W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2024 – 12:01 AM EST

PDB ID	:	1KFI
Title	:	Crystal Structure of the Exocytosis-Sensitive Phosphoprotein, pp63/Parafusin (phosphoglucomutase) from Paramecium
Authors	:	Mueller, S.; Diederichs, K.; Breed, J.; Kissmehl, R.; Hauser, K.; Plattner, H.; Welte, W.
Deposited on	:	2001-11-21
Resolution	:	2.40 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:

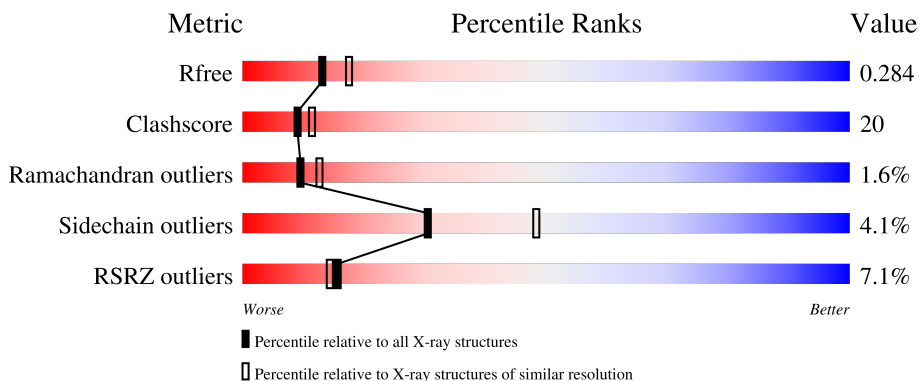|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
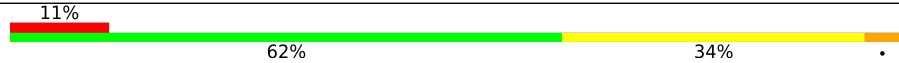*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	Percentile Ranks	Value
Rfree		0.284
Clashscore		20
Ramachandran outliers		1.6%
Sidechain outliers		4.1%
RSRZ outliers		7.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	572	3% 70% 27% •
1	B	572	11% 62% 34% •

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 9207 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 phosphoglucomutase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	570	Total	C	N	O	S	0	0	0
			4490	2858	769	850	13			
1	B	570	Total	C	N	O	S	0	0	0
			4490	2858	769	850	13			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
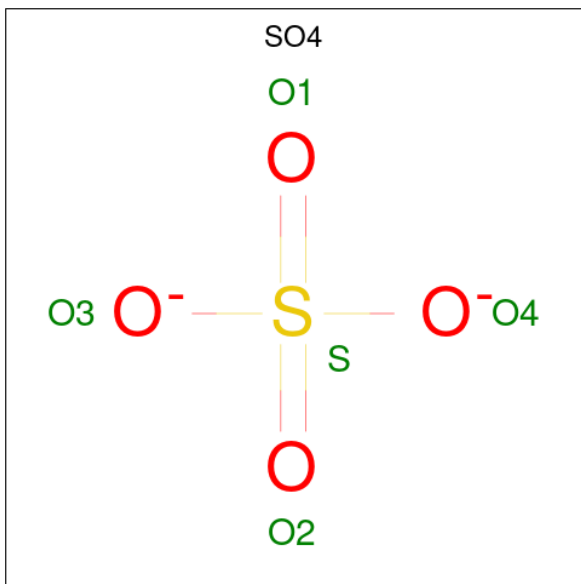
| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0

• Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	126	Total 126	O 126	0	0
4	B	79	Total 79	O 79	0	0

