A:506:ILE:HG21	1.56	0.87
1:B:488:ASN:HD21	1:B:501:ASN:H	1.18	0.86
1:A:497:GLY:HA2	1:A:591:LYS:HB2	1.59	0.85
1:B:226:MET:SD	1:B:249:LEU:HD11	2.18	0.83
1:A:438:ARG:HH11	1:A:438:ARG:HG2	1.43	0.83
1:B:472:ASP:OD1	1:B:484:ARG:HG2	1.80	0.81
1:A:493:LYS:HB3	1:A:496:ASN:HD22	1.45	0.80
1:B:372:SER:O	1:B:376:GLN:HG2	1.83	0.79
1:B:373:ASP:O	1:B:377:LYS:HG2	1.82	0.79
1:A:496:ASN:O	1:A:591:LYS:HD3	1.85	0.77
1:A:558:ARG:HG3	1:A:574:ILE:HD12	1.68	0.75
1:A:540:ARG:NH1	1:A:547:ILE:HD12	2.02	0.74
1:B:506:ILE:HB	1:B:509:ASP:OD2	1.87	0.74
1:B:532:GLU:HB2	1:B:534:ASN:ND2	2.03	0.73
1:B:542:GLU:HB2	1:B:545:THR:HG23	1.72	0.71
1:B:204:PHE:CD1	1:B:248:GLY:HA3	2.25	0.71
1:B:496:ASN:O	1:B:506:ILE:HD12	1.93	0.69
1:B:542:GLU:HG2	1:B:547:ILE:HD11	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:CYS:O	1:A:485:PHE:HB3	1.94	0.68
1:A:249:LEU:C	1:A:249:LEU:HD23	2.16	0.66
1:A:510:GLN:HE22	1:A:587:LEU:H	1.42	0.66
1:B:534:ASN:HB2	1:B:535:HIS:HD2	1.60	0.66
1:A:493:LYS:HB3	1:A:496:ASN:ND2	2.11	0.65
1:B:562:PHE:O	1:B:564:ASN:N	2.30	0.65
1:A:438:ARG:HG2	1:A:438:ARG:NH1	2.12	0.65
1:B:532:GLU:CB	1:B:534:ASN:ND2	2.60	0.64
1:A:542:GLU:HB2	1:A:547:ILE:CD1	2.26	0.63
1:A:606:VAL:HG13	1:A:607:THR:H	1.62	0.63
1:A:531:ARG:CZ	1:A:551:PRO:HG3	2.28	0.63
1:A:294:ILE:O	1:A:320:GLN:HG3	1.99	0.63
1:B:459:THR:O	1:B:473:VAL:HG13	1.98	0.63
1:A:188:THR:H	1:A:191:GLN:NE2	1.96	0.62
1:A:606:VAL:HG13	1:A:607:THR:N	2.14	0.62
1:B:530:ASN:HD21	1:B:558:ARG:HB3	1.64	0.62
1:B:563:PRO:HD2	1:B:573:ASN:ND2	2.15	0.62
1:A:532:GLU:HB2	1:A:534:ASN:HD22	1.65	0.61
1:B:275:ARG:HD2	1:B:288:ALA:HB3	1.82	0.61
1:B:454:PHE:HE1	1:B:479:ALA:HB2	1.66	0.61
1:A:300:THR:HG22	6:A:784:HOH:O	2.00	0.60
1:A:493:LYS:HD3	1:A:506:ILE:HD13	1.83	0.60
1:B:497:GLY:HA2	1:B:591:LYS:HB2	1.83	0.60
1:A:539:CYS:SG	1:A:553:ASP:O	2.59	0.59
1:A:202:LYS:HE3	1:A:393:LYS:O	2.02	0.59
1:B:488:ASN:HD21	1:B:501:ASN:N	1.97	0.59
1:B:486:GLN:NE2	1:B:490:GLN:HG2	2.18	0.59
1:B:447:LEU:HB3	1:B:461:CYS:HB2	1.84	0.59
1:A:530:ASN:HB3	1:A:549:CYS:SG	2.43	0.57
1:A:596:LYS:HB3	1:A:604:VAL:O	2.04	0.57
1:A:506:ILE:HD11	1:A:509:ASP:OD1	2.05	0.57
1:A:278:ASP:OD2	1:A:278:ASP:C	2.43	0.57
1:A:428:PRO:O	1:A:438:ARG:HD2	2.05	0.57
1:A:595:ARG:O	1:A:606:VAL:HG12	2.05	0.57
1:B:373:ASP:HA	1:B:376:GLN:HG3	1.85	0.56
1:A:527:PHE:HB3	1:A:554:VAL:HG22	1.87	0.56
1:B:241:ASN:HB2	6:B:741:HOH:O	2.06	0.56
1:B:202:LYS:HE3	1:B:393:LYS:O	2.06	0.56
1:B:497:GLY:HA3	1:B:506:ILE:HD11	1.88	0.56
1:A:507:MET:HE1	1:A:555:LYS:HB3	1.88	0.56
1:B:555:LYS:HB2	6:B:772:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:VAL:HG12	1:A:605:ASP:N	2.21	0.55
