



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:04 AM GMT

PDB ID : 2FGE
Title : Crystal structure of presequence protease PreP from Arabidopsis thaliana
Authors : Eneqvist, T.; Johnson, K.A.
Deposited on : 2005-12-21
Resolution : 2.10 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

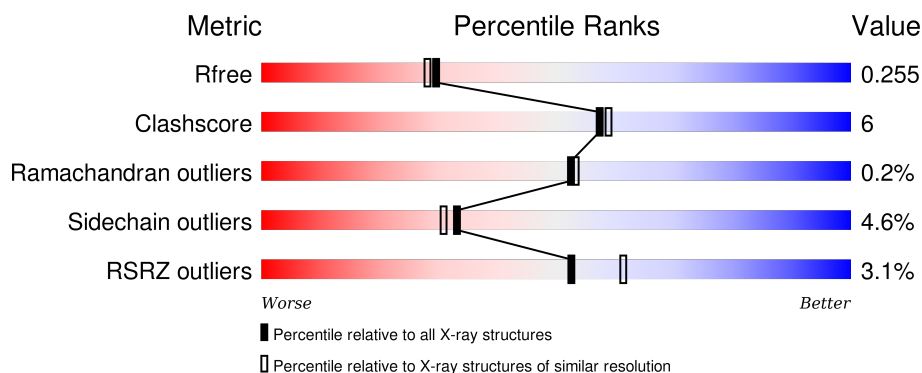
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	995	<div> <div>83%</div> <div>15%</div> <div>..</div> </div>
1	B	995	<div> <div>4%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>
2	D	6	<div> <div>67%</div> <div>83%</div> <div>17%</div> </div>
2	E	6	<div> <div>100%</div> <div>67%</div> <div>33%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16500 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 zinc metalloprotease (insulinase family).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	979	Total	C	N	O	S	Se	0	0	0
			7731	4901	1296	1502	12	20			
1	B	979	Total	C	N	O	S	Se	0	0	0
			7731	4901	1296	1502	12	20			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
A	80	GLN	GLU	ENGINEERED	UNP Q9LJL3
A	178	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
A	258	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
A	299	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
A	326	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
A	381	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
A	401	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
A	423	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
A	434	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
A	481	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
A	506	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
A	604	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
A	651	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
A	662	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
A	688	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
A	704	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
A	707	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
A	714	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
A	718	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
A	762	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
B	50	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
B	80	GLN	GLU	ENGINEERED	UNP Q9LJL3
B	178	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
B	258	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	299	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
B	326	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
B	381	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
B	401	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
B	423	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
B	434	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
B	481	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
B	506	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
B	604	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
B	651	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
B	662	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
B	688	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
B	704	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
B	707	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
B	714	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
B	718	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3
B	762	MSE	MET	MODIFIED RESIDUE	UNP Q9LJL3

- Molecule 2 is a protein called nonspecific peptide AALTRA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	6	Total	C	N	O	0	0	0
			41	25	9	7			
2	E	6	Total	C	N	O	0	0	0
			41	25	9	7			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

