



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 07:49 am BST

PDB ID : 2DWX
Title : Co-crystal Structure Analysis of GGA1-GAE with the WNSF motif
Authors : Inoue, M.; Shiba, T.; Yamada, Y.; Ihara, K.; Kawasaki, M.; Kato, R.;
Nakayama, K.; Wakatsuki, S.
Deposited on : 2006-08-21
Resolution : 2.55 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

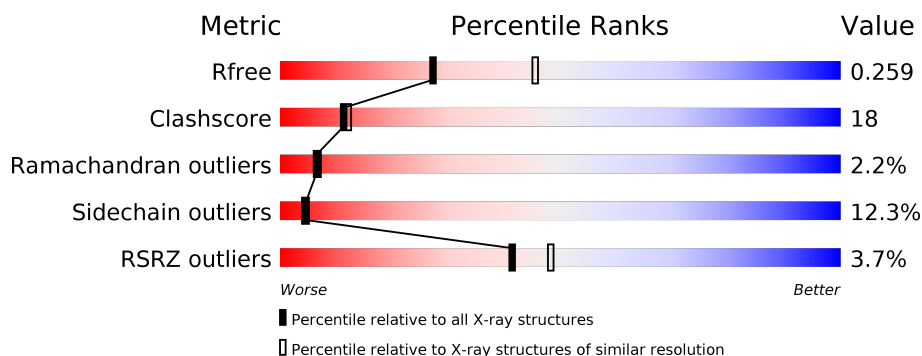
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 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	133	<div> <div>2%</div> <div>72% 18% 7%</div> </div>
1	B	133	<div> <div>7%</div> <div>48% 32% 8% 11%</div> </div>
1	C	133	<div> <div>2%</div> <div>65% 26% 5%</div> </div>
1	D	133	<div> <div>2%</div> <div>64% 26% 7%</div> </div>
2	P	13	<div> <div>8%</div> <div>46% 8% 8% 38%</div> </div>
2	Q	13	<div> <div>15%</div> <div>38% 8% 8% 46%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4235 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 ADP-ribosylation factor-binding protein GGA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			1020	662	173	181	4			
1	B	119	Total	C	N	O	S	0	0	0
			937	608	156	170	3			
1	C	128	Total	C	N	O	S	0	0	0
			1012	658	171	179	4			
1	D	129	Total	C	N	O	S	0	0	0
			1020	662	173	181	4			

- Molecule 2 is a protein called hinge peptide from ADP-ribosylation factor binding protein GGA1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	8	Total	C	N	O	0	0	0
			65	40	11	14			
2	Q	7	Total	C	N	O	0	0	0
			59	37	10	12			

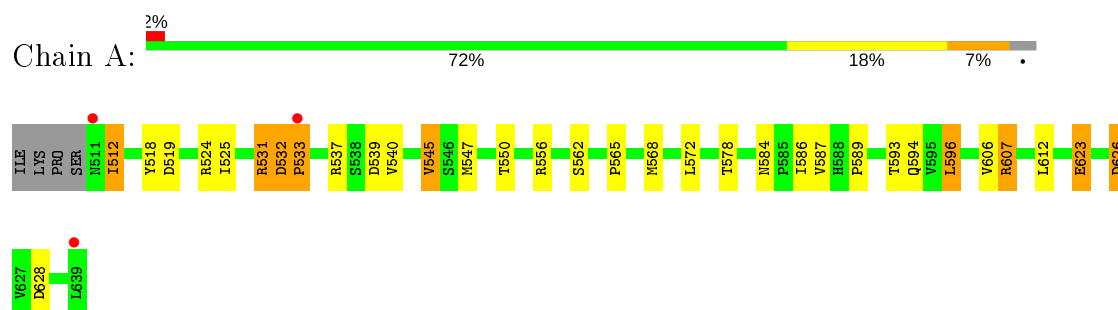
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	B	30	Total	O	0	0
			30	30		
3	C	30	Total	O	0	0
			30	30		
3	D	23	Total	O	0	0
			23	23		
3	P	6	Total	O	0	0
			6	6		
3	Q	3	Total	O	0	0
			3	3		