1:A:532:GLU:HB2	1:A:534:ASN:ND2	2.21	0.55
1:A:591:LYS:HE3	1:A:594:ASP:O	2.07	0.55
1:A:529:PHE:HB2	1:A:560:TYR:OH	2.07	0.55
1:B:534:ASN:HB2	1:B:535:HIS:CD2	2.41	0.54
1:A:324:LYS:NZ	1:B:320:GLN:HE22	2.06	0.54
1:B:465:LYS:HG2	1:B:469:ASP:OD1	2.08	0.54
1:B:490:GLN:HB3	1:B:499:CYS:SG	2.48	0.53
1:B:505:PRO:O	1:B:506:ILE:HD13	2.08	0.53
1:A:322:HIS:CE1	1:A:363:LEU:HD21	2.44	0.53
1:A:352:CYS:HB3	1:A:372:SER:HA	1.89	0.53
1:A:467:GLU:OE1	1:A:492:CYS:HA	2.08	0.53
1:B:565:SER:O	1:B:567:GLU:N	2.43	0.52
1:B:567:GLU:O	1:B:568:ASN:C	2.48	0.52
1:A:542:GLU:OE1	1:A:547:ILE:HD11	2.10	0.51
1:B:204:PHE:CE1	1:B:248:GLY:HA3	2.46	0.51
1:A:560:TYR:HD2	1:A:572:CYS:HB3	1.76	0.51
1:B:261:GLN:HB3	6:B:715:HOH:O	2.10	0.51
1:B:598:CYS:HA	1:B:602:GLN:O	2.11	0.51
1:B:564:ASN:O	1:B:565:SER:C	2.47	0.50
1:B:301:ALA:HB2	1:B:363:LEU:HD11	1.94	0.50
1:B:473:VAL:HG12	1:B:474:CYS:N	2.25	0.50
1:A:324:LYS:HZ3	1:B:320:GLN:HE22	1.57	0.50
1:A:535:HIS:HE1	1:A:576:TYR:OH	1.95	0.50
1:B:275:ARG:NE	1:B:285:HIS:NE2	2.54	0.50
1:A:249:LEU:HD23	1:A:249:LEU:O	2.12	0.49
1:A:356:PRO:HG2	1:A:367:ALA:HA	1.94	0.49
1:A:558:ARG:CG	1:A:574:ILE:HD12	2.39	0.49
1:B:410:PHE:HD2	1:B:412:GLU:HG3	1.78	0.49
1:A:497:GLY:HA2	1:A:591:LYS:CB	2.37	0.49
1:A:496:ASN:HB3	1:A:506:ILE:CG2	2.36	0.49
1:A:550:GLU:HA	1:A:550:GLU:OE1	2.13	0.49
1:A:355:ARG:HG3	1:A:355:ARG:HH11	1.77	0.49
1:B:188:THR:OG1	1:B:191:GLN:HG3	2.13	0.48
1:A:558:ARG:HD2	1:A:574:ILE:HG23	1.95	0.48
1:A:300:THR:O	1:B:324:LYS:HE2	2.13	0.48
1:B:259:ILE:O	1:B:261:GLN:HG3	2.14	0.47
1:B:311:ASN:ND2	1:B:314:TYR:HD2	2.11	0.47
1:A:278:ASP:OD2	1:A:282:ARG:HD3	2.13	0.47
1:B:512:ILE:HG23	1:B:517:PRO:HA	1.96	0.47
1:B:497:GLY:HA3	1:B:506:ILE:CD1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:MET:CE	1:B:249:LEU:HD11	2.44	0.47
1:B:341:LEU:O	1:B:379:HIS:HD2	1.97	0.47
1:B:466:ASP:OD1	1:B:468:CYS:N	2.47	0.47
1:A:187:LEU:HD12	1:A:191:GLN:NE2	2.30	0.47
1:A:438:ARG:NH1	1:A:438:ARG:CG	2.78	0.46
1:B:535:HIS:HB3	6:B:703:HOH:O	2.14	0.46
1:A:488:ASN:HD21	1:A:501:ASN:H	1.62	0.46
1:B:205:LEU:CD2	1:B:289:GLN:HB2	2.45	0.46
1:A:252:TRP:CE2	1:A:257:LYS:HG2	2.50	0.46
1:A:355:ARG:HB2	1:A:368:SER:HB3	1.97	0.46
1:A:550:GLU:O	1:A:553:ASP:N	2.47	0.46
1:B:226:MET:HE3	1:B:249:LEU:HD11	1.98	0.45
1:B:518:GLY:O	1:B:564:ASN:HB2	2.16	0.45
1:B:530:ASN:ND2	1:B:560:TYR:OH	2.49	0.45
1:B:396:LEU:HB2	1:B:399:ASP:OD2	2.16	0.45
1:B:290:LEU:HB3	1:B:318:ILE:HG22	1.99	0.45
1:A:593:ALA:HB3	1:A:596:LYS:HB2	1.98	0.45
1:A:557:GLY:O	1:A:586:VAL:HG23	2.16	0.45
1:B:475:THR:C	1:B:477:ARG:H	2.20	0.45
1:B:495:ASN:O	1:B:591:LYS:NZ	2.44	0.44
1:B:204:PHE:CD2	1:B:279:LEU:HD21	2.52	0.44