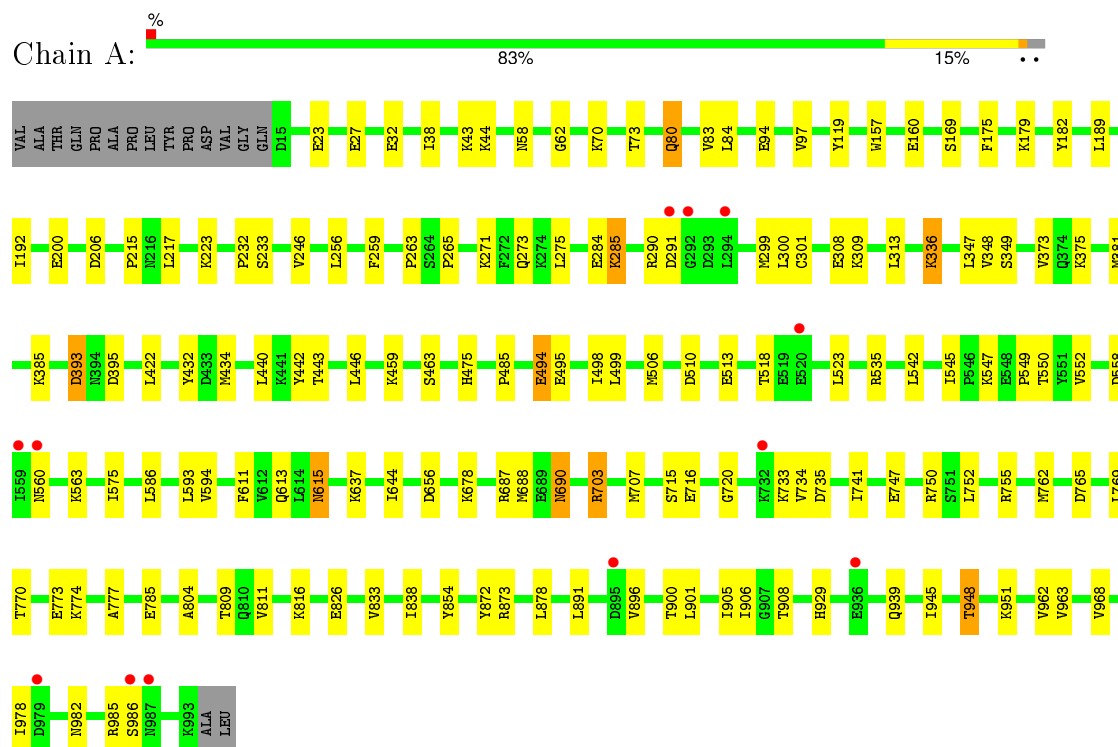
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	509	Total 509	O 509	0	0
6	B	438	Total 438	O 438	0	0
6	D	1	Total 1	O 1	0	0

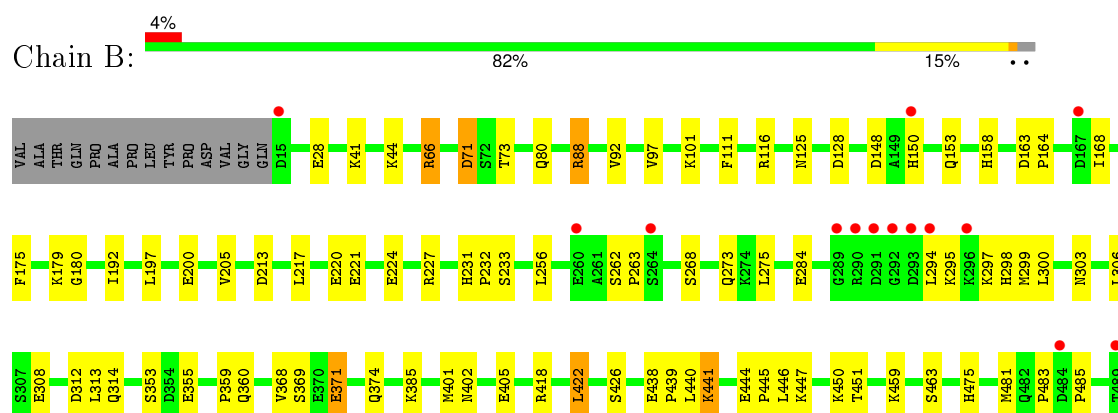
3 Residue-property plots

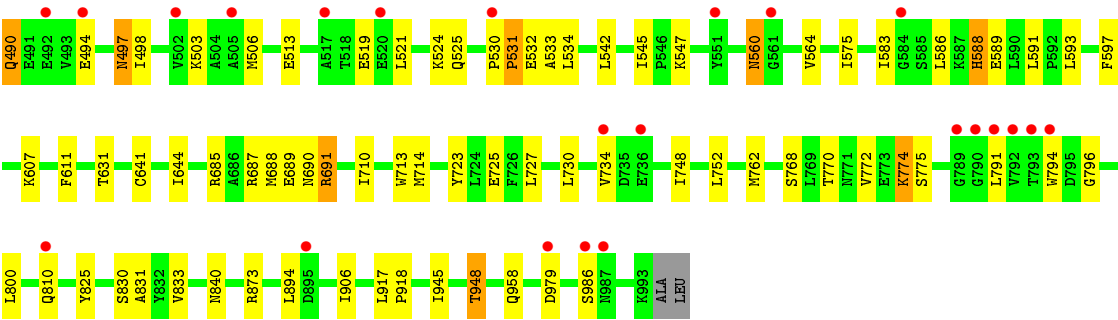
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). 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: zinc metalloprotease (insulinase family)