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: phosphoglucomutase 1
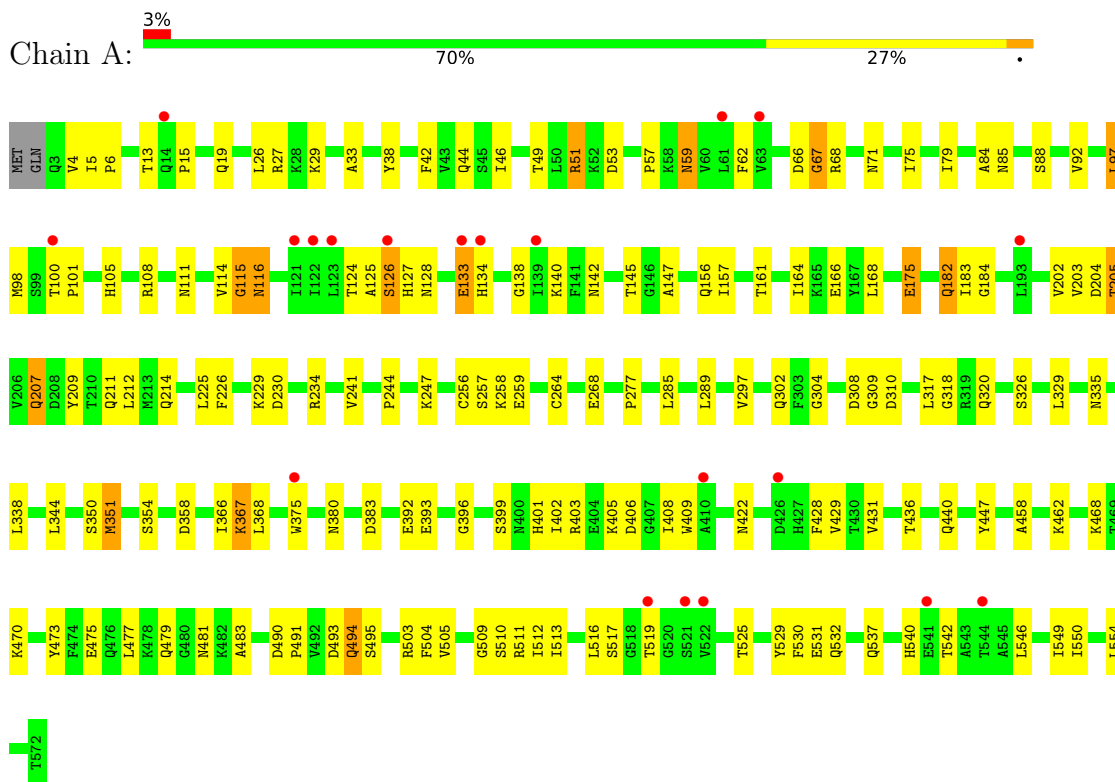
- Molecule 1: phosphoglucomutase 1
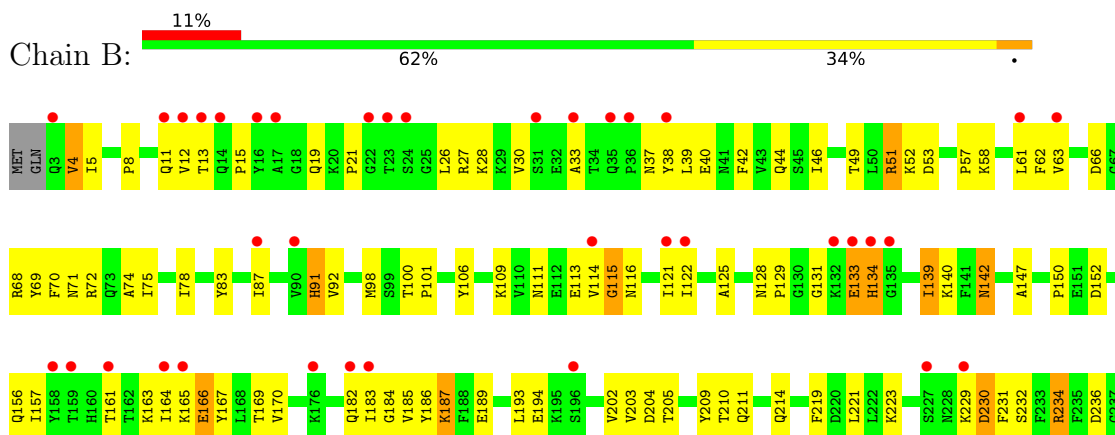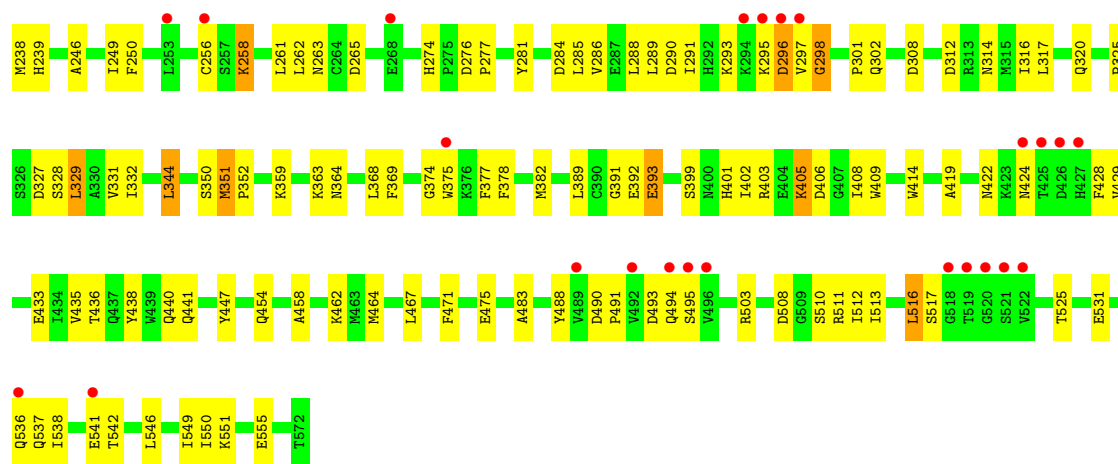
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.35Å 133.61Å 150.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 27.96 – 2.42	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.40) 93.8 (27.96-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.89 (at 2.42Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.286 0.233 , 0.284	Depositor DCC
R_{free} test set	974 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å^2)	25.4	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 58.6	EDS
L-test for twinning[2]	$< |L| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	9207	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, 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	0.37	0/4592	0.62	0/6207
1	B	0.36	0/4592	0.61	1/6207 (0.0%)
All	All	0.37	0/9184	0.61	1/12414 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	541	GLU	N-CA-C	-5.34	96.59	111.00

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	4490	0	4386	160	0
1	B	4490	0	4386	205	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	10	0	0	1	0
3	B	10	0	0	0	0
4	A	126	0	0	4	0
4	B	79	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9207	0	8772	358	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 20.