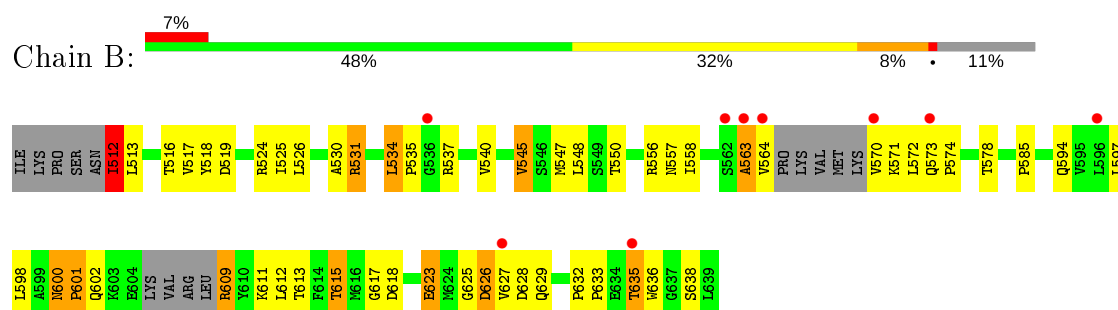
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

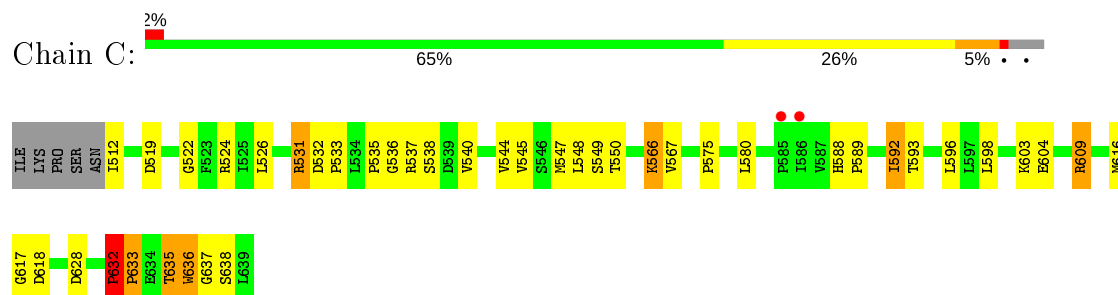
• Molecule 1: ADP-ribosylation factor-binding protein GGA1



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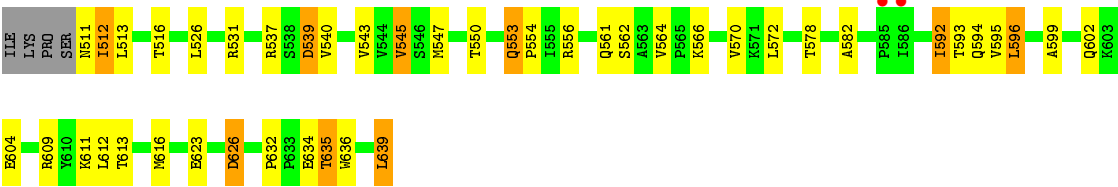


• Molecule 1: ADP-ribosylation factor-binding protein GGA1

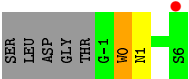


• Molecule 1: ADP-ribosylation factor-binding protein GGA1

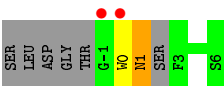
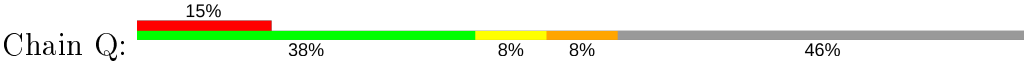




