



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:01 AM UTC

PDB ID : 1EF0 / pdb_00001ef0
Title : CRYSTAL STRUCTURE OF PI-SCEI MINIPRECURSOR
Authors : Poland, B.W.; Xu, M.-Q.; Quiocho, F.A.
Deposited on : 2000-02-04
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
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

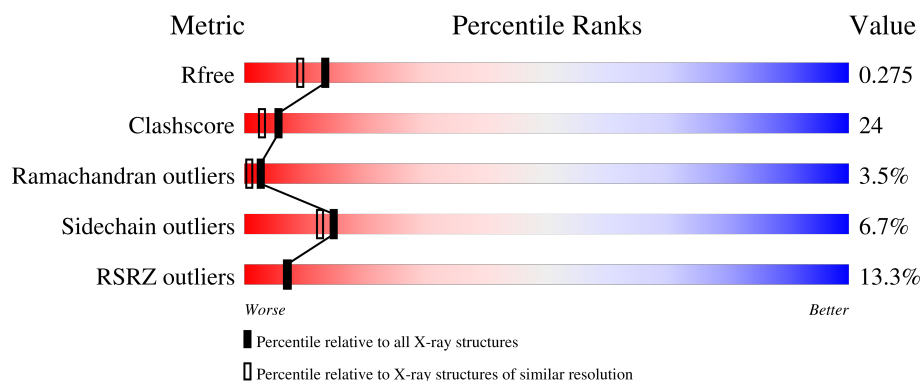
1 Overall quality at a glance

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	462	10% 52% 34% 6% 8%
1	B	462	14% 51% 27% 6% 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6887 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 PI-SCEI ENDONUCLEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	4	0
			3369	2124	584	647	14			
1	B	394	Total	C	N	O	S	0	0	0
			3106	1965	534	594	13			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	697	LYS	-	SEE REMARK 999	GB 172907
A	698	LEU	-	SEE REMARK 999	GB 172907
A	699	GLU	-	SEE REMARK 999	GB 172907
A	700	GLY	-	SEE REMARK 999	GB 172907
A	1	ALA	CYS	engineered mutation	GB 172907
A	454	ALA	ASN	engineered mutation	GB 172907
A	456	GLY	-	SEE REMARK 999	GB 172907
A	457	GLU	-	SEE REMARK 999	GB 172907
A	458	ARG	-	SEE REMARK 999	GB 172907
B	697	LYS	-	SEE REMARK 999	GB 172907
B	698	LEU	-	SEE REMARK 999	GB 172907
B	699	GLU	-	SEE REMARK 999	GB 172907
B	700	GLY	-	SEE REMARK 999	GB 172907
B	1	ALA	CYS	engineered mutation	GB 172907
B	454	ALA	ASN	engineered mutation	GB 172907
B	456	GLY	-	SEE REMARK 999	GB 172907
B	457	GLU	-	SEE REMARK 999	GB 172907
B	458	ARG	-	SEE REMARK 999	GB 172907

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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

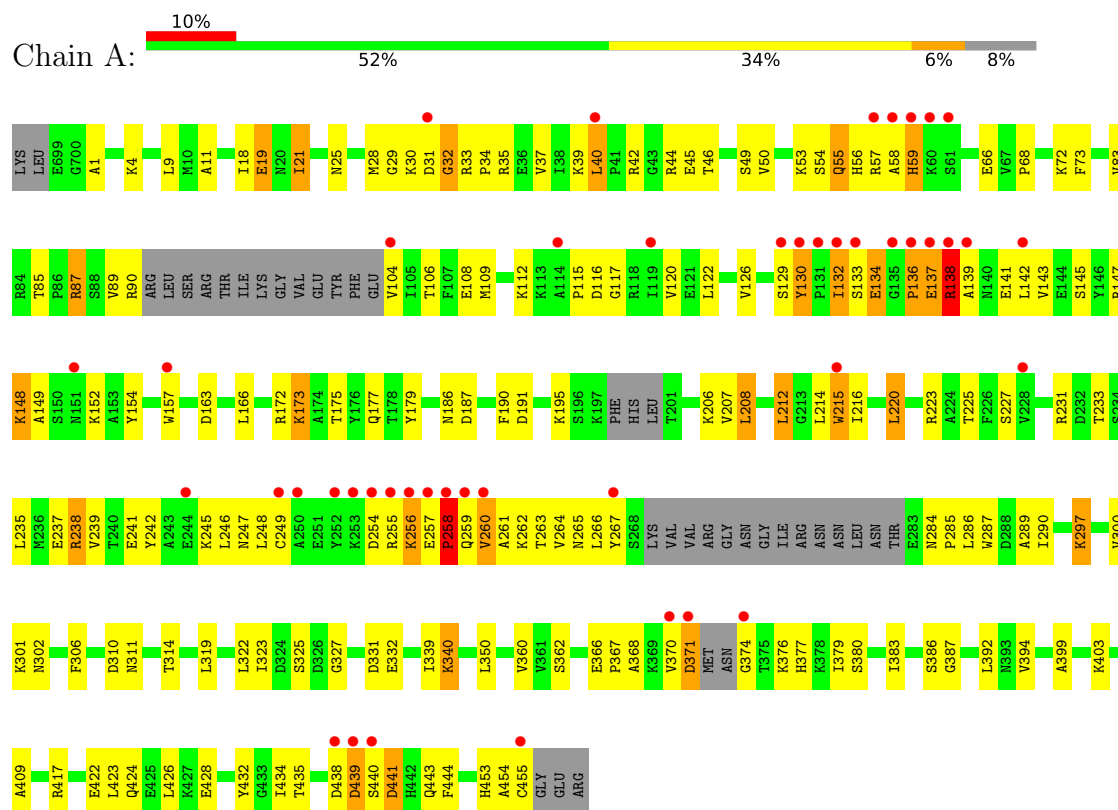
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	217	Total 218	O 218	0	1
3	B	191	Total 191	O 191	0	0