All (358) 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:124:THR:HG22	1:A:126:SER:H	1.12	1.10
1:B:375:TRP:CZ3	1:B:405:LYS:HB2	1.96	1.01
1:A:375:TRP:NE1	1:A:405:LYS:HE3	1.81	0.95
1:A:422:ASN:HD21	1:A:429:VAL:H	1.17	0.91
1:B:91:HIS:HD2	1:B:106:TYR:OH	1.55	0.89
1:A:422:ASN:HD21	1:A:429:VAL:N	1.76	0.83
1:A:59:ASN:ND2	1:A:88:SER:H	1.78	0.81
1:B:422:ASN:HD21	1:B:429:VAL:N	1.78	0.81
1:B:351:MET:CE	1:B:513:ILE:HG12	2.10	0.81
1:A:422:ASN:ND2	1:A:429:VAL:H	1.79	0.81
1:B:19:GLN:HE21	1:B:161:THR:HB	1.46	0.80
1:B:8:PRO:HA	1:B:170:VAL:HG12	1.64	0.78
1:B:169:THR:HG22	1:B:170:VAL:H	1.48	0.78
1:B:133:GLU:HG2	1:B:134:HIS:H	1.49	0.77
1:A:124:THR:HG22	1:A:126:SER:N	1.95	0.77
1:A:396:GLY:HA3	1:A:405:LYS:HE2	1.67	0.77
1:B:302:GLN:HG2	1:B:428:PHE:CE1	2.19	0.76
1:A:285:LEU:CD1	1:A:317:LEU:HD12	2.15	0.76
1:A:302:GLN:HG2	1:A:428:PHE:CE2	2.20	0.76
1:A:399:SER:HB3	1:A:401:HIS:HD2	1.51	0.75
1:B:285:LEU:HD12	1:B:317:LEU:HD12	1.67	0.75
1:B:232:SER:HB2	1:B:302:GLN:H	1.50	0.75
1:A:44:GLN:HE22	1:A:85:ASN:HD21	1.34	0.75
1:B:297:VAL:HG23	1:B:298:GLY:H	1.52	0.75
1:B:422:ASN:HD21	1:B:429:VAL:H	1.34	0.74
1:B:312:ASP:OD1	1:B:375:TRP:HH2	1.70	0.74
1:B:68:ARG:NH1	1:B:125:ALA:H	1.86	0.73
1:A:66:ASP:OD1	1:A:124:THR:HG23	1.87	0.73
1:B:236:ASP:HB2	1:B:285:LEU:HD23	1.70	0.73
1:B:351:MET:HE1	1:B:513:ILE:HG12	1.70	0.73
1:B:62:PHE:CZ	1:B:98:MET:HG2	2.23	0.73
1:B:182:GLN:O	1:B:202:VAL:HG11	1.89	0.73
1:A:140:LYS:HE2	1:A:142:ASN:HD21	1.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:PHE:HZ	1:B:98:MET:HG2	1.54	0.72
1:B:33:ALA:HA	1:B:38:TYR:CD2	2.25	0.71
1:A:19:GLN:HE21	1:A:161:THR:HB	1.55	0.71
1:A:182:GLN:O	1:A:202:VAL:HG11	1.93	0.69
1:A:542:THR:HG23	4:A:805:HOH:O	1.93	0.69
1:B:295:LYS:NZ	1:B:296:ASP:H	1.91	0.69
1:B:258:LYS:H	1:B:258:LYS:HE2	1.58	0.68
1:B:19:GLN:NE2	1:B:161:THR:HB	2.10	0.67
1:A:436:THR:O	1:A:440:GLN:HG3	1.93	0.67
1:B:133:GLU:CD	1:B:133:GLU:H	1.98	0.67
1:B:375:TRP:CH2	1:B:405:LYS:HB2	2.29	0.67
1:B:39:LEU:HD21	1:B:74:ALA:HA	1.76	0.66
1:B:183:ILE:HA	1:B:202:VAL:HG13	1.77	0.66
1:B:314:ASN:HD22	1:B:316:ILE:HD13	1.59	0.66
1:B:351:MET:HE3	1:B:513:ILE:HG12	1.77	0.66
1:B:83:TYR:CE1	1:B:170:VAL:HG11	2.31	0.66
1:B:350:SER:HB2	1:B:392:GLU:HG2	1.76	0.66
1:A:97:LEU:O	1:A:205:THR:HB	1.96	0.65
1:A:318:GLY:HA3	1:A:431:VAL:CG2	2.27	0.65
1:B:15:PRO:HG3	1:B:164:ILE:O	1.97	0.65
1:B:66:ASP:OD2	1:B:68:ARG:NH1	2.30	0.64
1:A:71:ASN:O	1:A:75:ILE:HG13	1.97	0.64
1:A:351:MET:HE2	1:A:351:MET:O	1.98	0.64
1:A:358:ASP:HA	1:A:368:LEU:HD22	1.80	0.64
1:A:68:ARG:CZ	1:A:125:ALA:HB3	2.28	0.64
1:A:105:HIS:CD2	1:A:212:LEU:HD22	2.34	0.63
1:A:29:LYS:NZ	1:A:134:HIS:HA	2.14	0.63
1:A:289:LEU:HD22	1:A:317:LEU:HB2	1.79	0.63
1:B:436:THR:O	1:B:440:GLN:HG3	2.00	0.62
1:A:15:PRO:HG3	1:A:164:ILE:O	2.00	0.62
1:B:285:LEU:CD1	1:B:317:LEU:HD12	2.29	0.62
1:A:375:TRP:HE1	1:A:405:LYS:HE3	1.61	0.61
1:B:351:MET:HE2	1:B:511:ARG:HH21	1.65	0.61
1:A:318:GLY:HA3	1:A:431:VAL:HG22	1.81	0.61
1:B:406:ASP:HB3	1:B:409:TRP:HB3	1.83	0.61
1:A:62:PHE:CZ	1:A:98:MET:HG2	2.36	0.60
1:A:351:MET:HE3	1:A:513:ILE:HG12	1.82	0.60
1:A:51:ARG:HH21	1:B:51:ARG:HH21	1.47	0.60
1:A:59:ASN:ND2	1:A:59:ASN:H	2.00	0.60
1:B:285:LEU:HD13	1:B:289:LEU:HD13	1.84	0.60
1:B:157:ILE:O	1:B:161:THR:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:VAL:HG13	1:B:291:ILE:CG1	2.32	0.60