- Molecule 2: hinge peptide from ADP-ribosylation factor binding protein GGA1



- Molecule 2: hinge peptide from ADP-ribosylation factor binding protein GGA1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.22Å 69.62Å 184.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.63 – 2.55 46.66 – 2.55	Depositor EDS
% Data completeness (in resolution range)	96.9 (38.63-2.55) 96.5 (46.66-2.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.95 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.238 , 0.287 0.242 , 0.259	Depositor DCC
R_{free} test set	1019 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.640	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4235	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% 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	0.77	0/1049	0.94	5/1433 (0.3%)
1	B	0.70	0/963	1.11	7/1316 (0.5%)
1	C	0.88	0/1041	1.00	4/1422 (0.3%)
1	D	0.69	0/1049	0.87	2/1433 (0.1%)
2	P	0.54	0/67	0.58	0/88
2	Q	0.71	0/60	0.56	0/77
All	All	0.76	0/4229	0.97	18/5769 (0.3%)

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	B	0	1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	512	ILE	O-C-N	-16.73	95.93	122.70
1	B	512	ILE	CA-C-N	12.31	144.27	117.20
1	D	539	ASP	CB-CG-OD2	8.00	125.50	118.30
1	C	632	PRO	N-CA-C	7.76	132.29	112.10
1	B	512	ILE	CA-C-O	-6.79	105.84	120.10
1	C	519	ASP	CB-CG-OD2	6.65	124.28	118.30
1	B	513	LEU	N-CA-C	-6.44	93.61	111.00
1	A	532	ASP	CB-CG-OD2	6.06	123.75	118.30
1	C	531	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	A	626	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	519	ASP	CB-CG-OD2	5.99	123.69	118.30
1	D	626	ASP	CB-CG-OD2	5.71	123.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	596	LEU	CA-CB-CG	5.66	128.33	115.30
1	B	628	ASP	CB-CG-OD2	5.45	123.21	118.30
1	A	628	ASP	CB-CG-OD2	5.40	123.16	118.30
1	C	632	PRO	CA-C-N	5.25	131.81	117.10
1	B	626	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	519	ASP	CB-CG-OD2	5.22	123.00	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	512	ILE	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	A	1020	0	1042	37	0
1	B	937	0	937	46	0
1	C	1012	0	1036	36	0
1	D	1020	0	1042	50	0
2	P	65	0	53	1	0
2	Q	59	0	47	2	0
3	A	30	0	0	0	0
3	B	30	0	0	1	0
3	C	30	0	0	1	0
3	D	23	0	0	1	0
3	P	6	0	0	0	0
3	Q	3	0	0	0	0
All	All	4235	0	4157	147	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 18.