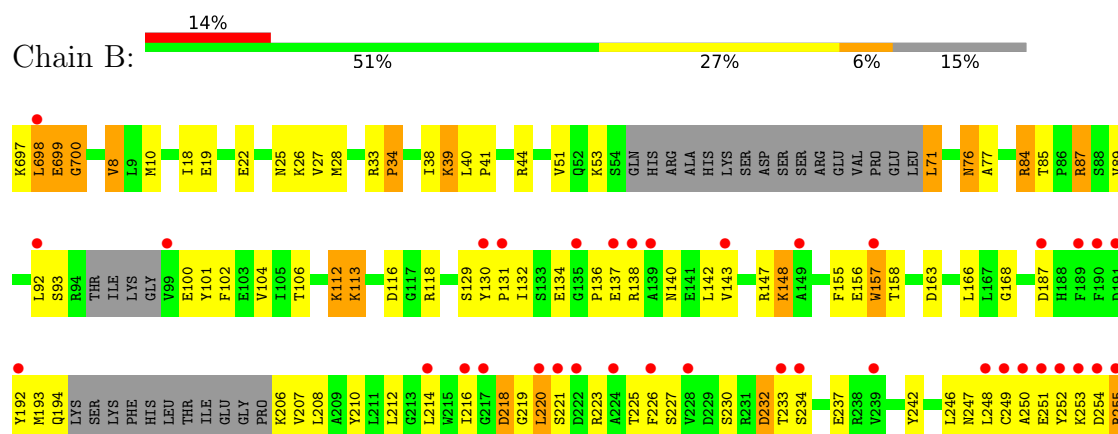
3 Residue-property plots

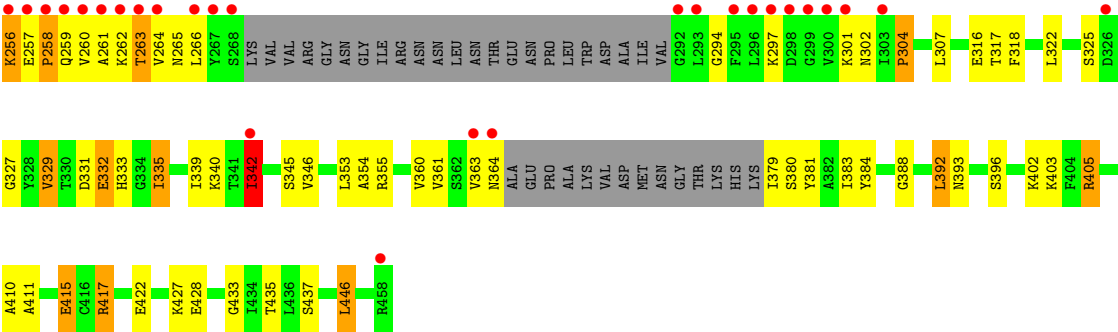
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: PI-SCEI ENDONUCLEASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.00Å 101.68Å 86.77Å 90.00° 93.51° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.3 (20.00-2.10) 88.2 (20.00-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.09Å)	Xtriage
Refinement program	CNS, XTALVIEW	Depositor
R, R_{free}	0.231 , 0.281 0.226 , 0.275	Depositor DCC
R_{free} test set	5333 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6887	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% 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: 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	0.40	0/3430	0.94	15/4626 (0.3%)
1	B	0.38	0/3157	0.91	8/4251 (0.2%)
All	All	0.39	0/6587	0.92	23/8877 (0.3%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	GLY	N-CA-C	-10.58	100.72	115.32
1	B	87	ARG	N-CA-C	-8.12	98.47	110.48
1	A	87	ARG	N-CA-C	-6.81	100.41	110.48
1	B	256	LYS	N-CA-C	-6.58	105.88	114.04
1	B	342	ILE	N-CA-C	-6.48	106.48	112.96
1	A	83	VAL	N-CA-C	6.18	117.73	108.96
1	B	77	ALA	N-CA-C	6.11	118.72	111.33
1	B	700	GLY	N-CA-C	-5.95	99.08	113.18
1	B	34	PRO	N-CA-C	5.66	119.91	111.41
1	B	446	LEU	N-CA-C	-5.65	103.24	110.53
1	A	186	ASN	N-CA-C	-5.64	102.57	110.35
1	A	130	TYR	CA-C-N	5.55	126.77	119.84
1	A	130	TYR	C-N-CA	5.55	126.77	119.84
1	B	168	GLY	N-CA-C	-5.54	105.45	112.54
1	A	379	ILE	N-CA-C	5.53	116.55	108.53
1	A	30	LYS	N-CA-C	-5.49	105.69	112.38
1	A	30	LYS	CA-C-N	5.48	127.62	120.28
1	A	30	LYS	C-N-CA	5.48	127.62	120.28
1	A	120	VAL	N-CA-C	5.47	115.83	108.17
1	A	394	VAL	N-CA-C	-5.40	106.42	111.45
1	A	371	ASP	N-CA-C	-5.33	108.03	114.75
1	A	374	GLY	N-CA-C	-5.12	101.05	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	360	VAL	N-CA-C	-5.08	101.27	108.58