1:B:406:ASP:OD2	1:B:409:TRP:HB2	2.02	0.60
1:B:422:ASN:ND2	1:B:429:VAL:H	1.99	0.60
1:B:83:TYR:CD1	1:B:170:VAL:HG11	2.36	0.59
1:A:358:ASP:CG	1:A:368:LEU:HD21	2.22	0.59
1:A:207:GLN:HE21	1:A:207:GLN:HA	1.68	0.59
1:B:314:ASN:ND2	1:B:316:ILE:HD13	2.18	0.59
1:A:75:ILE:O	1:A:79:ILE:HG13	2.02	0.59
1:B:91:HIS:CD2	1:B:106:TYR:OH	2.46	0.59
1:A:100:THR:HB	1:A:101:PRO:HD3	1.85	0.58
1:B:12:VAL:HA	1:B:166:GLU:HB3	1.85	0.58
1:B:312:ASP:OD1	1:B:375:TRP:CH2	2.53	0.58
1:A:124:THR:HG21	1:A:310:ASP:HB3	1.85	0.58
1:A:68:ARG:HD3	4:A:733:HOH:O	2.03	0.58
1:A:380:ASN:HD21	1:B:52:LYS:CE	2.15	0.58
1:B:511:ARG:NH1	1:B:531:GLU:OE1	2.36	0.58
1:A:375:TRP:CZ2	1:A:405:LYS:HB3	2.39	0.58
1:A:145:THR:HG23	1:B:53:ASP:HB2	1.86	0.58
1:B:27:ARG:NH1	1:B:128:ASN:ND2	2.52	0.58
1:B:74:ALA:O	1:B:78:ILE:HG13	2.03	0.58
1:A:126:SER:HB2	3:A:601:SO4:O1	2.04	0.57
1:A:209:TYR:OH	1:A:408:ILE:HB	2.05	0.57
1:A:59:ASN:HD21	1:A:88:SER:H	1.53	0.57
1:B:21:PRO:HG3	1:B:42:PHE:CZ	2.40	0.57
1:B:229:LYS:HG3	1:B:230:ASP:OD1	2.05	0.57
1:B:314:ASN:HD22	1:B:316:ILE:CD1	2.18	0.57
1:B:26:LEU:HD23	1:B:139:ILE:HD13	1.87	0.56
1:B:13:THR:HG22	1:B:166:GLU:CA	2.36	0.56
1:B:111:ASN:HA	1:B:115:GLY:HA2	1.87	0.56
1:A:75:ILE:HD13	1:A:92:VAL:HG21	1.86	0.56
1:B:140:LYS:NZ	1:B:142:ASN:HD21	2.03	0.56
1:B:142:ASN:N	1:B:142:ASN:HD22	2.02	0.56
1:B:256:CYS:SG	1:B:261:LEU:HD21	2.46	0.56
1:B:351:MET:CE	1:B:511:ARG:HH21	2.19	0.56
1:A:509:GLY:O	1:A:511:ARG:HG3	2.06	0.56
1:A:257:SER:OG	1:A:259:GLU:HG2	2.05	0.55
1:A:59:ASN:H	1:A:59:ASN:HD22	1.55	0.55
1:A:108:ARG:NH1	1:A:403:ARG:NH1	2.55	0.55
1:A:351:MET:CE	1:A:513:ILE:HD13	2.37	0.55
1:B:185:VAL:HG12	1:B:187:LYS:HD2	1.87	0.55
1:A:399:SER:HB3	1:A:401:HIS:CD2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LYS:HG3	1:A:230:ASP:OD1	2.07	0.55
1:B:152:ASP:O	1:B:156:GLN:HG2	2.07	0.55
1:B:114:VAL:O	1:B:116:ASN:N	2.40	0.55
1:B:258:LYS:H	1:B:258:LYS:CE	2.19	0.55
1:B:290:ASP:O	1:B:320:GLN:HG2	2.06	0.55
1:B:375:TRP:N	1:B:375:TRP:CD1	2.73	0.55
1:A:68:ARG:NH2	1:A:125:ALA:HB3	2.22	0.54
1:B:297:VAL:HG23	1:B:298:GLY:N	2.21	0.54
1:B:219:PHE:O	1:B:223:LYS:HB2	2.07	0.54
1:A:66:ASP:OD2	1:A:68:ARG:HD2	2.07	0.54
1:B:75:ILE:HD13	1:B:92:VAL:HG21	1.89	0.54
1:B:183:ILE:HG22	1:B:184:GLY:N	2.23	0.53
1:B:246:ALA:O	1:B:250:PHE:HB2	2.08	0.53
1:B:374:GLY:O	1:B:377:PHE:HD1	1.91	0.53
1:A:380:ASN:HD21	1:B:52:LYS:HE2	1.72	0.53
1:A:493:ASP:OD2	1:A:495:SER:HB2	2.08	0.53
1:B:13:THR:HG22	1:B:166:GLU:N	2.23	0.53
1:A:51:ARG:HH21	1:B:51:ARG:NH2	2.05	0.53
1:B:26:LEU:HD11	1:B:28:LYS:HE2	1.89	0.53
1:A:62:PHE:HZ	1:A:98:MET:HG2	1.73	0.53
1:A:473:TYR:CZ	1:A:477:LEU:HD21	2.44	0.53
1:A:517:SER:HB3	1:A:525:THR:HB	1.91	0.52
1:B:21:PRO:HG3	1:B:42:PHE:HZ	1.75	0.52
1:B:359:LYS:O	1:B:363:LYS:HG2	2.09	0.52
1:B:68:ARG:CZ	1:B:125:ALA:HB3	2.40	0.52
1:A:133:GLU:CD	1:A:133:GLU:H	2.12	0.52
1:B:42:PHE:CE2	1:B:139:ILE:HB	2.46	0.51
1:B:203:VAL:HG22	1:B:204:ASP:N	2.26	0.51
1:A:13:THR:HG22	1:A:166:GLU:HA	1.92	0.51
1:A:326:SER:HB3	1:A:354:SER:OG	2.11	0.51
1:A:447:TYR:HA	1:A:530:PHE:O	2.11	0.51
1:B:51:ARG:HD2	1:B:51:ARG:N	2.25	0.51
1:B:239:HIS:NE2	1:B:263:ASN:ND2	2.59	0.51
1:B:58:LYS:HE3	4:B:751:HOH:O	2.11	0.51
1:A:124:THR:CG2	1:A:126:SER:H	2.02	0.51
1:A:396:GLY:CA	1:A:405:LYS:HE2	2.38	0.51
1:B:286:VAL:HG13	1:B:291:ILE:HG13	1.92	0.51