All (147) 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:D:592:ILE:C	1:D:592:ILE:HD13	1.75	1.06
1:B:563:ALA:HB2	1:B:609:ARG:O	1.64	0.97
1:D:512:ILE:HD12	1:D:512:ILE:H	1.30	0.94
1:D:547:MET:HB2	1:D:592:ILE:HG23	1.50	0.91
1:D:632:PRO:O	1:D:635:THR:HG22	1.73	0.88
1:A:586:ILE:HG12	1:D:599:ALA:HB2	1.62	0.81
1:D:592:ILE:C	1:D:592:ILE:CD1	2.48	0.80
1:D:592:ILE:HD13	1:D:593:THR:N	1.95	0.79
1:D:512:ILE:N	1:D:512:ILE:HD12	1.95	0.79
1:A:586:ILE:HD11	1:D:540:VAL:HG22	1.63	0.79
1:B:609:ARG:HA	1:B:625:GLY:O	1.84	0.78
1:A:568:MET:HE1	1:A:606:VAL:HG13	1.66	0.75
1:A:586:ILE:CD1	1:D:540:VAL:HG22	2.16	0.74
1:A:586:ILE:CD1	1:D:599:ALA:HB2	2.18	0.73
1:B:563:ALA:HB2	1:B:609:ARG:C	2.09	0.73
1:D:512:ILE:CD1	1:D:512:ILE:H	2.00	0.72
1:D:636:TRP:HA	1:D:639:LEU:HD22	1.72	0.71
1:A:586:ILE:CG1	1:D:599:ALA:HB2	2.19	0.71
1:D:592:ILE:O	1:D:592:ILE:HD13	1.92	0.70
1:C:588:HIS:ND1	1:D:550:THR:CG2	2.55	0.69
1:A:589:PRO:HD2	1:B:550:THR:CG2	2.23	0.69
1:A:531:ARG:NH2	1:A:532:ASP:O	2.28	0.67
1:C:588:HIS:ND1	1:D:550:THR:HG22	2.11	0.66
1:B:512:ILE:O	1:B:512:ILE:HG12	1.96	0.65
1:D:545:VAL:HG13	1:D:594:GLN:O	1.98	0.64
1:C:580:LEU:HD21	1:C:592:ILE:HG22	1.79	0.64
1:C:633:PRO:C	1:C:635:THR:H	2.00	0.64
1:B:512:ILE:O	1:B:512:ILE:CG1	2.43	0.64
1:C:618:ASP:HB2	3:C:28:HOH:O	1.98	0.64
1:B:517:VAL:HG22	1:B:627:VAL:HG21	1.79	0.63
1:B:525:ILE:HG12	1:B:547:MET:HG2	1.79	0.63
1:A:584:ASN:ND2	1:A:587:VAL:HG13	2.15	0.62
1:A:531:ARG:HG2	1:A:540:VAL:O	1.99	0.62
1:A:518:TYR:HE1	1:A:623:GLU:HG2	1.65	0.62
1:D:511:ASN:CG	1:D:512:ILE:HD12	2.20	0.61
1:D:547:MET:HG3	1:D:592:ILE:HD12	1.83	0.61
1:A:532:ASP:HB2	1:A:533:PRO:HA	1.83	0.60
1:C:633:PRO:HB3	1:C:636:TRP:CZ3	2.37	0.59
1:D:632:PRO:O	1:D:635:THR:CG2	2.48	0.59
1:A:589:PRO:HD2	1:B:550:THR:HG23	1.84	0.59
1:B:632:PRO:O	1:B:635:THR:CG2	2.51	0.58
1:B:570:VAL:N	3:B:114:HOH:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:LEU:HB3	1:B:535:PRO:CD	2.35	0.57
1:D:596:LEU:O	1:D:596:LEU:HD12	2.04	0.57
1:C:588:HIS:ND1	1:D:550:THR:HG21	2.19	0.56
1:D:602:GLN:HB3	1:D:604:GLU:HG2	1.88	0.56
1:C:512:ILE:HD13	1:C:512:ILE:N	2.21	0.56
1:C:547:MET:HB2	1:C:592:ILE:HG23	1.87	0.56
1:A:545:VAL:HG13	1:A:594:GLN:HB3	1.88	0.56
1:B:601:PRO:HG2	1:B:633:PRO:HB3	1.89	0.55
1:C:589:PRO:HD2	1:D:550:THR:HG21	1.87	0.55