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	3369	0	3345	159	0
1	B	3106	0	3097	154	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	218	0	0	2	0
3	B	191	0	0	6	0
All	All	6887	0	6442	303	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 24.

All (303) 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:453[A]:HIS:HE1	1:A:455[A]:CYS:SG	1.55	1.29
1:A:453[A]:HIS:CE1	1:A:455[A]:CYS:SG	2.45	1.10
1:B:251:GLU:HG2	1:B:265:ASN:HB2	1.40	1.00
1:B:136:PRO:HB2	1:B:140:ASN:HD21	1.33	0.91
1:A:231:ARG:HH21	1:A:260:VAL:HG13	1.35	0.90
1:B:415:GLU:CD	1:B:415:GLU:H	1.82	0.88
1:A:130:TYR:HB2	1:A:138:ARG:HD2	1.59	0.84
1:B:28:MET:HE3	1:B:28:MET:HA	1.59	0.84
1:B:427:LYS:HD3	1:B:428:GLU:N	1.93	0.83
1:B:194:GLN:HB2	3:B:815:HOH:O	1.77	0.83
1:B:104:VAL:HG21	1:B:142:LEU:HD23	1.62	0.81
1:A:35:ARG:HG3	1:A:35:ARG:HH11	1.45	0.79
1:A:227:SER:HB3	1:A:256:LYS:NZ	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ILE:HG22	1:B:39:LYS:HG2	1.65	0.78
1:B:216:ILE:HG13	1:B:301:LYS:HB3	1.65	0.78
1:A:53:LYS:HA	1:A:57:ARG:NH2	1.98	0.77
1:A:227:SER:HB3	1:A:256:LYS:HZ3	1.49	0.77
1:A:231:ARG:NH1	1:A:231:ARG:HB2	1.99	0.77
1:A:297:LYS:O	1:A:300:VAL:HG12	1.84	0.77
1:A:53:LYS:HA	1:A:57:ARG:HH21	1.49	0.75
1:A:340:LYS:HZ3	1:A:340:LYS:HB3	1.51	0.75
1:A:108:GLU:OE2	1:A:126:VAL:HG21	1.86	0.75
1:A:148:LYS:HB2	1:A:148:LYS:NZ	2.01	0.75
1:A:147:ARG:HG2	1:B:410:ALA:HA	1.67	0.75
1:A:256:LYS:HB3	1:A:261:ALA:HB3	1.69	0.74
1:A:172:ARG:O	1:A:175:THR:HG22	1.87	0.74
1:B:251:GLU:CG	1:B:265:ASN:HB2	2.19	0.71
1:B:302:ASN:HD22	1:B:345:SER:HB2	1.55	0.71
1:A:366:GLU:HB2	1:A:367:PRO:HD2	1.73	0.69
1:B:219:GLY:HA2	1:B:226:PHE:HA	1.74	0.69
1:A:130:TYR:CB	1:A:138:ARG:HD2	2.22	0.69
1:A:231:ARG:HB2	1:A:231:ARG:HH11	1.58	0.68
1:B:113:LYS:HB2	1:B:113:LYS:HZ2	1.57	0.68
1:B:136:PRO:HB2	1:B:140:ASN:ND2	2.06	0.68
1:A:225:THR:HG22	1:A:265:ASN:HA	1.75	0.68
1:B:212:LEU:O	1:B:216:ILE:HG22	1.93	0.67
1:A:233:THR:O	1:A:237:GLU:HG3	1.95	0.67
1:A:311:ASN:HD22	1:A:314:THR:H	1.44	0.66
1:A:340:LYS:HB3	1:A:340:LYS:NZ	2.09	0.66
1:B:230:SER:OG	1:B:262:LYS:HB2	1.95	0.66
1:A:255:ARG:NH1	1:A:259:GLN:HE21	1.94	0.66
1:A:362:SER:HB3	1:B:333:HIS:HE1	1.60	0.66
1:A:238:ARG:NH1	1:A:399:ALA:HB2	2.11	0.65
1:A:152:LYS:HD2	1:A:154:TYR:CZ	2.31	0.65
1:B:102:PHE:CZ	1:B:132:ILE:HG23	2.30	0.65
1:B:342:ILE:HD12	1:B:342:ILE:N	2.11	0.65
1:A:35:ARG:HG3	1:A:35:ARG:NH1	2.10	0.65
1:A:257:GLU:O	1:A:259:GLN:N	2.29	0.65
1:A:55:GLN:H	1:A:55:GLN:HE21	1.45	0.65
1:B:100:GLU:HG2	1:B:132:ILE:HD12	1.79	0.65
1:A:134:GLU:O	1:A:138:ARG:HB2	1.97	0.65
1:B:698:LEU:O	1:B:699:GLU:HB3	1.96	0.64
1:A:40:LEU:HB2	1:A:42:ARG:NH1	2.13	0.64
1:B:254:ASP:HA	1:B:262:LYS:HG3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:LYS:HD3	1:B:428:GLU:O	1.98	0.63
