



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:50 AM UTC

PDB ID : 4BEV / pdb_00004bev
Title : ATPase crystal structure with bound phosphate analogue
Authors : Mattle, D.; Drachmann, N.D.; Liu, X.Y.; Gourdon, P.; Pedersen, B.P.; Morth, P.; Wang, J.; Nissen, P.
Deposited on : 2013-03-12
Resolution : 3.58 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

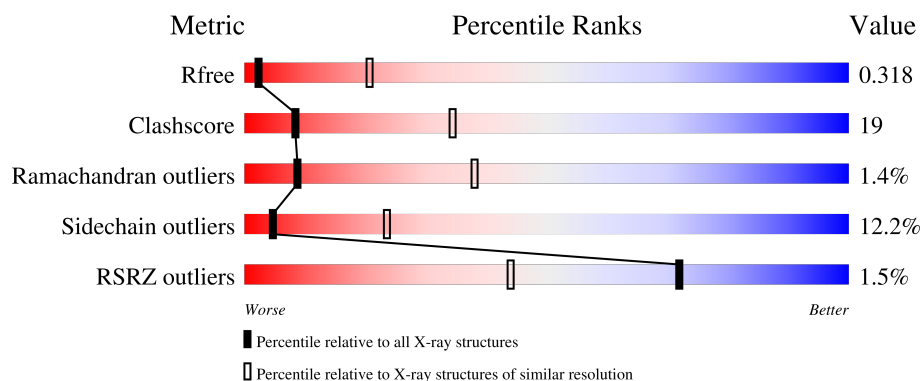
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.58 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	1521 (3.66-3.50)
Clashscore	190562	1595 (3.66-3.50)
Ramachandran outliers	187476	1551 (3.66-3.50)
Sidechain outliers	187428	1551 (3.66-3.50)
RSRZ outliers	180081	1520 (3.66-3.50)

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 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	736	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MGF	A	950	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4941 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.

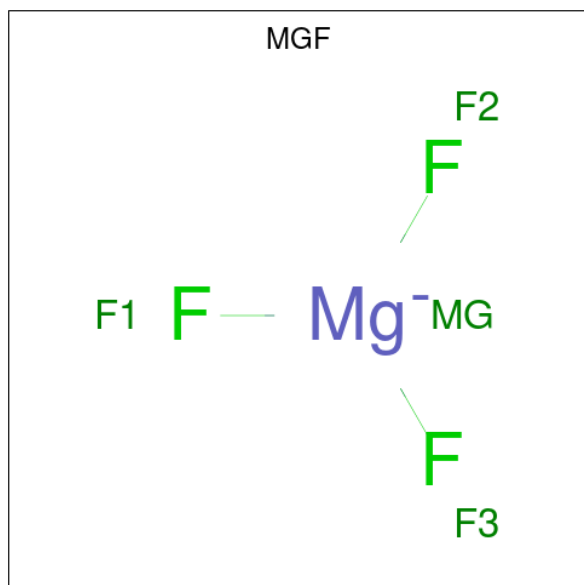
- Molecule 1 is a protein called COPPER EFFLUX ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	663	Total	C	N	O	S	0	0	0
			4934	3156	844	909	25			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is TRIFLUOROMAGNESATE (CCD ID: MGF) (formula: F₃Mg).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	F	Mg	0	0
			4	3	1		