1:C:633:PRO:HB3	1:C:636:TRP:CE3	2.41	0.55
1:D:561:GLN:HB2	1:D:611:LYS:HB3	1.88	0.55
1:A:532:ASP:OD1	1:A:532:ASP:C	2.43	0.55
1:B:600:ASN:ND2	1:B:602:GLN:OE1	2.39	0.55
1:B:632:PRO:O	1:B:635:THR:HG22	2.07	0.55
1:D:511:ASN:ND2	1:D:512:ILE:CD1	2.70	0.54
1:A:550:THR:HG21	1:C:537:ARG:CG	2.37	0.54
1:A:531:ARG:HH12	1:A:539:ASP:H	1.55	0.54
1:C:532:ASP:HB3	1:C:540:VAL:O	2.08	0.53
1:A:531:ARG:HH22	1:A:537:ARG:HE	1.55	0.53
1:A:589:PRO:HD2	1:B:550:THR:HG21	1.91	0.53
1:B:530:ALA:O	1:B:531:ARG:HB2	2.09	0.53
1:A:531:ARG:CZ	1:A:532:ASP:O	2.57	0.52
1:C:603:LYS:HG3	1:C:633:PRO:HG2	1.91	0.52
1:A:586:ILE:HD11	1:D:599:ALA:HB2	1.90	0.52
1:A:550:THR:O	1:A:550:THR:HG22	2.09	0.52
1:A:565:PRO:HA	2:P:0:TRP:HA	1.91	0.52
1:C:609:ARG:HB2	2:Q:0:TRP:CZ3	2.45	0.52
1:B:563:ALA:CB	1:B:609:ARG:C	2.79	0.51
1:B:573:GLN:HB3	1:B:574:PRO:CD	2.41	0.51
1:C:547:MET:SD	1:C:592:ILE:HG12	2.50	0.51
1:C:633:PRO:C	1:C:635:THR:N	2.62	0.51
1:D:562:SER:HB2	1:D:572:LEU:HD21	1.92	0.51
1:A:518:TYR:O	1:A:524:ARG:HA	2.12	0.50
1:A:607:ARG:NH2	1:A:626:ASP:HB3	2.26	0.50
1:D:592:ILE:HD13	1:D:593:THR:CA	2.41	0.50
1:C:575:PRO:HB2	1:C:592:ILE:HD12	1.93	0.50
1:B:633:PRO:HA	1:B:636:TRP:CD1	2.47	0.49
1:B:518:TYR:O	1:B:524:ARG:HA	2.12	0.49
1:D:547:MET:HB2	1:D:592:ILE:CG2	2.33	0.49
1:B:597:LEU:O	1:B:598:LEU:HD12	2.12	0.49
1:B:585:PRO:HG2	1:C:536:GLY:HA2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:532:ASP:HB2	1:C:533:PRO:HD2	1.96	0.48
1:C:532:ASP:HB3	1:C:540:VAL:HB	1.95	0.48
1:A:525:ILE:HG12	1:A:547:MET:HG2	1.93	0.48
1:B:534:LEU:CB	1:B:535:PRO:CD	2.91	0.48
1:D:554:PRO:HD3	1:D:582:ALA:HB2	1.95	0.48
1:A:518:TYR:CE1	1:A:623:GLU:HG2	2.46	0.47
1:A:562:SER:HB2	1:A:572:LEU:HD21	1.96	0.47
1:B:537:ARG:HB3	1:B:540:VAL:HG13	1.95	0.47
1:C:566:LYS:HA	2:Q:1:ASN:HD22	1.80	0.47
1:B:632:PRO:O	1:B:635:THR:HG23	2.13	0.47
1:D:543:VAL:HB	1:D:596:LEU:HG	1.96	0.47
1:B:563:ALA:O	1:B:564:VAL:HB	2.15	0.47
1:A:586:ILE:HD12	1:D:540:VAL:HG22	1.97	0.46
1:A:518:TYR:OH	1:A:623:GLU:OE1	2.23	0.46
1:D:553:GLN:HG3	1:D:616:MET:HE3	1.98	0.46
1:B:563:ALA:HB1	1:B:609:ARG:N	2.31	0.46
1:B:545:VAL:CG1	1:B:594:GLN:O	2.64	0.46
1:B:563:ALA:CB	1:B:609:ARG:N	2.79	0.46
1:C:524:ARG:CD	1:C:526:LEU:HD11	2.46	0.46
1:A:586:ILE:CD1	1:D:599:ALA:CB	2.92	0.46
1:B:547:MET:C	1:B:548:LEU:HD12	2.36	0.46