1:A:50:VAL:HG11	1:A:177:GLN:HE22	1.62	0.63
1:B:38:ILE:CD1	1:B:437:SER:HA	2.29	0.63
1:A:21:ILE:HD11	1:A:37:VAL:HG21	1.80	0.62
1:A:55:GLN:H	1:A:55:GLN:NE2	1.96	0.62
1:A:215:TRP:CZ3	1:A:220:LEU:O	2.52	0.62
1:B:329:VAL:HG11	1:B:403:LYS:HA	1.81	0.62
1:B:85:THR:OG1	1:B:157:TRP:CZ3	2.52	0.62
1:A:11:ALA:HA	1:A:28:MET:HG2	1.81	0.62
1:A:18:ILE:O	1:A:21:ILE:HG23	1.99	0.61
1:B:85:THR:OG1	1:B:157:TRP:HZ3	1.83	0.61
1:B:206:LYS:HG2	1:B:207:VAL:H	1.65	0.61
1:B:138:ARG:O	1:B:142:LEU:HD13	2.00	0.61
1:B:206:LYS:HD3	3:B:813:HOH:O	2.01	0.60
1:A:90:ARG:HH11	1:B:396:SER:HB2	1.66	0.60
1:A:440:SER:O	1:A:441:ASP:HB3	2.02	0.60
1:B:327:GLY:O	1:B:403:LYS:HE2	2.01	0.60
1:A:4:LYS:HG3	1:A:19:GLU:HG2	1.83	0.59
1:A:223:ARG:HG3	1:A:225:THR:HG23	1.85	0.59
1:A:206:LYS:HD3	1:A:242:TYR:OH	2.03	0.59
1:A:21:ILE:CD1	1:A:37:VAL:HG21	2.32	0.59
1:B:256:LYS:HB2	1:B:263:THR:OG1	2.03	0.58
1:B:116:ASP:OD1	1:B:118:ARG:HB2	2.03	0.58
1:B:253:LYS:O	1:B:253:LYS:HG3	2.02	0.58
1:B:297:LYS:HB3	1:B:302:ASN:HB3	1.84	0.58
1:A:53:LYS:HE3	1:A:422:GLU:OE2	2.04	0.58
1:A:247:ASN:O	1:A:248:LEU:HD23	2.04	0.58
1:A:255:ARG:NH1	1:A:259:GLN:NE2	2.51	0.57
1:B:112:LYS:HD3	1:B:113:LYS:N	2.18	0.57
1:A:130:TYR:HB2	1:A:138:ARG:CD	2.32	0.57
1:A:248:LEU:HD21	1:A:285:PRO:CG	2.34	0.57
1:B:225:THR:HG23	1:B:264:VAL:O	2.05	0.57
1:B:249:CYS:SG	3:B:845:HOH:O	2.57	0.57
1:A:31:ASP:HB3	1:A:33:ARG:H	1.70	0.56
1:A:323:ILE:HG12	1:A:339:ILE:HD11	1.86	0.56
1:B:415:GLU:CD	1:B:415:GLU:N	2.55	0.56
1:B:53:LYS:HE2	1:B:422:GLU:OE2	2.06	0.56
1:A:1:ALA:HB1	1:A:432:TYR:C	2.31	0.55
1:B:26:LYS:HD2	1:B:34:PRO:HB2	1.87	0.55
1:B:113:LYS:HB2	1:B:113:LYS:NZ	2.22	0.55
1:B:255:ARG:NH1	1:B:258:PRO:HA	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:ARG:O	1:B:148:LYS:HB3	2.06	0.55
1:A:173:LYS:HB2	1:A:173:LYS:NZ	2.22	0.54
1:A:284:ASN:HB3	1:A:287:TRP:HB3	1.90	0.54
1:A:441:ASP:O	1:A:443:GLN:HG3	2.08	0.54
1:B:163:ASP:HA	1:B:166:LEU:HD23	1.89	0.54
1:A:148:LYS:HB2	1:A:148:LYS:HZ3	1.70	0.54
1:B:38:ILE:HD11	1:B:437:SER:HA	1.89	0.54
1:A:257:GLU:O	1:A:258:PRO:C	2.50	0.54
1:A:29:GLY:C	1:A:31:ASP:N	2.63	0.54
1:A:386:SER:OG	1:B:333:HIS:HD2	1.90	0.54
1:A:147:ARG:HD3	1:B:411:ALA:N	2.22	0.54
1:B:89:VAL:HG23	1:B:106:THR:HG22	1.88	0.54
1:A:163:ASP:HA	1:A:166:LEU:HD13	1.88	0.54
1:B:307:LEU:HB3	1:B:353:LEU:HD13	1.87	0.54
1:B:104:VAL:HG23	1:B:104:VAL:O	2.07	0.54
1:B:163:ASP:O	1:B:166:LEU:HD23	2.08	0.54
1:A:246:LEU:O	1:A:247:ASN:HB2	2.08	0.53
1:B:256:LYS:HE2	3:B:850:HOH:O	2.08	0.53
1:B:379:ILE:HG12	1:B:380:SER:N	2.23	0.53
1:B:214:LEU:HA	1:B:325:SER:HB2	1.90	0.53
1:B:301:LYS:O	1:B:346:VAL:HG23	2.08	0.53
1:A:256:LYS:HD3	1:A:263:THR:OG1	2.08	0.52
1:B:39:LYS:C	1:B:41:PRO:HD3	2.34	0.52
