



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:32 PM UTC

PDB ID : 2FGE / pdb_00002fge
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

<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

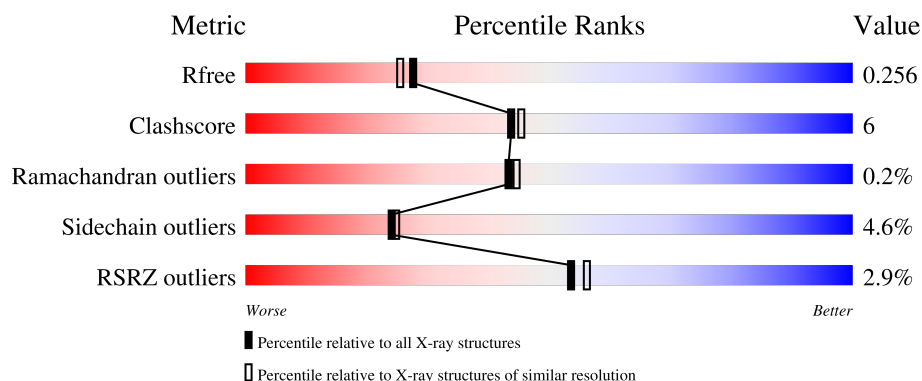
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	995	2% 82% 15% ..
1	B	995	3% 81% 16% ..
2	D	6	100% 83% 17%
2	E	6	83% 67% 33%

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 mutation	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 mutation	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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

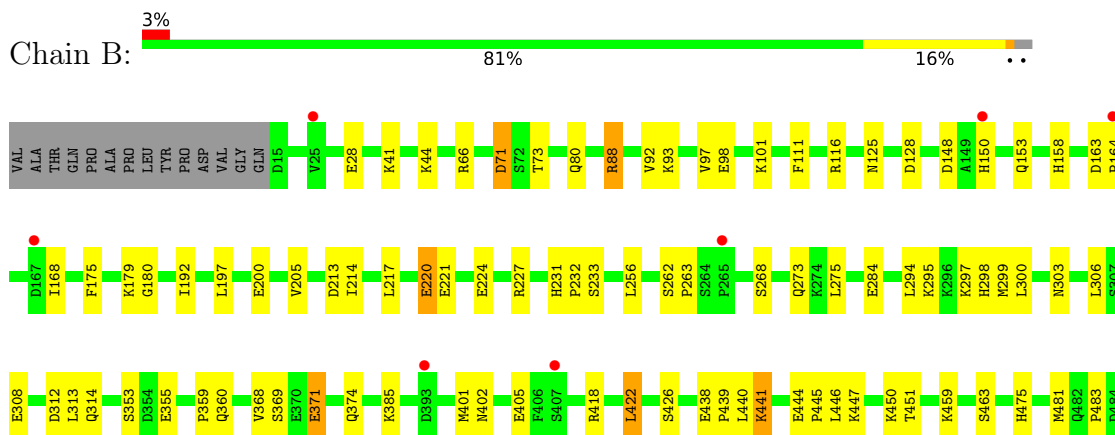
3 Residue-property plots [i](#)

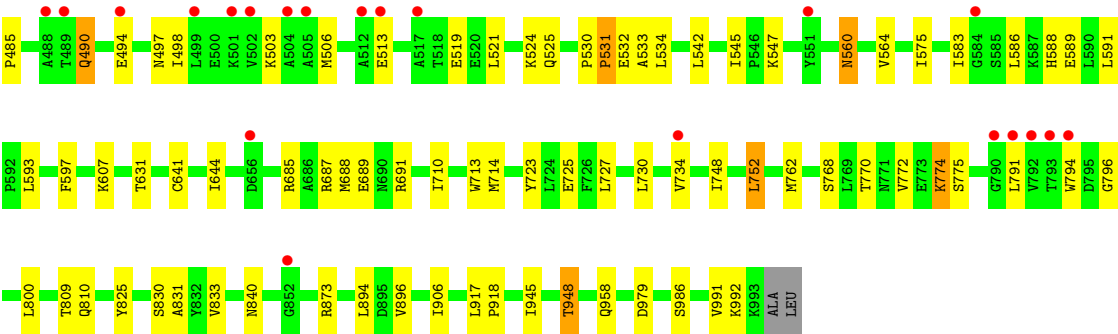
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: zinc metalloprotease (insulinase family)