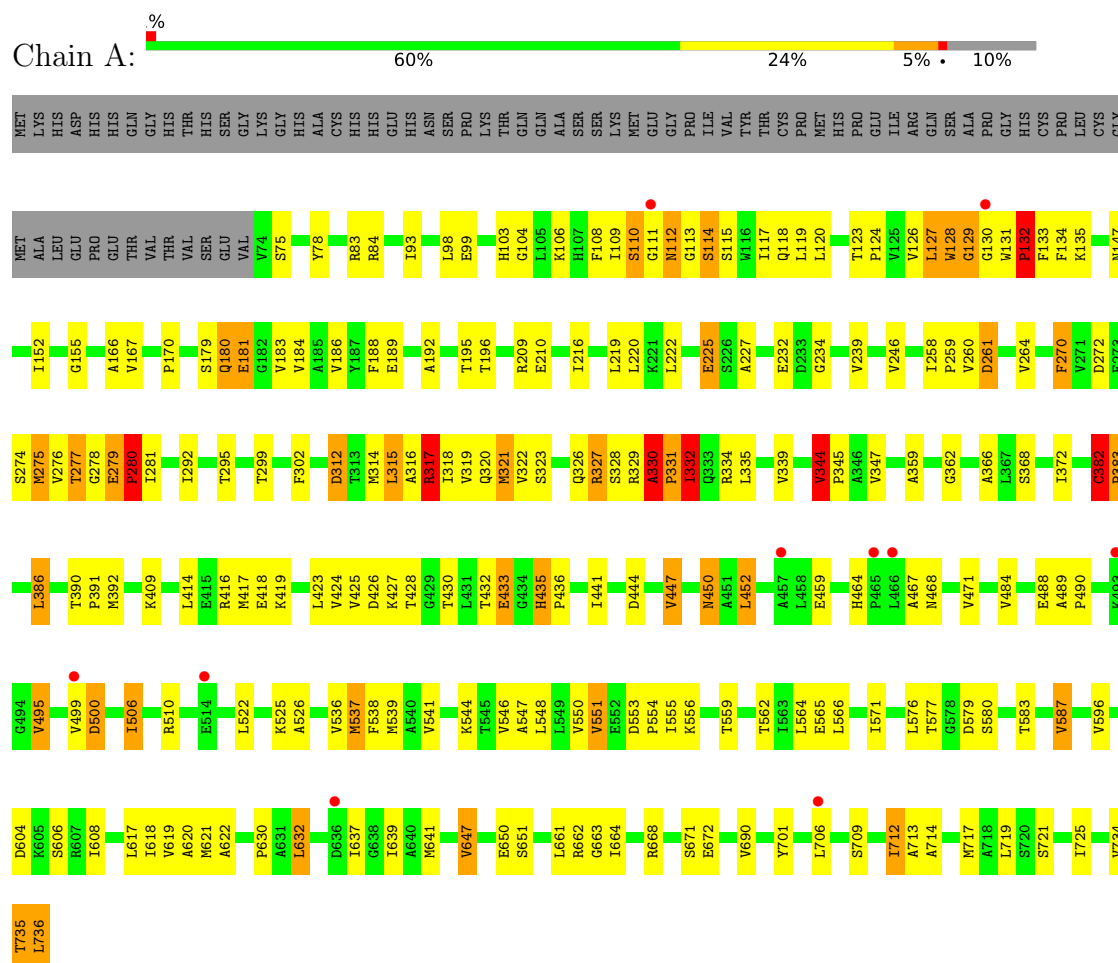
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		

3 Residue-property plots

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: COPPER EFFLUX ATPASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	44.36Å 72.65Å 328.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.45 – 3.58 29.45 – 3.60	Depositor EDS
% Data completeness (in resolution range)	96.5 (29.45-3.58) 97.7 (29.45-3.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 3.57Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.270 , 0.315 0.286 , 0.318	Depositor DCC
R_{free} test set	644 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	128.6	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 73.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4941	wwPDB-VP
Average B, all atoms (Å ²)	155.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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, MGF

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	0.78	12/5017 (0.2%)	1.05	34/6812 (0.5%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	435	HIS	C-N	26.03	1.67	1.33
1	A	332	ILE	C-N	-24.95	0.98	1.33
1	A	671	SER	C-N	-10.15	1.21	1.33
1	A	210	GLU	C-N	-9.70	1.20	1.33
1	A	147	ASN	C-N	-7.17	1.24	1.33
1	A	382	CYS	C-N	6.14	1.40	1.33
1	A	326	GLN	C-N	6.03	1.41	1.33
1	A	344	VAL	CA-CB	5.24	1.57	1.53
1	A	280	PRO	N-CD	5.23	1.55	1.47
1	A	131	TRP	C-N	5.14	1.41	1.34
1	A	551	VAL	C-N	5.08	1.40	1.33
1	A	132	PRO	N-CD	5.03	1.54	1.47