1:A:323:ILE:CG1	1:A:339:ILE:HD11	2.40	0.52
1:B:134:GLU:HB3	1:B:138:ARG:HH12	1.75	0.52
1:A:440:SER:O	1:A:441:ASP:CB	2.58	0.52
1:B:335:ILE:HD11	1:B:388:GLY:HA2	1.92	0.52
1:B:427:LYS:CD	1:B:428:GLU:N	2.71	0.52
1:A:40:LEU:HD12	1:A:40:LEU:O	2.09	0.52
1:B:227:SER:HB2	1:B:256:LYS:HD3	1.92	0.52
1:B:216:ILE:HG12	1:B:216:ILE:O	2.10	0.52
1:B:85:THR:HG1	1:B:157:TRP:HZ3	1.51	0.52
1:B:206:LYS:HG2	1:B:207:VAL:HG23	1.92	0.52
1:A:59:HIS:HB3	1:A:68:PRO:HB3	1.92	0.51
1:A:179:TYR:CZ	1:A:417:ARG:HB2	2.45	0.51
1:A:286:LEU:O	1:A:290:ILE:HG12	2.10	0.51
1:B:112:LYS:HD3	1:B:112:LYS:C	2.34	0.51
1:B:39:LYS:HA	1:B:39:LYS:HZ3	1.75	0.51
1:B:101:TYR:HB3	1:B:130:TYR:O	2.11	0.51
1:A:235:LEU:O	1:A:239:VAL:HG23	2.11	0.51
1:B:71:LEU:HD13	1:B:355:ARG:NH1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:VAL:HG22	1:B:364:ASN:N	2.26	0.51
1:A:44:ARG:NH1	1:A:428:GLU:OE2	2.44	0.51
1:B:102:PHE:CD2	1:B:132:ILE:HG12	2.46	0.51
1:A:28:MET:HE1	1:A:32:GLY:O	2.11	0.51
1:B:100:GLU:HG2	1:B:132:ILE:CD1	2.40	0.51
1:B:253:LYS:HG3	1:B:263:THR:HB	1.91	0.50
1:B:417:ARG:HD2	1:B:417:ARG:N	2.25	0.50
1:B:342:ILE:HG23	1:B:379:ILE:O	2.11	0.50
1:A:29:GLY:C	1:A:31:ASP:H	2.18	0.50
1:B:206:LYS:O	1:B:317:THR:HG21	2.11	0.50
1:B:76:ASN:C	1:B:76:ASN:HD22	2.20	0.50
1:B:102:PHE:CE2	1:B:132:ILE:HG23	2.47	0.50
1:B:331:ASP:O	1:B:332:GLU:C	2.54	0.50
1:A:115:PRO:C	1:A:117:GLY:H	2.19	0.50
1:A:173:LYS:HB2	1:A:173:LYS:HZ2	1.77	0.50
1:B:247:ASN:O	1:B:248:LEU:HD23	2.11	0.50
1:B:383:ILE:N	1:B:383:ILE:HD12	2.27	0.50
1:A:215:TRP:CD1	1:A:215:TRP:C	2.88	0.50
1:B:254:ASP:HB2	1:B:262:LYS:HE3	1.94	0.50
1:B:38:ILE:HD12	1:B:437:SER:HA	1.93	0.50
1:B:364:ASN:HB3	1:B:384:TYR:HE1	1.76	0.49
1:B:427:LYS:NZ	1:B:428:GLU:HB3	2.27	0.49
1:A:122:LEU:C	1:A:122:LEU:HD12	2.36	0.49
1:A:152:LYS:HD2	1:A:154:TYR:OH	2.12	0.49
1:A:191:ASP:O	1:A:195:LYS:HG2	2.11	0.49
1:B:41:PRO:HG2	1:B:435:THR:HG23	1.95	0.49
1:B:340:LYS:HA	1:B:381:TYR:O	2.12	0.49
1:A:122:LEU:HD12	1:A:122:LEU:O	2.13	0.49
1:A:49:SER:HB3	1:A:426:LEU:HD11	1.95	0.49
1:A:87:ARG:NH2	1:A:149:ALA:HB3	2.28	0.49
1:A:139:ALA:C	1:A:141:GLU:H	2.21	0.49
1:A:241:GLU:HG2	1:A:245:LYS:HE3	1.94	0.49
1:B:220:LEU:HD12	1:B:223:ARG:HG3	1.93	0.49
1:A:148:LYS:HB2	1:A:148:LYS:HZ2	1.78	0.49
1:B:302:ASN:O	1:B:304:PRO:HD3	2.13	0.49
1:A:21:ILE:HD12	1:A:25:ASN:HB2	1.95	0.48
1:A:55:GLN:HE21	1:A:55:GLN:N	2.10	0.48
1:B:415:GLU:N	1:B:415:GLU:OE1	2.45	0.48
1:B:18:ILE:HG23	1:B:19:GLU:N	2.28	0.48
1:A:137:GLU:O	1:A:141:GLU:HB3	2.13	0.48
1:A:207:VAL:HA	1:A:242:TYR:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ARG:HG2	1:A:138:ARG:HH11	1.79	0.48
1:A:4:LYS:HG3	1:A:19:GLU:CG	2.44	0.48
1:B:22:GLU:O	1:B:25:ASN:HB2	2.14	0.48
1:B:329:VAL:CG1	1:B:403:LYS:HA	2.42	0.48