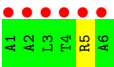
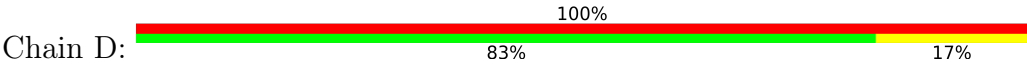


- Molecule 1: zinc metalloprotease (insulinase family)

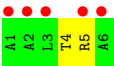
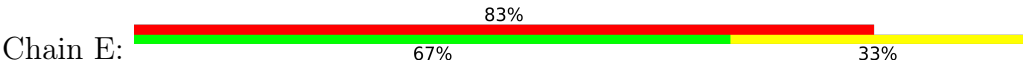




● Molecule 2: nonspecific peptide AALTRA



● 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 93.60 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.5 (93.66-2.10) 96.5 (93.60-2.10)	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 , 0.256	Depositor DCC
R_{free} test set	5876 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	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, 0.333 respectively for untwinned datasets, and 0.375, 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: MG, CL, ZN

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	0.70	1/7869 (0.0%)	0.89	4/10610 (0.0%)
1	B	0.67	1/7869 (0.0%)	0.89	1/10610 (0.0%)
2	D	0.53	0/40	0.59	0/53
2	E	0.55	0/40	0.63	0/53
All	All	0.68	2/15818 (0.0%)	0.89	5/21326 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214	ILE	CA-CB	5.46	1.56	1.54
1	B	214	ILE	CA-CB	5.30	1.56	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	ILE	CB-CA-C	-8.05	106.05	113.70
1	A	75	ILE	N-CA-CB	7.33	115.43	110.52
1	A	210	ASP	CA-C-N	5.67	126.05	119.47
1	A	210	ASP	C-N-CA	5.67	126.05	119.47
1	B	809	THR	N-CA-C	5.42	117.50	108.99