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	ALA	C-N-CD	-17.68	52.52	125.00
1	A	327	ARG	O-C-N	16.98	143.70	122.81
1	A	327	ARG	CA-C-N	-14.21	94.40	121.54
1	A	327	ARG	C-N-CA	-14.21	94.40	121.54
1	A	210	GLU	CA-C-N	11.79	138.72	122.34
1	A	210	GLU	C-N-CA	11.79	138.72	122.34
1	A	210	GLU	O-C-N	-10.85	107.77	122.74
1	A	332	ILE	O-C-N	-10.58	111.97	122.98
1	A	326	GLN	O-C-N	-10.23	111.04	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	GLY	CA-C-N	7.99	127.88	120.21
1	A	362	GLY	C-N-CA	7.99	127.88	120.21
1	A	435	HIS	CA-C-N	-7.81	111.96	119.85
1	A	435	HIS	C-N-CA	-7.81	111.96	119.85
1	A	279	GLU	N-CA-C	-7.67	98.88	110.07
1	A	317	ARG	N-CA-C	-7.66	102.93	111.28
1	A	435	HIS	O-C-N	7.60	128.34	121.35
1	A	112	ASN	N-CA-C	-7.39	101.32	110.41
1	A	382	CYS	CA-C-N	-6.92	113.53	120.31
1	A	382	CYS	C-N-CA	-6.92	113.53	120.31
1	A	734	VAL	N-CA-C	6.62	117.58	108.84
1	A	326	GLN	CA-C-N	6.18	130.08	120.75
1	A	326	GLN	C-N-CA	6.18	130.08	120.75
1	A	131	TRP	CA-C-N	-5.82	112.59	119.05
1	A	131	TRP	C-N-CA	-5.82	112.59	119.05
1	A	279	GLU	CA-C-N	-5.72	112.69	119.84
1	A	279	GLU	C-N-CA	-5.72	112.69	119.84
1	A	133	PHE	N-CA-C	5.60	117.38	111.28
1	A	332	ILE	CA-C-N	5.38	129.52	121.72
1	A	332	ILE	C-N-CA	5.38	129.52	121.72
1	A	129	GLY	N-CA-C	-5.28	106.39	112.73
1	A	277	THR	N-CA-C	-5.27	99.57	110.80
1	A	383	PRO	CA-N-CD	-5.13	104.81	112.00
1	A	93	ILE	CB-CA-C	-5.03	108.92	113.70
1	A	551	VAL	O-C-N	5.02	129.60	122.97

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	4934	0	5123	192	0
2	A	1	0	0	0	0
3	A	4	0	0	3	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4941	0	5123	192	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 19.