1:B:13:THR:HG22	1:B:166:GLU:HA	1.91	0.51
1:B:42:PHE:HE2	1:B:139:ILE:HB	1.76	0.50
1:B:546:LEU:O	1:B:549:ILE:HG22	2.11	0.50
1:A:114:VAL:O	1:A:116:ASN:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:GLY:HA3	1:A:405:LYS:CE	2.40	0.50
1:B:66:ASP:CG	1:B:68:ARG:NH1	2.65	0.50
1:B:291:ILE:HD11	1:B:317:LEU:HD13	1.92	0.50
1:A:289:LEU:HD22	1:A:317:LEU:CB	2.41	0.50
1:B:165:LYS:O	1:B:166:GLU:HB3	2.12	0.50
1:A:350:SER:HB3	1:A:392:GLU:HG2	1.92	0.50
1:A:277:PRO:CD	1:A:308:ASP:HB3	2.42	0.50
1:A:66:ASP:OD2	1:A:66:ASP:O	2.29	0.50
1:B:193:LEU:O	1:B:194:GLU:HB2	2.11	0.50
1:B:295:LYS:HZ2	1:B:296:ASP:H	1.58	0.50
1:A:211:GLN:HA	1:A:214:GLN:HE21	1.76	0.50
1:A:511:ARG:O	1:A:549:ILE:HD11	2.12	0.49
1:A:183:ILE:HA	1:A:202:VAL:HG13	1.95	0.49
1:A:126:SER:O	1:A:128:ASN:N	2.45	0.49
1:B:513:ILE:N	1:B:513:ILE:HD12	2.27	0.49
1:A:403:ARG:HG3	1:A:403:ARG:HH11	1.77	0.49
1:B:517:SER:HB3	1:B:525:THR:HB	1.94	0.49
1:B:39:LEU:CD2	1:B:74:ALA:HA	2.41	0.49
1:B:265:ASP:HB2	4:B:772:HOH:O	2.12	0.49
1:B:139:ILE:HD12	1:B:139:ILE:H	1.77	0.49
1:A:27:ARG:HB3	1:A:27:ARG:NH1	2.28	0.49
1:A:108:ARG:HH12	1:A:403:ARG:HH12	1.61	0.49
1:B:238:MET:HE1	1:B:276:ASP:N	2.28	0.48
1:A:44:GLN:HE22	1:A:85:ASN:ND2	2.07	0.48
1:B:100:THR:HB	1:B:101:PRO:HD3	1.96	0.48
1:B:517:SER:CB	1:B:525:THR:HB	2.43	0.48
1:A:258:LYS:HE2	1:A:258:LYS:H	1.78	0.48
1:A:483:ALA:HA	1:A:503:ARG:O	2.13	0.48
1:A:335:ASN:HD22	1:A:338:LEU:HD12	1.78	0.48
1:A:27:ARG:HB3	1:A:27:ARG:HH11	1.78	0.48
1:B:183:ILE:CG2	1:B:184:GLY:N	2.75	0.48
1:A:108:ARG:HH12	1:A:403:ARG:NH1	2.11	0.48
1:A:513:ILE:HB	1:A:529:TYR:HB2	1.96	0.48
1:B:4:VAL:HA	1:B:189:GLU:O	2.14	0.48
1:B:351:MET:HB3	1:B:352:PRO:HD3	1.96	0.48
1:B:150:PRO:HG3	4:B:775:HOH:O	2.13	0.48
1:A:289:LEU:HD21	1:A:304:GLY:N	2.29	0.47
1:B:131:GLY:HA3	1:B:133:GLU:OE2	2.14	0.47
1:A:458:ALA:O	1:A:462:LYS:HG3	2.14	0.47
1:B:186:TYR:HE1	1:B:202:VAL:HG12	1.79	0.47
1:B:139:ILE:HD12	1:B:139:ILE:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:ALA:O	1:B:462:LYS:HG3	2.14	0.47
1:B:234:ARG:CD	1:B:288:LEU:HD13	2.45	0.47
1:B:399:SER:HB3	1:B:401:HIS:ND1	2.30	0.47
1:B:464:MET:HA	1:B:467:LEU:HD12	1.97	0.47
1:A:203:VAL:HG22	1:A:204:ASP:N	2.29	0.47
1:B:378:PHE:O	1:B:382:MET:HG3	2.14	0.47
1:A:318:GLY:HA3	1:A:431:VAL:HG21	1.95	0.47
1:A:351:MET:HE2	1:A:511:ARG:NH2	2.30	0.47
1:A:403:ARG:HH11	1:A:403:ARG:CG	2.28	0.47
1:B:551:LYS:O	1:B:555:GLU:HG3	2.15	0.47
1:A:19:GLN:NE2	1:A:161:THR:HB	2.27	0.47
1:A:277:PRO:HD2	1:A:308:ASP:HB3	1.97	0.47
1:B:351:MET:HE3	1:B:513:ILE:CG1	2.43	0.47
1:B:471:PHE:O	1:B:475:GLU:HG3	2.14	0.47
1:A:285:LEU:HD13	1:A:317:LEU:HD12	1.92	0.47
1:A:205:THR:HG23	4:A:812:HOH:O	2.15	0.46
1:A:546:LEU:O	1:A:549:ILE:HG22	2.15	0.46
1:B:239:HIS:H	1:B:263:ASN:HB3	1.80	0.46
1:B:232:SER:HB2	1:B:302:GLN:N	2.27	0.46
1:A:510:SER:C	1:A:511:ARG:HG3	2.35	0.46
1:B:147:ALA:HB2	1:B:403:ARG:HB3	1.97	0.46
1:A:351:MET:HE1	1:A:513:ILE:HD13	1.96	0.46
1:B:185:VAL:CG1	1:B:187:LYS:HD2	2.45	0.46
1:B:209:TYR:OH	1:B:408:ILE:HB	2.15	0.46
1:B:295:LYS:HZ2	1:B:295:LYS:HB3	1.81	0.46
1:A:519:THR:O	1:A:519:THR:HG22	2.15	0.46
1:B:351:MET:O	1:B:511:ARG:NH2	2.48	0.46
1:A:84:ALA:HB1	1:A:168:LEU:HB3	1.97	0.46
1:A:111:ASN:HB3	1:B:57:PRO:HB3	1.98	0.46
1:A:383:ASP:OD2	1:A:403:ARG:NH1	2.48	0.46
1:A:66:ASP:O	1:A:71:ASN:ND2	2.49	0.46
1:A:67:GLY:O	1:A:268:GLU:HA	2.16	0.46