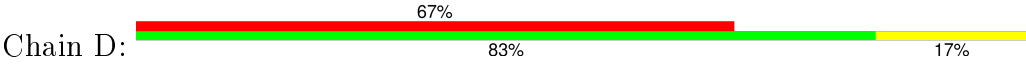


- Molecule 1: zinc metalloprotease (insulinase family)





● Molecule 2: nonspecific peptide AALTRA



● Molecule 2: nonspecific peptide AALTRA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.83Å 114.33Å 162.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.66 – 2.10 39.79 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.5 (93.66-2.10) 96.5 (39.79-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.206 , 0.256 0.206 , 0.255	Depositor DCC
R_{free} test set	5876 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.8	EDS
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 116872 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16500	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, CL

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	0.55	0/7869	0.64	1/10610 (0.0%)
1	B	0.54	0/7869	0.64	2/10610 (0.0%)
2	D	0.46	0/40	0.74	0/53
2	E	0.49	0/40	0.54	0/53
All	All	0.54	0/15818	0.64	3/21326 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	66	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	593	LEU	CA-CB-CG	5.07	126.95	115.30

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	7731	0	7652	84	0
1	B	7731	0	7652	101	0
2	D	41	0	48	0	0
2	E	41	0	48	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	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	509	0	0	7	0
6	B	438	0	0	9	0
6	D	1	0	0	0	0
All	All	16500	0	15400	185	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 (185) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:HD22	1:A:299:MSE:HE2	1.36	1.08
1:B:168:ILE:HD11	1:B:506:MSE:HE1	1.35	1.03
1:A:189:LEU:HD22	1:A:299:MSE:CE	1.88	1.02
1:A:189:LEU:CD2	1:A:299:MSE:CE	2.56	0.82
1:B:168:ILE:CD1	1:B:506:MSE:HE1	2.09	0.82
1:A:770:THR:O	1:A:773:GLU:HG2	1.80	0.81
1:B:422:LEU:HD22	1:B:440:LEU:HD22	1.62	0.80
1:B:545:ILE:HD11	1:B:906:ILE:HG12	1.63	0.79
1:A:80:GLN:O	1:A:84:LEU:HD23	1.83	0.77
1:A:733:LYS:HG2	1:A:741:ILE:HD11	1.67	0.76
1:A:44:LYS:HE2	1:A:259:PHE:O	1.85	0.76
1:B:224:GLU:OE1	1:B:227:ARG:NH1	2.20	0.74
1:A:945:ILE:O	1:A:948:THR:HG23	1.86	0.74
1:B:168:ILE:HD11	1:B:506:MSE:CE	2.16	0.74
1:A:336:LYS:NZ	6:A:1258:HOH:O	2.21	0.74
1:A:189:LEU:CD2	1:A:299:MSE:HE1	2.17	0.74
1:A:299:MSE:HE3	1:A:348:VAL:HG11	1.68	0.74
1:B:66:ARG:HD3	1:B:268:SER:O	1.90	0.72
1:A:83:VAL:HG23	1:A:84:LEU:HD22	1.70	0.72
1:A:432:TYR:HB2	1:A:434:MSE:HE2	1.73	0.70
1:B:401:MSE:HE2	1:B:450:LYS:HD2	1.71	0.70
1:A:200:GLU:H	1:A:273:GLN:HE22	1.40	0.69