1:A:215:TRP:CD1	1:A:216:ILE:N	2.81	0.48
1:A:248:LEU:HA	1:A:267:TYR:O	2.13	0.48
1:B:699:GLU:N	1:B:699:GLU:OE1	2.47	0.48
1:A:301:LYS:O	1:A:302:ASN:HB3	2.14	0.47
1:A:306:PHE:CD1	1:A:306:PHE:C	2.92	0.47
1:A:340:LYS:HE3	1:A:366:GLU:OE2	2.13	0.47
1:B:112:LYS:NZ	3:B:861:HOH:O	2.47	0.47
1:B:210:TYR:CE2	1:B:214:LEU:HD11	2.48	0.47
1:A:362:SER:CB	1:B:333:HIS:HE1	2.27	0.47
1:A:362:SER:HB3	1:B:333:HIS:CE1	2.44	0.47
1:A:238:ARG:HH11	1:A:238:ARG:HB2	1.79	0.47
1:B:227:SER:OG	1:B:261:ALA:HB1	2.15	0.47
1:B:101:TYR:HD2	1:B:131:PRO:N	2.13	0.47
1:A:138:ARG:NE	1:A:138:ARG:C	2.73	0.46
1:A:231:ARG:NH2	1:A:260:VAL:HG13	2.17	0.46
1:B:697:LYS:HA	3:B:812:HOH:O	2.15	0.46
1:B:251:GLU:HB3	1:B:265:ASN:O	2.14	0.46
1:A:44:ARG:HH11	1:A:44:ARG:HB3	1.81	0.46
1:B:227:SER:HB2	1:B:256:LYS:NZ	2.30	0.46
1:A:340:LYS:NZ	1:A:380:SER:OG	2.48	0.46
1:B:166:LEU:N	1:B:166:LEU:HD22	2.29	0.46
1:A:227:SER:HB3	1:A:256:LYS:HZ2	1.79	0.46
1:B:427:LYS:HD3	1:B:427:LYS:C	2.39	0.46
1:A:45:GLU:HG3	1:A:46:THR:N	2.30	0.46
1:A:90:ARG:NH1	1:B:396:SER:HB2	2.29	0.46
1:B:232:ASP:OD1	1:B:234:SER:HB3	2.16	0.46
1:B:157:TRP:CD1	1:B:158:THR:O	2.69	0.46
1:B:208:LEU:O	1:B:212:LEU:HG	2.16	0.46
1:A:39:LYS:HB3	1:A:435:THR:HB	1.99	0.45
1:A:56:HIS:C	1:A:57:ARG:HG3	2.41	0.45
1:B:192:TYR:CD1	1:B:192:TYR:C	2.94	0.45
1:A:264:VAL:HG12	1:A:266:LEU:HD12	1.99	0.45
1:A:254:ASP:O	1:A:255:ARG:CB	2.65	0.45
1:A:370:VAL:HG12	1:A:371:ASP:N	2.32	0.45
1:B:136:PRO:O	1:B:140:ASN:ND2	2.49	0.45
1:B:259:GLN:O	1:B:259:GLN:HG3	2.15	0.45
1:A:142:LEU:HA	1:A:145:SER:OG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:PHE:CD1	1:A:190:PHE:C	2.95	0.45
1:A:444:PHE:HE1	1:A:454:ALA:HB2	1.81	0.45
1:B:84:ARG:HA	1:B:155:PHE:O	2.16	0.45
1:A:44:ARG:NH1	1:A:428:GLU:HG2	2.32	0.45
1:B:259:GLN:HE21	1:B:259:GLN:HA	1.82	0.44
1:B:250:ALA:O	1:B:251:GLU:HB3	2.18	0.44
1:A:208:LEU:HD22	1:A:212:LEU:HD13	2.00	0.44
1:A:231:ARG:HH11	1:A:231:ARG:CB	2.26	0.44
1:A:332:GLU:HG3	3:A:772:HOH:O	2.18	0.44
1:B:138:ARG:HD3	1:B:138:ARG:H	1.82	0.44
1:B:265:ASN:C	1:B:266:LEU:HD22	2.42	0.44
1:B:216:ILE:HA	1:B:301:LYS:HD3	2.00	0.44
1:B:250:ALA:HB1	1:B:252:TYR:HE1	1.83	0.44
1:A:141:GLU:CG	1:A:142:LEU:N	2.80	0.44
1:A:264:VAL:HG12	1:A:266:LEU:CD1	2.48	0.44
1:A:368:ALA:HB3	1:A:377:HIS:O	2.17	0.44
1:B:33:ARG:HB3	1:B:34:PRO:HD2	1.99	0.44
1:A:139:ALA:C	1:A:141:GLU:N	2.76	0.44
1:B:76:ASN:C	1:B:76:ASN:ND2	2.76	0.44
1:B:92:LEU:HD12	1:B:93:SER:H	1.83	0.43
1:A:89:VAL:HG23	1:A:106:THR:HG22	2.00	0.43
1:B:257:GLU:HB2	1:B:261:ALA:H	1.83	0.43
1:A:104:VAL:O	1:A:104:VAL:HG13	2.18	0.43
1:A:133:SER:O	1:A:134:GLU:HB3	2.18	0.43
1:B:262:LYS:O	1:B:263:THR:C	2.62	0.43
1:A:19:GLU:CD	1:A:19:GLU:H	2.26	0.43
1:A:207:VAL:HG21	1:A:246:LEU:HG	2.01	0.43