1:B:518:TYR:HE1	1:B:623:GLU:HG2	1.81	0.46
1:C:550:THR:O	1:C:550:THR:HG22	2.16	0.45
1:B:534:LEU:HB3	1:B:535:PRO:HD2	1.96	0.45
1:C:522:GLY:O	1:C:549:SER:HA	2.16	0.45
1:D:531:ARG:HD3	1:D:636:TRP:O	2.17	0.45
1:A:550:THR:HG21	1:C:537:ARG:HG3	1.98	0.45
1:D:592:ILE:O	1:D:592:ILE:CD1	2.61	0.45
1:D:609:ARG:HD2	3:D:33:HOH:O	2.16	0.45
1:B:547:MET:O	1:B:548:LEU:HD12	2.18	0.44
1:A:586:ILE:HG12	1:D:599:ALA:CB	2.41	0.44
1:D:511:ASN:ND2	1:D:512:ILE:HD11	2.33	0.44
1:D:511:ASN:CG	1:D:512:ILE:CD1	2.84	0.44
1:D:547:MET:CG	1:D:592:ILE:HD12	2.45	0.44
1:A:531:ARG:HH12	1:A:540:VAL:H	1.66	0.44
1:C:538:SER:O	1:C:603:LYS:HE2	2.18	0.43
1:D:550:THR:O	1:D:550:THR:HG22	2.18	0.43
1:A:550:THR:CG2	1:C:537:ARG:HD3	2.49	0.43
1:B:601:PRO:CG	1:B:633:PRO:HB3	2.49	0.43
1:B:558:ILE:HA	1:B:613:THR:O	2.19	0.43
1:B:516:THR:HA	1:B:526:LEU:HD22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:ASN:HD22	1:B:615:THR:HB	1.84	0.43
1:B:601:PRO:HG3	1:B:636:TRP:CZ2	2.54	0.43
1:B:534:LEU:CB	1:B:535:PRO:HD2	2.49	0.42
1:B:563:ALA:HB1	1:B:609:ARG:HB2	2.01	0.42
1:C:589:PRO:HD2	1:D:550:THR:CG2	2.49	0.42
1:B:563:ALA:O	1:B:564:VAL:CB	2.67	0.42
1:D:516:THR:HA	1:D:526:LEU:HD22	2.00	0.42
1:D:596:LEU:C	1:D:596:LEU:HD12	2.40	0.42
1:D:564:VAL:HG22	1:D:570:VAL:HG12	2.00	0.42
1:C:538:SER:O	1:C:538:SER:OG	2.28	0.42
1:A:550:THR:HG21	1:C:537:ARG:HB2	2.01	0.42
1:C:532:ASP:CB	1:C:540:VAL:HB	2.50	0.42
1:D:595:VAL:HG12	1:D:596:LEU:N	2.35	0.42
1:C:596:LEU:HD23	1:C:596:LEU:C	2.41	0.41
1:A:584:ASN:HD21	1:A:587:VAL:HG13	1.83	0.41
1:B:550:THR:HG22	1:B:550:THR:O	2.19	0.41
1:B:530:ALA:O	1:B:531:ARG:CB	2.68	0.41
1:D:537:ARG:HB3	1:D:539:ASP:OD2	2.20	0.41
1:B:572:LEU:HD21	1:B:594:GLN:NE2	2.36	0.41
1:B:601:PRO:HG2	1:B:602:GLN:H	1.85	0.40
1:C:531:ARG:HH22	1:C:535:PRO:HA	1.85	0.40
1:C:538:SER:HB2	1:C:637:GLY:N	2.36	0.40
1:C:544:VAL:CG1	1:C:593:THR:HG23	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	127/133 (96%)	120 (94%)	5 (4%)	2 (2%)	9	12
1	B	113/133 (85%)	94 (83%)	12 (11%)	7 (6%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	126/133 (95%)	115 (91%)	9 (7%)	2 (2%)	9	12
1	D	127/133 (96%)	121 (95%)	6 (5%)	0	100	100
2	P	6/13 (46%)	5 (83%)	1 (17%)	0	100	100
2	Q	3/13 (23%)	3 (100%)	0	0	100	100
All	All	502/558 (90%)	458 (91%)	33 (7%)	11 (2%)	6	7