1:A:59:ASN:HD22	1:A:59:ASN:N	2.14	0.45
1:A:124:THR:HG21	1:A:310:ASP:CB	2.46	0.45
1:B:327:ASP:O	1:B:331:VAL:HG23	2.16	0.45
1:B:510:SER:C	1:B:511:ARG:HG3	2.36	0.45
1:B:109:LYS:O	1:B:113:GLU:HG3	2.16	0.45
1:B:210:THR:HG23	1:B:249:ILE:HG12	1.97	0.45
1:A:247:LYS:HE3	1:A:264:CYS:O	2.17	0.45
1:A:258:LYS:H	1:A:258:LYS:CE	2.29	0.45
1:B:288:LEU:O	1:B:301:PRO:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:PHE:O	1:A:46:ILE:HG13	2.15	0.45
1:A:511:ARG:CZ	1:A:513:ILE:HD11	2.47	0.45
1:B:122:ILE:HB	1:B:140:LYS:HG2	1.98	0.45
1:B:429:VAL:HG13	1:B:433:GLU:OE2	2.17	0.45
1:A:126:SER:C	1:A:128:ASN:H	2.20	0.45
1:B:234:ARG:HD3	1:B:288:LEU:HD13	1.98	0.45
1:A:157:ILE:O	1:A:161:THR:HG23	2.17	0.45
1:A:532:GLN:HB3	1:A:546:LEU:HD23	1.99	0.45
1:A:101:PRO:HG3	1:A:405:LYS:O	2.17	0.45
1:A:302:GLN:HG3	4:A:775:HOH:O	2.17	0.45
1:A:530:PHE:CE1	1:A:550:ILE:HA	2.51	0.45
1:B:33:ALA:O	1:B:38:TYR:HB3	2.17	0.45
1:B:71:ASN:O	1:B:75:ILE:HG13	2.16	0.45
1:B:393:GLU:HG3	1:B:447:TYR:OH	2.17	0.45
1:B:92:VAL:O	1:B:202:VAL:HA	2.17	0.44
1:B:236:ASP:OD1	1:B:238:MET:N	2.44	0.44
1:B:375:TRP:N	1:B:375:TRP:HD1	2.15	0.44
1:A:59:ASN:ND2	1:A:88:SER:N	2.58	0.44
1:B:202:VAL:HG13	1:B:202:VAL:O	2.17	0.44
1:B:290:ASP:OD1	1:B:293:LYS:HA	2.17	0.44
1:A:125:ALA:O	1:A:126:SER:O	2.35	0.44
1:A:490:ASP:HA	1:A:491:PRO:HD3	1.87	0.44
1:A:504:PHE:HB2	1:A:512:ILE:HB	1.99	0.44
1:B:11:GLN:O	1:B:166:GLU:HA	2.18	0.44
1:B:285:LEU:HD12	1:B:317:LEU:CD1	2.43	0.44
1:A:111:ASN:HA	1:A:115:GLY:HA2	1.99	0.44
1:A:490:ASP:O	1:A:494:GLN:HA	2.17	0.44
1:A:537:GLN:HB3	1:A:540:HIS:NE2	2.32	0.44
1:B:312:ASP:OD1	1:B:312:ASP:C	2.56	0.44
1:B:69:TYR:O	1:B:70:PHE:HB3	2.17	0.44
1:B:68:ARG:NH2	1:B:128:ASN:O	2.51	0.44
1:A:59:ASN:HD21	1:A:88:SER:N	2.14	0.44
1:B:368:LEU:HD13	1:B:369:PHE:N	2.33	0.44
1:A:26:LEU:O	1:A:138:GLY:HA2	2.17	0.43
1:B:37:ASN:HA	1:B:40:GLU:OE2	2.18	0.43
1:B:295:LYS:HZ3	1:B:296:ASP:H	1.64	0.43
1:B:375:TRP:CD2	1:B:405:LYS:HD3	2.53	0.43
1:A:241:VAL:HG12	1:A:309:GLY:O	2.18	0.43
1:A:297:VAL:HG12	1:A:320:GLN:NE2	2.33	0.43
1:B:66:ASP:OD1	1:B:68:ARG:HG2	2.18	0.43
1:A:380:ASN:HD21	1:B:52:LYS:HE3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:MET:CE	1:B:511:ARG:NH2	2.82	0.43
1:B:284:ASP:HB2	4:B:731:HOH:O	2.17	0.43
1:A:13:THR:HG22	1:A:166:GLU:CA	2.48	0.43
1:B:302:GLN:HG3	4:B:750:HOH:O	2.18	0.43
1:B:42:PHE:O	1:B:46:ILE:HG13	2.19	0.43
1:B:488:TYR:OH	1:B:491:PRO:HD3	2.18	0.43
1:B:66:ASP:OD1	1:B:68:ARG:NH1	2.51	0.43
1:B:27:ARG:NH1	1:B:128:ASN:HD21	2.17	0.43
1:B:49:THR:HG23	1:B:156:GLN:HB2	2.01	0.43
1:B:546:LEU:O	1:B:550:ILE:HG13	2.19	0.43
1:A:49:THR:HG23	1:A:156:GLN:HB2	1.99	0.43
1:B:5:ILE:N	1:B:189:GLU:O	2.50	0.43
1:B:328:SER:O	1:B:332:ILE:HG13	2.19	0.43
1:B:239:HIS:N	1:B:263:ASN:HB3	2.34	0.43
1:A:5:ILE:HA	1:A:6:PRO:HD3	1.84	0.42
1:B:129:PRO:HG3	1:B:274:HIS:HA	2.01	0.42
1:B:221:LEU:HG	1:B:419:ALA:HB1	2.01	0.42
1:B:276:ASP:HB3	1:B:281:TYR:CD2	2.54	0.42
1:B:375:TRP:NE1	1:B:392:GLU:OE1	2.52	0.42
1:A:184:GLY:N	1:A:202:VAL:HG13	2.34	0.42
1:B:100:THR:N	1:B:101:PRO:CD	2.83	0.42
1:B:510:SER:O	1:B:511:ARG:HG3	2.19	0.42
1:A:351:MET:O	1:A:511:ARG:NH2	2.46	0.42
1:A:406:ASP:HB3	1:A:409:TRP:HB3	2.02	0.42
1:A:344:LEU:HD23	1:A:366:ILE:HG21	2.02	0.42
1:A:422:ASN:ND2	1:A:428:PHE:HA	2.35	0.42
1:B:39:LEU:HD21	1:B:74:ALA:CA	2.47	0.42