1:B:140:ASN:O	1:B:143:VAL:HG22	2.18	0.43
1:B:254:ASP:OD1	1:B:255:ARG:N	2.52	0.43
1:A:85:THR:HG1	1:A:157:TRP:HH2	1.59	0.43
1:B:39:LYS:HA	1:B:39:LYS:NZ	2.34	0.43
1:B:210:TYR:HE2	1:B:214:LEU:HD11	1.84	0.43
1:B:246:LEU:O	1:B:248:LEU:HG	2.19	0.43
1:A:138:ARG:HG2	1:A:138:ARG:NH1	2.34	0.43
1:B:22:GLU:HA	1:B:40:LEU:HD11	2.00	0.43
1:B:257:GLU:O	1:B:259:GLN:N	2.52	0.43
1:B:132:ILE:C	1:B:134:GLU:H	2.27	0.42
1:A:49:SER:HG	1:A:424:GLN:HB3	1.84	0.42
1:A:143:VAL:O	1:A:147:ARG:HG3	2.18	0.42
1:B:700:GLY:O	1:B:433:GLY:HA2	2.19	0.42
1:A:134:GLU:C	1:A:136:PRO:HD2	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ILE:N	1:A:383:ILE:HD12	2.34	0.42
1:B:327:GLY:HA2	1:B:339:ILE:HD13	2.01	0.42
1:B:354:ALA:HB3	1:B:361:VAL:HG21	2.01	0.42
1:B:255:ARG:CZ	1:B:258:PRO:HA	2.49	0.42
1:A:11:ALA:O	1:A:28:MET:HE3	2.19	0.42
1:B:100:GLU:OE2	1:B:132:ILE:HD12	2.20	0.42
1:B:294:GLY:C	1:B:304:PRO:HG3	2.44	0.42
1:A:289:ALA:O	1:A:290:ILE:C	2.62	0.42
1:A:147:ARG:CG	1:B:410:ALA:HA	2.42	0.42
1:A:4:LYS:HB2	1:A:432:TYR:CE1	2.54	0.41
1:A:50:VAL:HG22	1:A:423:LEU:CD1	2.51	0.41
1:B:259:GLN:HA	1:B:259:GLN:NE2	2.36	0.41
1:B:402:LYS:O	1:B:405:ARG:NH2	2.53	0.41
1:A:254:ASP:O	1:A:255:ARG:HB3	2.20	0.41
1:B:318:PHE:CE1	1:B:322:LEU:HD12	2.55	0.41
1:A:54:SER:H	1:A:57:ARG:HH21	1.66	0.41
1:A:248:LEU:HD21	1:A:285:PRO:HG2	2.01	0.41
1:A:311:ASN:HD22	1:A:314:THR:N	2.16	0.41
1:B:392:LEU:HD12	1:B:392:LEU:HA	1.85	0.41
1:A:34:PRO:O	1:A:35:ARG:HG3	2.20	0.41
1:B:316:GLU:OE2	1:B:393:ASN:ND2	2.38	0.41
1:B:360:VAL:HG23	1:B:417:ARG:NH1	2.36	0.41
1:A:115:PRO:C	1:A:117:GLY:N	2.79	0.41
1:A:220:LEU:HD12	1:A:220:LEU:HA	1.89	0.41
1:A:214:LEU:HA	1:A:325:SER:HB2	2.03	0.41
1:A:215:TRP:HZ3	1:A:220:LEU:O	2.01	0.41
1:B:218:ASP:CG	1:B:227:SER:HB3	2.45	0.41
1:B:233:THR:HG22	1:B:237:GLU:HG3	2.03	0.41
1:A:409:ALA:HB1	1:B:87:ARG:HB2	2.02	0.41
1:B:102:PHE:O	1:B:129:SER:HA	2.21	0.41
1:A:18:ILE:HD11	1:A:434:ILE:HG23	2.03	0.40
1:A:21:ILE:CD1	1:A:25:ASN:HB2	2.50	0.40
1:A:72:LYS:O	1:A:73:PHE:HB3	2.21	0.40
1:A:262:LYS:HB2	1:A:262:LYS:HE3	1.90	0.40
1:A:132:ILE:O	1:A:134:GLU:HG2	2.21	0.40
1:B:8:VAL:HA	1:B:446:LEU:HA	2.04	0.40
1:A:50:VAL:CG1	1:A:177:GLN:HE22	2.32	0.40
1:A:187:ASP:HA	3:A:760:HOH:O	2.20	0.40
1:A:438:ASP:O	1:A:439:ASP:C	2.64	0.40
1:B:207:VAL:HG13	1:B:242:TYR:CD2	2.56	0.40
1:A:109:MET:HE3	1:A:122:LEU:C	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:GLY:O	1:A:403:LYS:HE2	2.22	0.40
1:B:699:GLU:HG2	1:B:700:GLY:N	2.35	0.40
1:B:10:MET:HA	1:B:27:VAL:HA	2.04	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	420/462 (91%)	372 (89%)	35 (8%)	13 (3%)	3	1
1	B	382/462 (83%)	346 (91%)	21 (6%)	15 (4%)	2	0
All	All	802/924 (87%)	718 (90%)	56 (7%)	28 (4%)	3	1