1:B:92:VAL:HG12	1:B:533:ALA:HB1	1.73	0.69
1:B:494:GLU:O	1:B:498:ILE:HG12	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:CYS:HG	1:A:349:SER:HG	1.40	0.68
1:A:275:LEU:HG	1:A:308:GLU:HG3	1.78	0.66
1:A:549:PRO:HD3	1:A:939:GLN:OE1	1.95	0.66
1:B:294:LEU:HD23	1:B:483:PRO:HB2	1.77	0.65
1:B:66:ARG:HD2	1:B:268:SER:OG	1.96	0.65
1:B:447:LYS:O	1:B:451:THR:HG23	1.96	0.65
1:B:231:HIS:HD2	1:B:233:SER:H	1.44	0.65
1:B:401:MSE:HE1	1:B:446:LEU:HG	1.79	0.64
1:A:896:VAL:HG13	1:A:900:THR:HB	1.79	0.64
1:B:945:ILE:O	1:B:948:THR:HG23	1.99	0.62
1:B:101:LYS:HG2	1:B:840:ASN:HB3	1.81	0.62
1:B:564:VAL:CG1	1:B:762:MSE:HE2	2.29	0.62
1:A:27:GLU:HG3	1:A:38:ILE:HG12	1.83	0.61
1:A:200:GLU:H	1:A:273:GLN:NE2	1.97	0.61
1:A:301:CYS:SG	1:A:349:SER:OG	2.55	0.60
1:A:542:LEU:HD23	1:A:545:ILE:HD12	1.82	0.60
1:A:545:ILE:HD11	1:A:906:ILE:HG12	1.83	0.60
1:B:687:ARG:NH2	6:B:1347:HOH:O	2.33	0.60
1:B:591:LEU:HD11	1:B:714:MSE:HG2	1.83	0.59
1:A:833:VAL:HG21	1:A:948:THR:HG21	1.84	0.59
1:B:401:MSE:O	1:B:405:GLU:HG2	2.02	0.58
1:B:227:ARG:HD2	6:B:1275:HOH:O	2.02	0.58
1:A:246:VAL:HG23	6:A:1386:HOH:O	2.04	0.58
1:B:401:MSE:CE	6:B:1382:HOH:O	2.52	0.57
1:B:542:LEU:HA	1:B:545:ILE:HD12	1.85	0.57
1:B:73:THR:HB	1:B:217:LEU:HB2	1.87	0.57
1:A:678:LYS:HG2	1:A:734:VAL:HG11	1.86	0.57
1:A:422:LEU:HD22	1:A:440:LEU:HD22	1.87	0.56
1:B:299:MSE:HB2	1:B:481:MSE:HB2	1.87	0.56
1:B:444:GLU:HB2	1:B:445:PRO:HD3	1.88	0.56
1:B:768:SER:O	1:B:772:VAL:HG23	2.05	0.55
1:A:755:ARG:NH2	1:A:785:GLU:OE2	2.32	0.55
1:A:189:LEU:HD23	1:A:299:MSE:HE1	1.87	0.55
1:B:275:LEU:HA	1:B:475:HIS:ND1	2.21	0.55
1:B:402:ASN:HB3	6:B:1077:HOH:O	2.06	0.55
1:B:295:LYS:O	1:B:369:SER:HA	2.07	0.54
1:A:189:LEU:HD22	1:A:299:MSE:HE1	1.73	0.54
1:B:294:LEU:O	1:B:483:PRO:HG3	2.07	0.54
1:A:613:GLN:NE2	6:A:1133:HOH:O	2.40	0.54
1:A:896:VAL:HG12	1:A:901:LEU:HG	1.90	0.54
1:B:71:ASP:HA	1:B:205:VAL:HG11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:GLU:HB2	1:A:43:LYS:HE2	1.90	0.54
1:A:94:GLU:HG2	1:A:97:VAL:HG23	1.88	0.53
1:A:816:LYS:HE2	1:A:963:VAL:O	2.09	0.53
1:B:116:ARG:NH1	1:B:355:GLU:HG2	2.23	0.53
1:B:200:GLU:H	1:B:273:GLN:HE22	1.55	0.53
1:B:312:ASP:OD2	1:B:314:GLN:HG2	2.08	0.53
1:B:530:PRO:O	1:B:532:GLU:N	2.43	0.52
1:A:854:TYR:HD2	1:A:872:TYR:CD2	2.27	0.52
1:B:28:GLU:OE1	1:B:441:LYS:NZ	2.27	0.52
1:B:525:GLN:NE2	6:B:1199:HOH:O	2.38	0.52
1:B:688:MSE:HE1	1:B:691:ARG:CZ	2.39	0.52
1:A:690:ASN:HD22	1:A:690:ASN:C	2.13	0.52
1:B:583:ILE:HG21	1:B:644:ILE:HD12	1.93	0.51