All (192) 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:435:HIS:C	1:A:436:PRO:N	1.67	1.50
1:A:441:ILE:CD1	1:A:452:LEU:HD22	1.53	1.39
1:A:130:GLY:CA	1:A:134:PHE:HE1	1.23	1.34
1:A:123:THR:CG2	1:A:127:LEU:HD11	1.63	1.25
1:A:123:THR:HG22	1:A:127:LEU:CD1	1.67	1.24
1:A:441:ILE:HD11	1:A:452:LEU:CD2	1.66	1.23
1:A:274:SER:CA	1:A:278:GLY:HA2	1.71	1.21
1:A:130:GLY:CA	1:A:134:PHE:CE1	2.13	1.19
1:A:123:THR:O	1:A:127:LEU:CD1	1.89	1.17
1:A:123:THR:C	1:A:127:LEU:HD12	1.69	1.17
1:A:130:GLY:HA3	1:A:134:PHE:CE1	1.78	1.14
1:A:123:THR:HG23	1:A:127:LEU:HD11	1.15	1.14
1:A:123:THR:O	1:A:127:LEU:HD12	0.97	1.14
1:A:123:THR:CG2	1:A:127:LEU:CD1	2.23	1.08
1:A:130:GLY:HA3	1:A:134:PHE:HE1	0.97	1.06
1:A:327:ARG:O	1:A:328:SER:OG	1.74	1.06
1:A:274:SER:HA	1:A:278:GLY:HA2	1.11	1.05
1:A:111:GLY:HA3	1:A:183:VAL:HG11	1.40	1.03
1:A:536:VAL:HG22	1:A:550:VAL:HG12	1.39	1.02
1:A:126:VAL:O	1:A:130:GLY:HA3	1.61	1.00
1:A:123:THR:HG22	1:A:127:LEU:HD13	1.45	0.99
1:A:274:SER:HA	1:A:278:GLY:CA	1.92	0.99
1:A:447:VAL:CG2	1:A:450:ASN:HB2	1.97	0.94
1:A:280:PRO:CD	1:A:281:ILE:H	1.79	0.94
1:A:280:PRO:CG	1:A:281:ILE:H	1.80	0.93
1:A:441:ILE:CD1	1:A:452:LEU:CD2	2.35	0.92
1:A:277:THR:HG22	1:A:279:GLU:HB2	1.51	0.91
1:A:276:VAL:O	1:A:277:THR:HB	1.70	0.90
1:A:441:ILE:HD11	1:A:452:LEU:HD22	0.90	0.89
1:A:327:ARG:C	1:A:328:SER:HG	1.79	0.89
1:A:274:SER:C	1:A:278:GLY:HA2	1.97	0.89
1:A:276:VAL:C	1:A:278:GLY:H	1.82	0.86
1:A:277:THR:CG2	1:A:279:GLU:HB2	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLY:O	1:A:117:ILE:HG13	1.77	0.85
1:A:277:THR:HG22	1:A:279:GLU:H	1.42	0.84
1:A:327:ARG:C	1:A:328:SER:OG	2.20	0.83
1:A:180:GLN:HG2	1:A:181:GLU:OE1	1.78	0.83
1:A:130:GLY:HA2	1:A:134:PHE:HE1	1.44	0.82
1:A:280:PRO:HG2	1:A:281:ILE:H	1.44	0.81
1:A:276:VAL:C	1:A:278:GLY:N	2.36	0.80
1:A:447:VAL:HG22	1:A:450:ASN:HB2	1.61	0.79
1:A:280:PRO:HD2	1:A:281:ILE:H	1.47	0.79
1:A:280:PRO:CG	1:A:281:ILE:N	2.43	0.78
1:A:126:VAL:O	1:A:130:GLY:CA	2.31	0.78
1:A:315:LEU:O	1:A:318:ILE:HB	1.85	0.76
1:A:536:VAL:HG22	1:A:550:VAL:CG1	2.16	0.76
1:A:735:THR:HA	1:A:736:LEU:HB2	1.66	0.75
1:A:129:GLY:O	1:A:132:PRO:HD2	1.87	0.74
1:A:435:HIS:C	1:A:436:PRO:CA	2.60	0.73
1:A:119:LEU:HD23	1:A:119:LEU:C	2.13	0.73
1:A:495:VAL:HG23	1:A:506:ILE:HG23	1.69	0.72
1:A:111:GLY:HA3	1:A:183:VAL:CG1	2.16	0.72
1:A:99:GLU:HG2	1:A:118:GLN:HE22	1.54	0.71
1:A:114:SER:O	1:A:118:GLN:HG3	1.91	0.70
1:A:500:ASP:N	1:A:500:ASP:OD1	2.24	0.70
1:A:106:LYS:H	1:A:109:ILE:HD13	1.56	0.70
1:A:280:PRO:HG2	1:A:281:ILE:N	2.05	0.69
1:A:123:THR:C	1:A:127:LEU:CD1	2.54	0.69
1:A:181:GLU:OE1	1:A:181:GLU:N	2.26	0.69
1:A:577:THR:HA	3:A:950:MGF:F1	1.82	0.69
1:A:274:SER:O	1:A:278:GLY:HA2	1.92	0.69
1:A:280:PRO:CD	1:A:281:ILE:N	2.46	0.68
1:A:274:SER:O	1:A:278:GLY:CA	2.42	0.68
1:A:344:VAL:HG13	1:A:345:PRO:HD3	1.76	0.67