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	86	0
1	B	7731	0	7652	104	0
2	D	41	0	48	0	0
2	E	41	0	48	1	0
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	10	0
6	D	1	0	0	0	0
All	All	16500	0	15400	190	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 (190) 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:A:945:ILE:O	1:A:948:THR:HG23	1.86	0.74
1:B:224:GLU:OE1	1:B:227:ARG:NH1	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:246:VAL:HG23	6:A:1386:HOH:O	2.04	0.58
1:B:227:ARG:HD2	6:B:1275:HOH:O	2.02	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:A:678:LYS:HG2	1:A:734:VAL:HG11	1.86	0.57
1:B:73:THR:HB	1:B:217:LEU:HB2	1.87	0.57
1:A:422:LEU:HD22	1:A:440:LEU:HD22	1.87	0.56
1:A:690:ASN:C	1:A:690:ASN:HD22	2.13	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:A:263:PRO:C	1:A:265:PRO:HD2	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:23:GLU:HB2	1:A:43:LYS:HE2	1.90	0.54
1:B:71:ASP:HA	1:B:205:VAL:HG11	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: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:A:73:THR:HB	1:A:217:LEU:HB2	1.94	0.50
1:A:300:LEU:HD23	1:A:373:VAL:HG13	1.92	0.50
1:B:560:ASN:HB2	6:B:1359:HOH:O	2.12	0.50
1:B:833:VAL:HG21	1:B:948:THR:HG21	1.93	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: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:B:830:SER:HB2	1:B:948:THR:HB	1.96	0.47
1:B:66:ARG:HD3	1:B:268:SER:C	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:CYS:HG	1:A:349:SER:HG	1.45	0.47
1:B:713:TRP:CD2	1:B:796:GLY:HA3	2.50	0.47
1:B:371:GLU:H	1:B:371:GLU:HG3	1.45	0.47
1:B:945:ILE:O	1:B:948:THR:CG2	2.62	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
1:B:275:LEU:HG	1:B:308:GLU:HB2	1.97	0.46
1:A:687:ARG:NH1	1:A:688:MSE:HE3	2.30	0.46
1:A:854:TYR:HD2	1:A:872:TYR:HD2	1.64	0.46
1:B:588:HIS:NE2	1:B:714:MSE:HE3	2.30	0.46
1:A:615:ASN:ND2	6:A:1091:HOH:O	2.49	0.46
1:A:804:ALA:HB1	1:A:978:ILE:HG12	1.96	0.46
1:A:563:LYS:HE3	1:A:929:HIS:NE2	2.30	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:150:HIS:CE1	1:B:521:LEU:CD1	2.99	0.46
1:A:690:ASN:HB3	6:A:1191:HOH:O	2.15	0.46
1:B:313:LEU:HD13	1:B:438:GLU:OE2	2.16	0.46
1:A:878:LEU:HD22	1:A:985:ARG:CZ	2.46	0.46
1:B:774:LYS:HZ2	1:B:774:LYS:H	1.64	0.46
1:A:690:ASN:C	1:A:690:ASN:ND2	2.74	0.45
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:169:SER:HA	1:A:499:LEU:HD13	1.98	0.45
1:A:285:LYS:N	1:A:285:LYS:HD2	2.32	0.45
1:B:224:GLU:CD	1:B:227:ARG:HH12	2.17	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:A:552:VAL:HG21	6:A:1281:HOH:O	2.17	0.45
1:B:71:ASP:OD2	1:B:73:THR:HG23	2.15	0.45
1:B:93:LYS:NZ	6:B:1151:HOH:O	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:ASN:ND2	6:B:1090:HOH:O	2.50	0.43
1:A:410:GLU:CD	1:A:412:ASN:HB2	2.43	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:A:275:LEU:HA	1:A:475:HIS:ND1	2.34	0.43
1:B:530:PRO:O	1:B:533:ALA:N	2.49	0.43
1:A:459:LYS:O	1:A:463:SER:HB2	2.19	0.43
1:A:833:VAL:HA	1:A:908:THR:OG1	2.19	0.43
1:A:309:LYS:O	1:A:309:LYS:HG3	2.18	0.42
1:B:98:GLU:CD	1:B:534:LEU:HD22	2.44	0.42
1:B:220:GLU:CD	1:B:220:GLU:H	2.27	0.42
1:B:153:GLN:HB3	1:B:158:HIS:HB3	2.01	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: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:730:LEU:O	1:B:734:VAL:HG23	2.20	0.42
1:A:756:ASN:HD22	1:A:786:ASN:CG	2.28	0.41
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:232:PRO:HB3	1:B:256:LEU:HD22	2.02	0.41
1:B:418:ARG:NH2	6:B:1385:HOH:O	2.52	0.41
1:A:542:LEU:HD21	1:A:905:ILE:HG21	2.01	0.41
1:A:160:GLU:HG2	1:A:518:THR:HG23	2.02	0.41
1:B:830:SER:CB	1:B:948:THR:HB	2.50	0.41
1:A:594:VAL:HG13	1:A:644:ILE:HD11	2.03	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:442:TYR:O	1:A:446:LEU:HB2	2.21	0.41
1:B:125:ASN:HB3	1:B:128:ASP:HB3	2.02	0.40
1:B:503:LYS:HA	1:B:506:MSE:CE	2.51	0.40
1:A:175:PHE:CE2	1:A:179:LYS:HD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:ARG:HA	1:A:703:ARG:HD2	1.75	0.40
1:B:192:ILE:HG21	1:B:284:GLU:HG3	2.04	0.40
1:B:531:PRO:HA	1:B:534:LEU:HB2	2.03	0.40
1:A:506:MSE:HB3	1:A:510:ASP:HB2	2.04	0.40
1:B:631:THR:HA	1:B:641:CYS:O	2.21	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 [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	977/995 (98%)	952 (97%)	25 (3%)	0	100	100
1	B	977/995 (98%)	951 (97%)	23 (2%)	3 (0%)	36	36
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%)	43	44

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 [i](#)

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%)	26	27
1	B	859/851 (101%)	819 (95%)	40 (5%)	23	24
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%)	1645 (95%)	79 (5%)	24	25

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLU
1	A	70	LYS
1	A	80	GLN
1	A	223	LYS
1	A	271	LYS
1	A	284	GLU
1	A	291	ASP
1	A	313	LEU
1	A	329	THR
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	575	ILE
1	A	586	LEU
1	A	589	GLU
1	A	611	PHE
1	A	656	ASP
1	A	668	GLU
1	A	690	ASN
1	A	703	ARG
1	A	715	SER

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Mol	Chain	Res	Type
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
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	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	607	LYS
1	B	710	ILE
1	B	725	GLU
1	B	752	LEU
1	B	770	THR
1	B	774	LYS
1	B	775	SER
1	B	791	LEU
1	B	800	LEU