1:B:344:LEU:HB2	4:B:738:HOH:O	2.19	0.42
1:A:468:LYS:C	1:A:470:LYS:H	2.23	0.42
1:B:147:ALA:HB2	1:B:403:ARG:CB	2.50	0.42
1:B:295:LYS:NZ	1:B:295:LYS:HB3	2.35	0.42
1:B:493:ASP:O	1:B:495:SER:N	2.53	0.42
1:A:33:ALA:HA	1:A:38:TYR:CD2	2.55	0.42
1:A:351:MET:HE2	1:A:511:ARG:HH21	1.85	0.42
1:B:163:LYS:O	1:B:163:LYS:HG2	2.19	0.42
1:A:59:ASN:ND2	1:A:59:ASN:N	2.60	0.42
1:A:29:LYS:HZ3	1:A:134:HIS:HA	1.82	0.41
1:A:124:THR:CG2	1:A:310:ASP:HB3	2.48	0.41
1:B:512:ILE:C	1:B:513:ILE:HD12	2.41	0.41
1:A:147:ALA:HB2	1:A:403:ARG:HB3	2.02	0.41
1:B:61:LEU:HD22	1:B:87:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LYS:HZ1	1:A:134:HIS:HA	1.82	0.41
1:A:367:LYS:HD2	1:A:367:LYS:HA	1.87	0.41
1:B:63:VAL:HA	1:B:121:ILE:O	2.20	0.41
1:B:211:GLN:HA	1:B:214:GLN:NE2	2.35	0.41
1:A:175:GLU:H	1:A:175:GLU:HG2	1.45	0.41
1:A:207:GLN:HE21	1:A:207:GLN:CA	2.33	0.41
1:B:30:VAL:O	1:B:33:ALA:N	2.54	0.41
1:B:133:GLU:HB2	1:B:134:HIS:CE1	2.55	0.41
1:B:508:ASP:C	1:B:508:ASP:OD1	2.58	0.41
1:B:536:GLN:O	1:B:538:ILE:N	2.53	0.41
1:A:53:ASP:O	1:A:57:PRO:HD3	2.20	0.41
1:A:401:HIS:HE1	1:A:406:ASP:OD2	2.04	0.41
1:A:511:ARG:NH1	1:A:531:GLU:OE2	2.50	0.41
1:B:26:LEU:HD11	1:B:28:LYS:CE	2.50	0.41
1:B:364:ASN:N	1:B:364:ASN:HD22	2.18	0.41
1:B:167:TYR:CE1	1:B:169:THR:OG1	2.73	0.41
1:B:375:TRP:HZ2	4:B:702:HOH:O	2.03	0.41
1:B:277:PRO:CD	1:B:308:ASP:HB3	2.50	0.41
1:B:516:LEU:HA	1:B:516:LEU:HD12	1.85	0.41
1:A:226:PHE:HE2	1:A:256:CYS:HB3	1.86	0.41
1:A:475:GLU:HA	1:A:481:ASN:HB2	2.02	0.41
1:B:435:VAL:O	1:B:438:TYR:HB3	2.20	0.41
1:A:473:TYR:CE1	1:A:477:LEU:HD21	2.56	0.41
1:B:49:THR:HG23	1:B:156:GLN:CB	2.50	0.41
1:B:231:PHE:HD1	1:B:428:PHE:HZ	1.69	0.41
1:B:277:PRO:HD3	1:B:308:ASP:CA	2.51	0.41
1:B:329:LEU:HG	1:B:391:GLY:HA3	2.03	0.41
1:A:66:ASP:O	1:A:68:ARG:N	2.48	0.40
1:B:490:ASP:HA	1:B:491:PRO:HD3	1.90	0.40
1:B:44:GLN:HG2	1:B:167:TYR:CB	2.51	0.40
1:B:203:VAL:CG2	1:B:204:ASP:N	2.84	0.40
1:B:72:ARG:O	1:B:75:ILE:HB	2.22	0.40
1:B:331:VAL:HG11	1:B:414:TRP:CH2	2.57	0.40
1:A:241:VAL:O	1:A:244:PRO:HD2	2.22	0.40
1:B:211:GLN:HA	1:B:214:GLN:HE21	1.86	0.40
1:A:380:ASN:HD22	1:A:380:ASN:HA	1.69	0.40
1:A:550:ILE:O	1:A:554:LEU:HG	2.22	0.40
1:B:483:ALA:HA	1:B:503:ARG:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	568/572 (99%)	531 (94%)	28 (5%)	9 (2%)	9	13
1	B	568/572 (99%)	515 (91%)	44 (8%)	9 (2%)	9	13
All	All	1136/1144 (99%)	1046 (92%)	72 (6%)	18 (2%)	9	13

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	SER
1	A	127	HIS
1	B	494	GLN
1	A	115	GLY
1	A	133	GLU
1	B	115	GLY
1	B	424	ASN
1	A	479	GLN
1	B	166	GLU
1	A	4	VAL
1	A	67	GLY
1	B	4	VAL
1	B	133	GLU
1	B	537	GLN
1	A	402	ILE
1	A	494	GLN
1	B	402	ILE
1	B	298	GLY

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	479/481 (100%)	463 (97%)	16 (3%)	38	57
1	B	479/481 (100%)	456 (95%)	23 (5%)	25	41
All	All	958/962 (100%)	919 (96%)	39 (4%)	30	48

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ARG
1	A	59	ASN
1	A	97	LEU
1	A	116	ASN
1	A	175	GLU
1	A	182	GLN
1	A	205	THR
1	A	207	GLN
1	A	225	LEU
1	A	234	ARG
1	A	329	LEU
1	A	351	MET
1	A	367	LYS
1	A	393	GLU
1	A	505	VAL
1	A	516	LEU
1	B	51	ARG
1	B	91	HIS
1	B	134	HIS
1	B	139	ILE
1	B	142	ASN
1	B	187	LYS
1	B	205	THR
1	B	230	ASP
1	B	234	ARG
1	B	258	LYS
1	B	262	LEU
1	B	296	ASP
1	B	325	PRO
1	B	329	LEU
1	B	344	LEU
1	B	351	MET
1	B	389	LEU