1:B:564:VAL:HG12	1:B:762:MSE:HE2	1.92	0.51
1:A:747:GLU:HB3	1:A:750:ARG:NH2	2.26	0.50
1:A:762:MSE:HE2	1:A:769:LEU:HD22	1.92	0.50
1:B:200:GLU:H	1:B:273:GLN:NE2	2.09	0.50
1:B:833:VAL:HG21	1:B:948:THR:HG21	1.93	0.50
1:B:560:ASN:HB2	6:B:1359:HOH:O	2.12	0.50
1:A:300:LEU:HD23	1:A:373:VAL:HG13	1.92	0.50
1:A:263:PRO:C	1:A:265:PRO:HD2	2.32	0.50
1:A:73:THR:HB	1:A:217:LEU:HB2	1.94	0.50
1:B:180:GLY:HA3	1:B:873:ARG:HD3	1.92	0.50
1:A:189:LEU:CD2	1:A:299:MSE:HE2	2.21	0.50
1:B:521:LEU:O	1:B:525:GLN:HG2	2.11	0.49
1:A:192:ILE:HG21	1:A:284:GLU:HG3	1.94	0.49
1:B:588:HIS:HB2	1:B:794:TRP:CH2	2.47	0.48
1:A:182:TYR:OH	1:A:206:ASP:OD2	2.25	0.48
1:B:685:ARG:O	1:B:689:GLU:HG3	2.14	0.48
1:B:593:LEU:HB3	1:B:748:ILE:HD11	1.95	0.48
1:B:830:SER:HB2	1:B:948:THR:HB	1.96	0.47
1:B:192:ILE:HD13	1:B:284:GLU:HG3	1.96	0.47
1:B:262:SER:HB2	1:B:263:PRO:HD2	1.96	0.47
1:A:838:ILE:HD11	1:A:891:LEU:HD11	1.96	0.47
1:B:401:MSE:HE3	1:B:405:GLU:OE1	2.14	0.47
1:A:179:LYS:NZ	1:A:495:GLU:OE1	2.48	0.47
1:B:713:TRP:CD2	1:B:796:GLY:HA3	2.50	0.47
1:B:945:ILE:O	1:B:948:THR:CG2	2.62	0.47
1:B:371:GLU:H	1:B:371:GLU:HG3	1.45	0.47
1:A:393:ASP:OD2	1:A:395:ASP:HB2	2.15	0.47
1:B:917:LEU:HB3	1:B:918:PRO:HD2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:LEU:HG	1:B:308:GLU:HB2	1.97	0.46
1:B:588:HIS:NE2	1:B:714:MSE:HE3	2.30	0.46
1:A:854:TYR:HD2	1:A:872:TYR:HD2	1.64	0.46
1:A:687:ARG:NH1	1:A:688:MSE:HE3	2.30	0.46
1:A:804:ALA:HB1	1:A:978:ILE:HG12	1.96	0.46
1:A:615:ASN:ND2	6:A:1091:HOH:O	2.49	0.46
1:A:563:LYS:HE3	1:A:929:HIS:NE2	2.30	0.46
1:B:150:HIS:CE1	1:B:521:LEU:CD1	2.99	0.46
1:A:232:PRO:HB3	1:A:256:LEU:HD22	1.97	0.46
1:A:982:ASN:O	1:A:986:SER:HA	2.15	0.46
1:B:313:LEU:HD13	1:B:438:GLU:OE2	2.16	0.46
1:A:690:ASN:HB3	6:A:1191:HOH:O	2.15	0.46
1:A:878:LEU:HD22	1:A:985:ARG:CZ	2.46	0.46
1:B:459:LYS:O	1:B:463:SER:HB2	2.15	0.45
1:B:490:GLN:O	1:B:490:GLN:NE2	2.48	0.45
1:A:707:MSE:SE	1:A:968:VAL:HG21	2.66	0.45
1:A:285:LYS:HD2	1:A:285:LYS:N	2.32	0.45
1:A:169:SER:HA	1:A:499:LEU:HD13	1.98	0.45
1:A:290:ARG:HG3	1:A:485:PRO:HB2	1.97	0.45
1:A:811:VAL:HB	1:A:873:ARG:HA	1.98	0.45
1:B:71:ASP:OD2	1:B:73:THR:HG23	2.15	0.45
1:A:552:VAL:HG21	6:A:1281:HOH:O	2.17	0.45
1:B:825:TYR:OH	1:B:831:ALA:HB2	2.17	0.44
1:A:157:TRP:CE2	1:A:215:PRO:HA	2.53	0.44
1:A:434:MSE:HE1	6:A:1418:HOH:O	2.17	0.44
1:B:589:GLU:O	1:B:589:GLU:HG2	2.18	0.44
1:B:217:LEU:HD12	1:B:221:GLU:OE2	2.17	0.44
1:B:306:LEU:HB2	1:B:359:PRO:HG2	1.99	0.44
1:A:560:ASN:ND2	1:A:777:ALA:O	2.50	0.44
1:B:168:ILE:CD1	1:B:506:MSE:CE	2.88	0.44