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Mol	Chain	Res	Type
1	B	810	GLN
1	B	896	VAL
1	B	948	THR
1	B	958	GLN
1	B	979	ASP
1	B	991	VAL
1	B	992	LYS
2	D	5	ARG
2	E	5	ARG

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

Mol	Chain	Res	Type
1	A	58	ASN
1	A	154	GLN
1	A	228	GLN
1	A	273	GLN
1	A	360	GLN
1	A	411	ASN
1	A	525	GLN
1	A	588	HIS
1	A	615	ASN
1	A	663	ASN
1	A	667	GLN
1	A	675	GLN
1	A	690	ASN
1	A	756	ASN
1	A	771	ASN
1	A	810	GLN
1	A	840	ASN
1	B	231	HIS
1	B	234	ASN
1	B	247	HIS
1	B	273	GLN
1	B	360	GLN
1	B	411	ASN
1	B	482	GLN
1	B	490	GLN
1	B	497	ASN
1	B	560	ASN
1	B	690	ASN
1	B	771	ASN

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Mol	Chain	Res	Type
1	B	810	GLN
1	B	840	ASN
1	B	916	GLN
1	B	958	GLN

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 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 [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	959/995 (96%)	0.16	17 (1%) 67 70	21, 34, 53, 68	0
1	B	959/995 (96%)	0.37	28 (2%) 53 56	23, 38, 60, 73	0
2	D	6/6 (100%)	3.79	6 (100%) 0 0	78, 79, 80, 80	0
2	E	6/6 (100%)	3.43	5 (83%) 0 0	71, 72, 74, 76	0
All	All	1930/2002 (96%)	0.28	56 (2%) 53 56	21, 36, 58, 80	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1	ALA	5.4
2	E	6	ALA	5.3
2	D	6	ALA	4.7
2	E	1	ALA	4.5
1	A	560	ASN	4.3
1	B	794	TRP	4.1
2	E	5	ARG	3.6
2	D	2	ALA	3.6
1	A	292	GLY	3.6
2	D	5	ARG	3.5
1	B	793	THR	3.5
2	D	3	LEU	3.3
1	B	792	VAL	3.2
2	E	2	ALA	3.2
1	B	791	LEU	3.1
2	E	3	LEU	3.1
1	B	852	GLY	3.0
1	A	291	ASP	2.7
1	A	559	ILE	2.7
1	B	551	TYR	2.6
1	A	301	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	790	GLY	2.6
1	B	505	ALA	2.6
1	B	167	ASP	2.6
1	B	502	VAL	2.5
1	A	561	GLY	2.5
1	B	504	ALA	2.5
1	B	499	LEU	2.5
1	A	895	ASP	2.4
1	B	584	GLY	2.4
1	A	25	VAL	2.3
1	B	488	ALA	2.3
1	A	393	ASP	2.3
1	A	545	ILE	2.3
1	B	164	PRO	2.3
1	A	313	LEU	2.3
1	B	150	HIS	2.3
2	D	4	THR	2.3
1	B	265	PRO	2.2
1	B	489	THR	2.2
1	A	266	ASN	2.2
1	B	656	ASP	2.2
1	A	991	VAL	2.1
1	B	407	SER	2.1
1	A	988	PHE	2.1
1	B	512	ALA	2.1
1	A	936	GLU	2.1
1	B	494	GLU	2.1
1	B	25	VAL	2.1
1	B	517	ALA	2.1
1	A	730	LEU	2.0
1	B	393	ASP	2.0
1	B	513	GLU	2.0
1	B	734	VAL	2.0
1	A	992	LYS	2.0
1	B	501	LYS	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
4	CL	A	997	1/1	0.96	0.05	36,36,36,36	0
4	CL	B	997	1/1	0.96	0.07	42,42,42,42	0
3	ZN	A	996	1/1	0.98	0.05	50,50,50,50	0
3	ZN	B	996	1/1	0.98	0.07	56,56,56,56	0
5	MG	A	998	1/1	0.99	0.03	38,38,38,38	0
5	MG	A	999	1/1	0.99	0.02	29,29,29,29	0
5	MG	B	998	1/1	0.99	0.06	35,35,35,35	0
5	MG	B	999	1/1	0.99	0.02	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.