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Mol	Chain	Res	Type
1	B	393	GLU
1	B	405	LYS
1	B	441	GLN
1	B	454	GLN
1	B	516	LEU
1	B	542	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	19	GLN
1	A	37	ASN
1	A	41	ASN
1	A	59	ASN
1	A	73	GLN
1	A	85	ASN
1	A	105	HIS
1	A	116	ASN
1	A	128	ASN
1	A	142	ASN
1	A	207	GLN
1	A	214	GLN
1	A	239	HIS
1	A	263	ASN
1	A	320	GLN
1	A	335	ASN
1	A	337	ASN
1	A	364	ASN
1	A	380	ASN
1	A	401	HIS
1	A	422	ASN
1	A	441	GLN
1	A	461	ASN
1	A	472	GLN
1	A	476	GLN
1	A	479	GLN
1	A	500	GLN
1	A	561	GLN
1	A	566	ASN
1	B	14	GLN
1	B	19	GLN

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Mol	Chain	Res	Type
1	B	37	ASN
1	B	44	GLN
1	B	48	ASN
1	B	85	ASN
1	B	91	HIS
1	B	142	ASN
1	B	179	ASN
1	B	207	GLN
1	B	214	GLN
1	B	263	ASN
1	B	314	ASN
1	B	320	GLN
1	B	335	ASN
1	B	337	ASN
1	B	364	ASN
1	B	380	ASN
1	B	422	ASN
1	B	461	ASN
1	B	472	GLN
1	B	479	GLN
1	B	481	ASN
1	B	561	GLN
1	B	566	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	SO4	A	603	-	4,4,4	0.25	0	6,6,6	0.11	0
3	SO4	B	604	-	4,4,4	0.27	0	6,6,6	0.08	0
3	SO4	A	601	2	4,4,4	0.28	0	6,6,6	0.10	0
3	SO4	B	602	2	4,4,4	0.23	0	6,6,6	0.10	0

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 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	SO4	1	0

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(Å²)	Q<0.9
1	A	570/572 (99%)	0.21	20 (3%)	44	43	11, 29, 52, 85	0
1	B	570/572 (99%)	0.52	61 (10%)	6	5	10, 31, 54, 86	0
All	All	1140/1144 (99%)	0.37	81 (7%)	16	14	10, 30, 53, 86	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	522	VAL	7.6
1	A	522	VAL	7.3
1	B	521	SER	6.2
1	B	520	GLY	5.6
1	B	134	HIS	4.5
1	B	295	LYS	4.4
1	B	227	SER	4.2
1	B	296	ASP	4.2
1	B	426	ASP	4.0
1	A	121	ILE	3.9
1	B	519	THR	3.8
1	B	424	ASN	3.7
1	B	518	GLY	3.7
1	B	133	GLU	3.7
1	B	132	LYS	3.6
1	B	375	TRP	3.6
1	B	12	VAL	3.6
1	B	294	LYS	3.5
1	B	14	GLN	3.5
1	A	521	SER	3.5
1	B	229	LYS	3.4
1	A	544	THR	3.4
1	B	13	THR	3.3
1	B	427	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	23	THR	3.3
1	B	496	VAL	3.3
1	B	161	THR	3.2
1	B	495	SER	3.2
1	A	63	VAL	3.2
1	B	16	TYR	3.0
1	B	22	GLY	3.0
1	B	425	THR	3.0
1	B	3	GLN	3.0
1	A	375	TRP	3.0
1	B	33	ALA	3.0
1	A	139	ILE	2.8
1	B	196	SER	2.8
1	B	114	VAL	2.8
1	B	541	GLU	2.8
1	B	297	VAL	2.8
1	B	121	ILE	2.8
1	B	164	ILE	2.8
1	B	36	PRO	2.8
1	B	489	VAL	2.7
1	B	90	VAL	2.6
1	A	134	HIS	2.6
1	B	183	ILE	2.6
1	A	14	GLN	2.6
1	A	123	LEU	2.5
1	B	165	LYS	2.5
1	B	11	GLN	2.5
1	A	133	GLU	2.5
1	A	541	GLU	2.5
1	B	268	GLU	2.5
1	A	126	SER	2.4
1	B	17	ALA	2.4
1	A	193	LEU	2.4
1	B	35	GLN	2.4
1	A	426	ASP	2.3
1	B	494	GLN	2.3
1	A	519	THR	2.3
1	B	38	TYR	2.3
1	B	536	GLN	2.3
1	B	256	CYS	2.3
1	B	492	VAL	2.3
1	B	159	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	61	LEU	2.2
1	B	158	TYR	2.2
1	A	410	ALA	2.2
1	B	24	SER	2.2
1	B	63	VAL	2.2
1	B	182	GLN	2.2
1	B	253	LEU	2.2
1	B	61	LEU	2.1
1	B	135	GLY	2.1
1	B	87	ILE	2.1
1	A	100	THR	2.0
1	A	122	ILE	2.0
1	B	31	SER	2.0
1	B	122	ILE	2.0
1	B	176	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å^2)	Q<0.9
3	SO4	B	602	5/5	0.93	0.23	71,73,77,80	0
3	SO4	A	603	5/5	0.97	0.13	38,39,41,42	0
3	SO4	A	601	5/5	0.98	0.12	38,41,50,52	0
3	SO4	B	604	5/5	0.98	0.07	47,47,52,54	0
2	ZN	A	700	1/1	0.99	0.11	21,21,21,21	0
2	ZN	B	700	1/1	0.99	0.09	33,33,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.