1:B:175:PHE:CE2	1:B:179:LYS:HE3	2.52	0.44
1:B:497:ASN:ND2	6:B:1090:HOH:O	2.50	0.43
1:B:426:SER:HA	1:B:439:PRO:HG2	2.00	0.43
1:A:381:MSE:O	1:A:385:LYS:HG3	2.19	0.43
1:B:97:VAL:O	1:B:101:LYS:HG3	2.18	0.43
1:B:298:HIS:HB2	1:B:368:VAL:O	2.19	0.43
1:B:438:GLU:HA	1:B:441:LYS:HE3	2.01	0.43
1:A:494:GLU:O	1:A:498:ILE:HG12	2.18	0.43
1:B:530:PRO:O	1:B:533:ALA:N	2.49	0.43
1:A:275:LEU:HA	1:A:475:HIS:ND1	2.34	0.43
1:B:774:LYS:HZ2	1:B:774:LYS:H	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:833:VAL:HA	1:A:908:THR:OG1	2.19	0.43
1:A:459:LYS:O	1:A:463:SER:HB2	2.19	0.43
1:A:309:LYS:HG3	1:A:309:LYS:O	2.18	0.42
1:B:294:LEU:CD2	1:B:485:PRO:HD3	2.50	0.42
1:B:588:HIS:CE1	1:B:714:MSE:HE3	2.55	0.42
1:B:153:GLN:HB3	1:B:158:HIS:HB3	2.01	0.42
1:B:723:TYR:CE2	1:B:727:LEU:HD11	2.55	0.42
1:B:116:ARG:HH12	1:B:355:GLU:HG2	1.84	0.42
1:B:197:LEU:HD11	1:B:303:ASN:HB3	2.01	0.42
1:A:716:GLU:HG2	1:A:720:GLY:HA3	2.02	0.42
1:B:163:ASP:OD1	1:B:164:PRO:HD2	2.20	0.42
1:B:503:LYS:HA	1:B:506:MSE:HE3	2.02	0.42
1:B:66:ARG:HD3	1:B:268:SER:C	2.39	0.42
1:B:730:LEU:O	1:B:734:VAL:HG23	2.20	0.42
1:A:233:SER:O	1:A:265:PRO:HG3	2.20	0.41
1:A:32:GLU:HG3	1:A:443:THR:HG23	2.02	0.41
1:B:418:ARG:NH2	6:B:1385:HOH:O	2.52	0.41
1:B:232:PRO:HB3	1:B:256:LEU:HD22	2.02	0.41
1:A:542:LEU:HD21	1:A:905:ILE:HG21	2.01	0.41
1:B:830:SER:CB	1:B:948:THR:HB	2.50	0.41
1:A:160:GLU:HG2	1:A:518:THR:HG23	2.02	0.41
1:B:73:THR:HG22	1:B:213:ASP:O	2.20	0.41
1:B:111:PHE:HD2	2:E:4:THR:HG22	1.85	0.41
1:B:894:LEU:HA	6:B:1223:HOH:O	2.21	0.41
1:A:594:VAL:HG13	1:A:644:ILE:HD11	2.03	0.41
1:B:224:GLU:CD	1:B:227:ARG:HH12	2.17	0.41
1:A:690:ASN:C	1:A:690:ASN:ND2	2.74	0.41
1:A:442:TYR:O	1:A:446:LEU:HB2	2.21	0.41
1:B:503:LYS:HA	1:B:506:MSE:CE	2.51	0.40
1:B:125:ASN:HB3	1:B:128:ASP:HB3	2.02	0.40
1:B:192:ILE:HG21	1:B:284:GLU:HG3	2.04	0.40
1:A:175:PHE:CE2	1:A:179:LYS:HD2	2.56	0.40
1:A:703:ARG:HD2	1:A:703:ARG:HA	1.75	0.40
1:B:531:PRO:HA	1:B:534:LEU:HB2	2.03	0.40
1:B:631:THR:HA	1:B:641:CYS:O	2.21	0.40
1:A:506:MSE:HB3	1:A:510:ASP:HB2	2.04	0.40
1:A:62:GLY:HA2	1:A:119:TYR:O	2.22	0.40
1:B:597:PHE:CE2	1:B:752:LEU:HD21	2.56	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	977/995 (98%)	952 (97%)	25 (3%)	0	100	100
1	B	977/995 (98%)	951 (97%)	23 (2%)	3 (0%)	46	45
2	D	4/6 (67%)	4 (100%)	0	0	100	100
2	E	4/6 (67%)	4 (100%)	0	0	100	100
All	All	1962/2002 (98%)	1911 (97%)	48 (2%)	3 (0%)	52	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	531	PRO
1	B	88	ARG
1	B	986	SER