1:B:590:THR:O	1:B:597:ALA:HA	2.17	0.44
1:B:564:ASN:O	1:B:566:PRO:N	2.50	0.44
1:A:550:GLU:O	1:A:552:GLN:N	2.50	0.44
1:B:202:LYS:HD3	1:B:395:PRO:HB3	1.98	0.44
1:B:565:SER:C	1:B:567:GLU:N	2.71	0.44
1:B:380:ARG:HH11	1:B:380:ARG:HG3	1.83	0.44
1:B:312:THR:HG22	1:B:313:MET:HG3	1.99	0.44
1:B:608:THR:HB	1:B:609:PRO:HD2	2.00	0.44
1:A:536:TYR:CD1	1:A:536:TYR:C	2.91	0.44
1:A:346:ASP:OD1	1:A:372:SER:OG	2.35	0.43
1:A:309:ILE:O	1:A:310:CYS:HB2	2.18	0.43
1:A:488:ASN:ND2	1:A:501:ASN:H	2.16	0.43
1:A:491:PRO:HA	1:A:498:TYR:HD2	1.84	0.43
1:B:320:GLN:HG2	1:B:322:HIS:HB3	2.00	0.43
1:A:493:LYS:O	1:A:494:ASN:HB2	2.19	0.43
1:B:226:MET:SD	1:B:249:LEU:CD1	2.98	0.43
1:B:373:ASP:OD1	1:B:373:ASP:N	2.52	0.43
1:A:600:ASN:C	1:A:602:GLN:H	2.21	0.43
1:A:212:TYR:CE1	1:A:217:ARG:HA	2.54	0.43
1:B:533:GLY:HA2	1:B:538:TYR:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:ASP:HB2	1:B:349:THR:H	1.61	0.42
1:A:531:ARG:NH2	1:A:551:PRO:HG3	2.34	0.42
1:A:540:ARG:NH1	6:A:752:HOH:O	2.53	0.42
1:B:203:LEU:HD11	1:B:289:GLN:HG2	2.00	0.42
1:A:206:VAL:HG11	1:A:252:TRP:CZ2	2.54	0.42
1:A:515:PHE:CZ	1:A:575:TYR:HB2	2.54	0.42
1:A:535:HIS:HE1	1:A:576:TYR:CZ	2.38	0.42
1:A:552:GLN:NE2	1:A:596:LYS:HZ3	2.18	0.42
1:B:469:ASP:OD2	1:B:470:MET:N	2.53	0.42
1:A:238:HIS:HE1	1:A:243:HIS:ND1	2.18	0.42
1:B:576:TYR:OH	1:B:581:GLU:HG2	2.20	0.42
1:A:542:GLU:HB2	1:A:547:ILE:CG1	2.50	0.42
1:A:290:LEU:HB3	1:A:318:ILE:HG22	2.01	0.42
1:B:397:LYS:NZ	1:B:413:VAL:HA	2.35	0.42
1:A:508:ALA:HA	1:A:521:VAL:HG23	2.02	0.41
1:B:447:LEU:N	1:B:447:LEU:HD12	2.34	0.41
1:A:600:ASN:C	1:A:602:GLN:N	2.72	0.41
1:B:596:LYS:HB3	1:B:596:LYS:HE2	1.85	0.41
1:B:332:ALA:O	1:B:335:HIS:HB3	2.21	0.41
1:A:564:ASN:HD22	1:A:564:ASN:N	2.16	0.41
1:B:373:ASP:O	1:B:376:GLN:HB2	2.21	0.41
1:B:518:GLY:O	1:B:564:ASN:CB	2.68	0.41
1:A:606:VAL:CG1	1:A:607:THR:N	2.83	0.41
1:A:238:HIS:CE1	1:A:243:HIS:ND1	2.88	0.41
1:A:205:LEU:O	1:A:249:LEU:HA	2.20	0.41
1:A:604:VAL:CG1	1:A:605:ASP:N	2.84	0.41
1:B:202:LYS:NZ	1:B:286:ASP:OD1	2.54	0.41
1:A:422:PRO:HA	1:A:432:ALA:HB3	2.02	0.41
1:A:510:GLN:NE2	1:A:587:LEU:H	2.14	0.41
1:A:320:GLN:C	1:A:322:HIS:N	2.74	0.41
1:B:478:SER:OG	1:B:480:GLU:HG2	2.20	0.41
1:B:204:PHE:O	1:B:288:ALA:HA	2.21	0.40
1:A:496:ASN:CB	1:A:506:ILE:HG21	2.39	0.40
1:B:373:ASP:HA	1:B:376:GLN:CG	2.51	0.40
1:B:473:VAL:CG1	1:B:474:CYS:N	2.84	0.40
1:B:447:LEU:CB	1:B:461:CYS:HB2	2.49	0.40
1:A:455:LYS:O	1:A:476:GLY:HA2	2.21	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	422/427 (99%)	388 (92%)	28 (7%)	6 (1%)	14	24
1	B	421/427 (99%)	390 (93%)	24 (6%)	7 (2%)	11	19
All	All	843/854 (99%)	778 (92%)	52 (6%)	13 (2%)	13	22