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	512	ILE
1	B	531	ARG
1	B	601	PRO
1	B	617	GLY
1	C	617	GLY
1	B	563	ALA
1	C	632	PRO
1	B	638	SER
1	A	533	PRO
1	B	600	ASN
1	B	534	LEU

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	117/121 (97%)	107 (92%)	10 (8%)	10	13
1	B	107/121 (88%)	93 (87%)	14 (13%)	4	3
1	C	116/121 (96%)	101 (87%)	15 (13%)	4	3
1	D	117/121 (97%)	101 (86%)	16 (14%)	3	3
2	P	7/11 (64%)	5 (71%)	2 (29%)	0	0
2	Q	6/11 (54%)	5 (83%)	1 (17%)	2	2
All	All	470/506 (93%)	412 (88%)	58 (12%)	4	4

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

Mol	Chain	Res	Type
1	A	512	ILE
1	A	531	ARG
1	A	545	VAL
1	A	556	ARG
1	A	578	THR
1	A	593	THR
1	A	596	LEU
1	A	607	ARG
1	A	612	LEU
1	A	623	GLU
1	B	512	ILE
1	B	545	VAL
1	B	556	ARG
1	B	571	LYS
1	B	578	THR
1	B	609	ARG
1	B	611	LYS
1	B	612	LEU
1	B	615	THR
1	B	618	ASP
1	B	623	GLU
1	B	626	ASP
1	B	629	GLN
1	B	635	THR
1	C	545	VAL
1	C	548	LEU
1	C	566	LYS
1	C	567	VAL
1	C	592	ILE
1	C	598	LEU
1	C	604	GLU
1	C	609	ARG
1	C	616	MET
1	C	628	ASP
1	C	632	PRO
1	C	633	PRO
1	C	635	THR
1	C	636	TRP
1	C	638	SER
1	D	512	ILE
1	D	513	LEU
1	D	545	VAL

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Mol	Chain	Res	Type
1	D	553	GLN
1	D	556	ARG
1	D	566	LYS
1	D	578	THR
1	D	592	ILE
1	D	596	LEU
1	D	612	LEU
1	D	613	THR
1	D	623	GLU
1	D	626	ASP
1	D	634	GLU
1	D	635	THR
1	D	639	LEU
2	P	0	TRP
2	P	1	ASN
2	Q	1	ASN

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

Mol	Chain	Res	Type
1	A	588	HIS
1	A	602	GLN
1	A	629	GLN
1	B	553	GLN
1	B	557	ASN
1	B	561	GLN
1	B	588	HIS
1	B	600	ASN
1	B	629	GLN
1	C	521	HIS
1	D	511	ASN
1	D	553	GLN
1	D	588	HIS
1	D	629	GLN
2	Q	1	ASN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	129/133 (96%)	-0.02	3 (2%) 60 67	23, 37, 69, 79	0
1	B	119/133 (89%)	0.31	9 (7%) 13 17	29, 57, 87, 93	0
1	C	128/133 (96%)	-0.07	2 (1%) 72 78	22, 36, 53, 67	0
1	D	129/133 (96%)	0.15	2 (1%) 72 78	27, 50, 72, 76	0
2	P	8/13 (61%)	1.01	1 (12%) 3 5	75, 81, 84, 86	0
2	Q	7/13 (53%)	1.36	2 (28%) 0 0	69, 71, 94, 94	0
All	All	520/558 (93%)	0.12	19 (3%) 41 48	22, 43, 81, 94	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	586	ILE	4.6
1	A	639	LEU	4.4
1	B	562	SER	4.0
1	B	596	LEU	3.9
1	A	533	PRO	3.7
2	Q	-1	GLY	3.0
1	C	586	ILE	3.0
2	P	6	SER	2.8
1	C	585	PRO	2.4
1	B	573	GLN	2.3
1	B	563	ALA	2.2
1	D	585	PRO	2.2
1	B	570	VAL	2.2
1	B	564	VAL	2.2
1	A	511	ASN	2.2
1	B	635	THR	2.1
1	B	627	VAL	2.1
2	Q	0	TRP	2.1
1	B	536	GLY	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.