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	859/851 (101%)	822 (96%)	37 (4%)	35	34
1	B	859/851 (101%)	818 (95%)	41 (5%)	31	29
2	D	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	E	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	1724/1708 (101%)	1644 (95%)	80 (5%)	33	31

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	70	LYS
1	A	80	GLN
1	A	223	LYS
1	A	271	LYS
1	A	285	LYS
1	A	291	ASP
1	A	313	LEU
1	A	336	LYS
1	A	347	LEU
1	A	375	LYS
1	A	393	ASP
1	A	494	GLU
1	A	513	GLU
1	A	523	LEU
1	A	535	ARG
1	A	547	LYS
1	A	550	THR
1	A	558	ASP
1	A	575	ILE
1	A	586	LEU
1	A	611	PHE
1	A	615	ASN
1	A	637	LYS
1	A	656	ASP
1	A	690	ASN
1	A	703	ARG
1	A	715	SER
1	A	735	ASP
1	A	752	LEU
1	A	765	ASP
1	A	774	LYS
1	A	809	THR
1	A	826	GLU
1	A	948	THR
1	A	951	LYS
1	A	962	VAL
1	B	41	LYS
1	B	44	LYS
1	B	71	ASP
1	B	80	GLN
1	B	88	ARG
1	B	148	ASP