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	534	ASN
1	B	348	ASP
1	B	564	ASN
1	A	432	ALA
1	A	542	GLU
1	B	568	ASN
1	A	594	ASP
1	B	534	ASN
1	A	551	PRO
1	A	607	THR
1	B	551	PRO
1	B	563	PRO
1	B	566	PRO

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	360/363 (99%)	352 (98%)	8 (2%)	60	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	359/363 (99%)	346 (96%)	13 (4%)	42	69
All	All	719/726 (99%)	698 (97%)	21 (3%)	50	77

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	249	LEU
1	A	292	THR
1	A	349	THR
1	A	363	LEU
1	A	370	LEU
1	A	539	CYS
1	A	562	PHE
1	A	564	ASN
1	B	300	THR
1	B	312	THR
1	B	323	SER
1	B	348	ASP
1	B	365	CYS
1	B	390	CYS
1	B	451	GLN
1	B	461	CYS
1	B	490	GLN
1	B	494	ASN
1	B	539	CYS
1	B	545	THR
1	B	563	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	192	GLN
1	A	196	ASN
1	A	238	HIS
1	A	297	ASN
1	A	327	HIS
1	A	451	GLN
1	A	488	ASN
1	A	496	ASN
1	A	510	GLN

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Mol	Chain	Res	Type
1	A	523	GLN
1	A	535	HIS
1	A	552	GLN
1	A	564	ASN
1	A	579	ASN
1	A	602	GLN
1	B	191	GLN
1	B	289	GLN
1	B	320	GLN
1	B	376	GLN
1	B	439	GLN
1	B	451	GLN
1	B	486	GLN
1	B	488	ASN
1	B	490	GLN
1	B	494	ASN
1	B	501	ASN
1	B	523	GLN
1	B	530	ASN
1	B	535	HIS
1	B	568	ASN
1	B	573	ASN
1	B	602	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 ⓘ

2 carbohydrates are modelled in this entry.