1:A:383:PRO:HD2	1:A:386:LEU:HD11	1.75	0.67
1:A:186:VAL:HG21	1:A:188:PHE:CD2	2.29	0.67
1:A:276:VAL:O	1:A:277:THR:CB	2.43	0.67
1:A:130:GLY:HA2	1:A:134:PHE:CE1	2.25	0.64
1:A:277:THR:HG22	1:A:279:GLU:CB	2.27	0.63
1:A:155:GLY:HA3	1:A:382:CYS:SG	2.38	0.62
1:A:314:MET:HE1	1:A:317:ARG:NH2	2.15	0.62
1:A:506:ILE:HD11	1:A:537:MET:HB3	1.83	0.61
1:A:186:VAL:CG2	1:A:188:PHE:CD2	2.83	0.61
1:A:426:ASP:OD2	3:A:950:MGF:F2	2.07	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:GLY:CA	1:A:183:VAL:HG11	2.25	0.61
1:A:416:ARG:HB2	1:A:637:ILE:HD11	1.82	0.61
1:A:314:MET:CE	1:A:317:ARG:NH2	2.64	0.60
1:A:98:LEU:HB3	1:A:118:GLN:HE21	1.66	0.60
1:A:124:PRO:O	1:A:128:TRP:HB2	2.02	0.59
1:A:662:ARG:N	1:A:663:GLY:HA3	2.17	0.59
1:A:84:ARG:NH1	1:A:132:PRO:HD3	2.18	0.59
1:A:447:VAL:HG23	1:A:450:ASN:H	1.67	0.59
1:A:314:MET:HE1	1:A:317:ARG:HH22	1.66	0.58
1:A:128:TRP:O	1:A:132:PRO:HD3	2.04	0.58
1:A:276:VAL:O	1:A:278:GLY:N	2.25	0.58
1:A:279:GLU:OE2	1:A:428:THR:OG1	2.07	0.57
1:A:435:HIS:CA	1:A:436:PRO:N	2.63	0.57
1:A:170:PRO:HB3	1:A:184:VAL:HG23	1.86	0.56
1:A:258:ILE:HD12	1:A:295:THR:HB	1.87	0.56
1:A:606:SER:HB2	1:A:630:PRO:HB2	1.87	0.56
1:A:277:THR:HG22	1:A:279:GLU:N	2.18	0.56
1:A:425:VAL:HG12	1:A:622:ALA:HB3	1.87	0.56
1:A:359:ALA:HA	1:A:366:ALA:HB1	1.88	0.56
1:A:134:PHE:HD1	1:A:134:PHE:H	1.51	0.56
1:A:272:ASP:OD1	1:A:280:PRO:O	2.24	0.55
1:A:280:PRO:O	1:A:281:ILE:C	2.50	0.55
1:A:166:ALA:HB1	1:A:184:VAL:HB	1.88	0.55
1:A:280:PRO:HD2	1:A:281:ILE:N	2.16	0.55
1:A:166:ALA:HB1	1:A:184:VAL:CG1	2.38	0.54
1:A:261:ASP:HB3	1:A:292:ILE:HA	1.89	0.54
1:A:426:ASP:CG	3:A:950:MGF:F2	2.40	0.54
1:A:219:LEU:HD12	1:A:650:GLU:HG3	1.89	0.54
1:A:126:VAL:O	1:A:130:GLY:N	2.41	0.54
1:A:419:LYS:HB3	1:A:618:ILE:HD13	1.91	0.53
1:A:447:VAL:HG23	1:A:450:ASN:HB2	1.89	0.53
1:A:318:ILE:O	1:A:322:VAL:HG23	2.09	0.53
1:A:316:ALA:HA	1:A:319:VAL:HG22	1.90	0.52
1:A:468:ASN:HA	1:A:471:VAL:HG22	1.90	0.52
1:A:124:PRO:O	1:A:128:TRP:CB	2.58	0.52
1:A:386:LEU:HD12	1:A:386:LEU:H	1.75	0.52
1:A:418:GLU:HG3	1:A:672:GLU:HG2	1.90	0.51
1:A:75:SER:HB3	1:A:78:TYR:HB3	1.91	0.51
1:A:275:MET:HE1	1:A:315:LEU:HD23	1.93	0.51
1:A:409:LYS:NZ	1:A:650:GLU:OE1	2.43	0.51
1:A:316:ALA:O	1:A:319:VAL:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:MET:HG3	1:A:668:ARG:HA	1.94	0.49
1:A:314:MET:O	1:A:318:ILE:HG12	2.12	0.49
1:A:427:LYS:HD2	1:A:587:VAL:HG11	1.95	0.49
1:A:183:VAL:HG23	1:A:183:VAL:O	2.12	0.49
1:A:209:ARG:HH12	1:A:334:ARG:HH21	1.59	0.49
1:A:418:GLU:HG3	1:A:672:GLU:CG	2.43	0.49
1:A:417:MET:HE2	1:A:637:ILE:HG21	1.94	0.49
1:A:714:ALA:HA	1:A:717:MET:HE2	1.95	0.49
1:A:274:SER:O	1:A:278:GLY:HA3	2.11	0.49
1:A:319:VAL:HG23	1:A:320:GLN:N	2.27	0.49
1:A:330:ALA:O	1:A:331:PRO:CB	2.55	0.49
1:A:134:PHE:CD1	1:A:134:PHE:N	2.78	0.48
1:A:621:MET:HG3	1:A:632:LEU:HD13	1.95	0.48
1:A:441:ILE:HD12	1:A:452:LEU:CD2	2.38	0.48