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Mol	Chain	Res	Type
1	B	220	GLU
1	B	297	LYS
1	B	300	LEU
1	B	353	SER
1	B	360	GLN
1	B	371	GLU
1	B	374	GLN
1	B	385	LYS
1	B	422	LEU
1	B	441	LYS
1	B	490	GLN
1	B	497	ASN
1	B	513	GLU
1	B	519	GLU
1	B	524	LYS
1	B	547	LYS
1	B	560	ASN
1	B	575	ILE
1	B	586	LEU
1	B	588	HIS
1	B	607	LYS
1	B	611	PHE
1	B	690	ASN
1	B	691	ARG
1	B	710	ILE
1	B	725	GLU
1	B	770	THR
1	B	774	LYS
1	B	775	SER
1	B	791	LEU
1	B	800	LEU
1	B	810	GLN
1	B	948	THR
1	B	958	GLN
1	B	979	ASP
2	D	5	ARG
2	E	5	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN

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Mol	Chain	Res	Type
1	A	80	GLN
1	A	194	GLN
1	A	228	GLN
1	A	234	ASN
1	A	273	GLN
1	A	360	GLN
1	A	411	ASN
1	A	525	GLN
1	A	690	ASN
1	A	756	ASN
1	A	771	ASN
1	A	876	ASN
1	B	231	HIS
1	B	234	ASN
1	B	273	GLN
1	B	360	GLN
1	B	411	ASN
1	B	490	GLN
1	B	497	ASN
1	B	560	ASN
1	B	690	ASN
1	B	771	ASN
1	B	958	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	959/995 (96%)	0.09	12 (1%) 79 84	21, 34, 53, 68	0
1	B	959/995 (96%)	0.22	37 (3%) 43 52	23, 38, 60, 73	0
2	D	6/6 (100%)	2.91	4 (66%) 0 0	78, 79, 80, 80	0
2	E	6/6 (100%)	4.00	6 (100%) 0 0	71, 72, 74, 76	0
All	All	1930/2002 (96%)	0.17	59 (3%) 52 61	21, 36, 58, 80	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	6	ALA	6.4
1	B	793	THR	5.3
2	E	1	ALA	5.1
1	B	789	GLY	4.8
1	A	560	ASN	4.7
1	A	292	GLY	4.6
1	A	291	ASP	4.5
2	D	1	ALA	4.4
1	B	294	LEU	4.2
2	D	6	ALA	4.1
2	E	5	ARG	4.0
1	B	291	ASP	3.7
1	B	292	GLY	3.7
1	B	293	ASP	3.6
1	B	584	GLY	3.6
1	B	794	TRP	3.5
1	A	987	ASN	3.5
1	B	792	VAL	3.5
2	E	3	LEU	3.5
1	A	986	SER	3.3
1	B	791	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	790	GLY	3.3
1	B	492	GLU	3.2
1	B	734	VAL	3.1
1	B	986	SER	3.0
2	D	5	ARG	2.9
1	B	551	TYR	2.8
1	B	561	GLY	2.8
1	B	264	SER	2.8
1	A	559	ILE	2.8
1	B	260	GLU	2.7
1	B	987	ASN	2.7
1	B	289	GLY	2.7
1	A	294	LEU	2.7
2	E	2	ALA	2.7
1	A	979	ASP	2.6
1	A	895	ASP	2.6
1	B	517	ALA	2.6
1	B	296	LYS	2.5
1	B	810	GLN	2.5
1	A	936	GLU	2.5
1	B	502	VAL	2.4
1	B	15	ASP	2.4
1	B	484	ASP	2.4
1	A	520	GLU	2.3
2	E	4	THR	2.3
2	D	4	THR	2.3
1	B	505	ALA	2.3
1	B	150	HIS	2.3
1	B	895	ASP	2.2
1	B	489	THR	2.2
1	A	732	LYS	2.2
1	B	736	GLU	2.2
1	B	290	ARG	2.2
1	B	494	GLU	2.2
1	B	167	ASP	2.1
1	B	979	ASP	2.1
1	B	520	GLU	2.0
1	B	530	PRO	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 carbohydrates 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. 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(\AA^2)	Q<0.9
3	ZN	A	996	1/1	0.97	0.07	-1.24	50,50,50,50	0
3	ZN	B	996	1/1	0.99	0.06	-1.43	56,56,56,56	0
4	CL	B	997	1/1	0.97	0.06	-2.42	42,42,42,42	0
5	MG	A	999	1/1	0.99	0.03	-3.17	29,29,29,29	0
5	MG	B	999	1/1	0.97	0.06	-	40,40,40,40	0
5	MG	B	998	1/1	0.96	0.03	-	35,35,35,35	0
5	MG	A	998	1/1	0.96	0.05	-	38,38,38,38	0
4	CL	A	997	1/1	0.97	0.09	-	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.