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	NAG	A	1	1,2	14,14,15	0.50	0	15,19,21	0.98	1 (6%)
2	NAG	A	2	2	14,14,15	0.50	0	15,19,21	0.69	1 (6%)

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	NAG	A	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2	NAG	C2-N2-C7	-2.12	120.32	123.04
2	A	1	NAG	C2-N2-C7	-2.10	120.34	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 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
3	NAG	B	3	1	14,14,15	0.64	0	15,19,21	0.88	1 (6%)

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
3	NAG	B	3	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3	NAG	C2-N2-C7	-2.55	119.77	123.04

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 [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	A	424/427 (99%)	0.63	33 (7%) 16 17	17, 49, 87, 112	0
1	B	423/427 (99%)	0.51	31 (7%) 18 20	23, 50, 86, 107	0
All	All	847/854 (99%)	0.57	64 (7%) 17 18	17, 50, 87, 112	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	554	VAL	7.7
1	A	542	GLU	7.5
1	B	497	GLY	7.2
1	B	609	PRO	5.9
1	A	496	ASN	5.6
1	B	447	LEU	5.1
1	B	494	ASN	4.8
1	B	465	LYS	4.5
1	B	607	THR	4.2
1	A	594	ASP	4.2
1	A	593	ALA	4.1
1	B	496	ASN	4.0
1	A	604	VAL	3.9
1	A	552	GLN	3.5
1	A	606	VAL	3.5
1	A	499	CYS	3.3
1	A	423	ARG	3.3
1	B	543	GLN	3.3
1	A	596	LYS	3.2
1	B	563	PRO	3.2
1	B	459	THR	3.2
1	B	464	ALA	3.1
1	A	607	THR	3.1
1	B	608	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	567	GLU	3.0
1	A	489	GLY	3.0
1	B	532	GLU	3.0
1	A	426	ARG	3.0
1	A	498	TYR	2.8
1	A	595	ARG	2.8
1	A	543	GLN	2.8
1	B	187	LEU	2.8
1	B	468	CYS	2.8
1	A	487	ARG	2.8
1	A	365	CYS	2.8
1	A	574	ILE	2.7
1	B	542	GLU	2.7
1	B	499	CYS	2.7
1	A	551	PRO	2.6
1	A	605	ASP	2.6
1	B	498	TYR	2.5
1	B	599	SER	2.5
1	B	593	ALA	2.5
1	B	384	ILE	2.4
1	B	477	ARG	2.4
1	B	544	ASN	2.4
1	B	461	CYS	2.4
1	B	606	VAL	2.4
1	B	564	ASN	2.4
1	A	464	ALA	2.3
1	A	497	GLY	2.3
1	A	553	ASP	2.3
1	B	493	LYS	2.3
1	A	603	CYS	2.3
1	B	472	ASP	2.3
1	A	470	MET	2.2
1	B	485	PHE	2.2
1	A	586	VAL	2.2
1	A	547	ILE	2.2
1	A	599	SER	2.2
1	A	575	TYR	2.1
1	A	468	CYS	2.1
1	A	549	CYS	2.1
1	B	587	LEU	2.0

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](#)

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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	A	2	14/15	0.88	0.22	-	70,74,79,79	0
2	NAG	A	1	14/15	0.87	0.16	-	55,64,68,68	0

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, 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	LLDF	B-factors(Å ²)	Q<0.9
5	CA	A	701	1/1	0.98	0.16	0.55	34,34,34,34	0
5	CA	B	701	1/1	0.99	0.14	-0.59	33,33,33,33	0
5	CA	A	702	1/1	0.97	0.06	-3.42	58,58,58,58	0
5	CA	B	702	1/1	0.88	0.05	-4.54	82,82,82,82	0
3	NAG	B	3	14/15	0.89	0.19	-	49,53,63,65	0
4	ZN	A	700	1/1	0.97	0.24	-	36,36,36,36	0
4	ZN	B	700	1/1	0.96	0.17	-	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.