1:A:430:THR:HA	1:A:641:MET:HE2	1.95	0.48
1:A:432:THR:OG1	1:A:553:ASP:OD1	2.32	0.48
1:A:112:ASN:OD1	1:A:112:ASN:N	2.46	0.48
1:A:484:VAL:HG12	1:A:499:VAL:HG22	1.96	0.48
1:A:562:THR:HG21	1:A:662:ARG:HA	1.94	0.47
1:A:576:LEU:HD21	1:A:608:ILE:HB	1.96	0.47
1:A:277:THR:C	1:A:279:GLU:N	2.72	0.47
1:A:292:ILE:O	1:A:295:THR:OG1	2.26	0.47
1:A:129:GLY:C	1:A:132:PRO:HD2	2.39	0.47
1:A:433:GLU:H	1:A:433:GLU:HG2	1.60	0.47
1:A:709:SER:HB3	1:A:712:ILE:HG23	1.96	0.47
1:A:459:GLU:HB3	1:A:467:ALA:HB1	1.97	0.46
1:A:84:ARG:NH1	1:A:128:TRP:O	2.45	0.46
1:A:390:THR:HB	1:A:391:PRO:HD3	1.98	0.46
1:A:522:LEU:HB3	1:A:548:LEU:HD13	1.99	0.45
1:A:526:ALA:HB2	1:A:548:LEU:HD21	1.98	0.45
1:A:721:SER:O	1:A:725:ILE:HG12	2.15	0.45
1:A:225:GLU:H	1:A:225:GLU:HG2	1.53	0.45
1:A:499:VAL:HA	1:A:500:ASP:HA	1.66	0.45
1:A:84:ARG:NH1	1:A:132:PRO:CD	2.80	0.44
1:A:432:THR:OG1	1:A:554:PRO:O	2.31	0.44
1:A:99:GLU:HG3	1:A:189:GLU:HB2	1.98	0.44
1:A:317:ARG:O	1:A:321:MET:HG3	2.17	0.44
1:A:275:MET:C	1:A:276:VAL:HG13	2.43	0.44
1:A:128:TRP:O	1:A:132:PRO:CD	2.66	0.44
1:A:277:THR:C	1:A:279:GLU:H	2.25	0.44
1:A:329:ARG:O	1:A:330:ALA:HB3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:THR:CG2	1:A:662:ARG:HA	2.47	0.43
1:A:275:MET:HE2	1:A:275:MET:HB3	1.61	0.43
1:A:735:THR:HG22	1:A:736:LEU:C	2.43	0.43
1:A:368:SER:O	1:A:372:ILE:HG12	2.19	0.43
1:A:119:LEU:HD23	1:A:120:LEU:N	2.33	0.43
1:A:330:ALA:O	1:A:331:PRO:HB3	2.19	0.42
1:A:566:LEU:HB3	1:A:571:ILE:HB	2.02	0.42
1:A:103:HIS:CG	1:A:109:ILE:HG21	2.53	0.42
1:A:166:ALA:HB1	1:A:184:VAL:CB	2.50	0.42
1:A:264:VAL:HG13	1:A:302:PHE:HB2	2.02	0.42
1:A:417:MET:HE1	1:A:639:ILE:HD11	2.02	0.42
1:A:556:LYS:HB2	1:A:559:THR:OG1	2.20	0.42
1:A:332:ILE:H	1:A:332:ILE:HG13	1.69	0.42
1:A:119:LEU:O	1:A:123:THR:OG1	2.27	0.42
1:A:335:LEU:O	1:A:339:VAL:HG12	2.19	0.42
1:A:579:ASP:OD1	1:A:580:SER:N	2.43	0.41
1:A:604:ASP:O	1:A:608:ILE:HG12	2.19	0.41
1:A:506:ILE:HD12	1:A:538:PHE:O	2.21	0.41
1:A:152:ILE:HD11	1:A:386:LEU:HD13	2.03	0.41
1:A:270:PHE:HE1	1:A:464:HIS:CE1	2.39	0.41
1:A:98:LEU:O	1:A:103:HIS:NE2	2.53	0.41
1:A:115:SER:HB3	1:A:167:VAL:HG22	2.02	0.41
1:A:123:THR:O	1:A:127:LEU:CG	2.64	0.41
1:A:227:ALA:HB3	1:A:239:VAL:HG23	2.03	0.41
1:A:539:MET:HB3	1:A:547:ALA:HB3	2.03	0.41
1:A:423:LEU:HD12	1:A:620:ALA:O	2.20	0.41
1:A:220:LEU:HD13	1:A:647:VAL:HG21	2.03	0.41
1:A:489:ALA:HA	1:A:490:PRO:HD3	1.82	0.41
1:A:661:LEU:HD23	1:A:661:LEU:H	1.85	0.41
1:A:444:ASP:OD1	1:A:444:ASP:N	2.53	0.41
1:A:192:ALA:O	1:A:195:THR:OG1	2.32	0.40
1:A:712:ILE:HG13	1:A:713:ALA:N	2.34	0.40
1:A:103:HIS:HA	1:A:104:GLY:HA3	1.85	0.40
1:A:544:LYS:O	1:A:546:VAL:HG13	2.21	0.40
1:A:109:ILE:C	1:A:110:SER:OG	2.63	0.40
1:A:119:LEU:C	1:A:119:LEU:CD2	2.85	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	661/736 (90%)	611 (92%)	41 (6%)	9 (1%)	9 38

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	ALA
1	A	331	PRO
1	A	280	PRO
1	A	232	GLU
1	A	108	PHE
1	A	299	THR
1	A	312	ASP
1	A	259	PRO
1	A	234	GLY

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	523/586 (89%)	459 (88%)	64 (12%)	5 23

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ARG
1	A	110	SER

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Mol	Chain	Res	Type
1	A	114	SER
1	A	127	LEU
1	A	128	TRP
1	A	132	PRO
1	A	135	LYS
1	A	179	SER
1	A	180	GLN
1	A	181	GLU
1	A	196	THR
1	A	216	ILE
1	A	222	LEU
1	A	225	GLU
1	A	246	VAL
1	A	260	VAL
1	A	261	ASP
1	A	270	PHE
1	A	275	MET
1	A	312	ASP
1	A	315	LEU
1	A	317	ARG
1	A	321	MET
1	A	323	SER
1	A	332	ILE
1	A	344	VAL
1	A	347	VAL
1	A	382	CYS
1	A	386	LEU
1	A	392	MET
1	A	414	LEU
1	A	424	VAL
1	A	433	GLU
1	A	447	VAL
1	A	450	ASN
1	A	452	LEU
1	A	488	GLU
1	A	495	VAL
1	A	500	ASP
1	A	506	ILE
1	A	510	ARG
1	A	525	LYS
1	A	537	MET
1	A	541	VAL

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Mol	Chain	Res	Type
1	A	551	VAL
1	A	555	ILE
1	A	564	LEU
1	A	565	GLU
1	A	583	THR
1	A	587	VAL
1	A	596	VAL
1	A	617	LEU
1	A	619	VAL
1	A	632	LEU
1	A	647	VAL
1	A	651	SER
1	A	664	ILE
1	A	690	VAL
1	A	701	TYR
1	A	706	LEU
1	A	712	ILE
1	A	719	LEU
1	A	735	THR
1	A	736	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	139	GLN
1	A	464	HIS
1	A	513	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is 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	MGF	A	950	4,1	0,3,3	-	-	-		

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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	950	MGF	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	435:HIS	C	436:PRO	N	1.67

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	210:GLU	C	211:GLN	N	1.20
1	A	332:ILE	C	333:GLN	N	0.98

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	663/736 (90%)	0.12	10 (1%) 72 44	86, 148, 227, 293	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	466	LEU	3.0
1	A	457	ALA	2.4
1	A	130	GLY	2.3
1	A	493	LYS	2.2
1	A	465	PRO	2.2
1	A	499	VAL	2.2
1	A	111	GLY	2.1
1	A	706	LEU	2.1
1	A	636	ASP	2.1
1	A	514	GLU	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](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MGF	A	950	4/4	0.89	0.09	110,129,141,173	0
2	MG	A	900	1/1	0.94	0.05	101,101,101,101	0

6.5 Other polymers [i](#)

There are no such residues in this entry.