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	GLU
1	A	138	ARG
1	A	258	PRO
1	A	441	ASP
1	B	148	LYS
1	B	258	PRO
1	B	332	GLU
1	A	136	PRO
1	A	256	LYS
1	B	698	LEU
1	B	193	MET
1	B	218	ASP
1	B	220	LEU
1	B	232	ASP
1	B	255	ARG

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Mol	Chain	Res	Type
1	A	58	ALA
1	A	59	HIS
1	A	439	ASP
1	B	137	GLU
1	A	132	ILE
1	B	699	GLU
1	B	221	SER
1	B	260	VAL
1	B	263	THR
1	A	116	ASP
1	A	387	GLY
1	B	304	PRO
1	A	260	VAL

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	367/396 (93%)	339 (92%)	28 (8%)	12	9
1	B	337/396 (85%)	318 (94%)	19 (6%)	19	18
All	All	704/792 (89%)	657 (93%)	47 (7%)	15	12

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	19	GLU
1	A	21	ILE
1	A	40	LEU
1	A	55	GLN
1	A	66	GLU
1	A	112	LYS
1	A	129	SER
1	A	137	GLU
1	A	138	ARG

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Mol	Chain	Res	Type
1	A	148	LYS
1	A	173	LYS
1	A	208	LEU
1	A	212	LEU
1	A	215	TRP
1	A	220	LEU
1	A	238	ARG
1	A	249	CYS
1	A	258	PRO
1	A	297	LYS
1	A	310	ASP
1	A	319	LEU
1	A	322	LEU
1	A	331	ASP
1	A	340	LYS
1	A	350	LEU
1	A	376	LYS
1	A	392	LEU
1	B	8	VAL
1	B	39	LYS
1	B	44	ARG
1	B	51	VAL
1	B	71	LEU
1	B	76	ASN
1	B	84	ARG
1	B	112	LYS
1	B	113	LYS
1	B	156	GLU
1	B	157	TRP
1	B	187	ASP
1	B	329	VAL
1	B	335	ILE
1	B	342	ILE
1	B	392	LEU
1	B	405	ARG
1	B	415	GLU
1	B	417	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN

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Mol	Chain	Res	Type
1	A	79	HIS
1	A	177	GLN
1	A	259	GLN
1	A	311	ASN
1	A	443	GLN
1	B	7	ASN
1	B	52	GLN
1	B	76	ASN
1	B	111	GLN
1	B	140	ASN
1	B	194	GLN
1	B	259	GLN
1	B	302	ASN
1	B	333	HIS
1	B	364	ASN
1	B	424	GLN
1	B	443	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 3 ligands modelled in this entry, 3 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	425/462 (91%)	0.49	45 (10%)	11 12	7, 28, 62, 81	4 (0%)
1	B	394/462 (85%)	0.65	64 (16%)	4 4	14, 30, 73, 92	0
All	All	819/924 (88%)	0.57	109 (13%)	7 7	7, 29, 68, 92	4 (0%)

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	58	ALA	6.6
1	A	61	SER	5.4
1	B	250	ALA	5.3
1	B	249	CYS	4.9
1	A	455[A]	CYS	4.9
1	B	99	VAL	4.6
1	A	374	GLY	4.6
1	B	258	PRO	4.5
1	B	253	LYS	4.5
1	B	298	ASP	4.4
1	A	135	GLY	4.3
1	A	132	ILE	4.2
1	A	257	GLU	4.2
1	B	143	VAL	4.1
1	A	59	HIS	4.1
1	B	296	LEU	4.0
1	A	57	ARG	4.0
1	A	438	ASP	4.0
1	A	249	CYS	3.9
1	B	292	GLY	3.9
1	B	252	TYR	3.9
1	A	142	LEU	3.8
1	A	139	ALA	3.7
1	B	220	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	248	LEU	3.7
1	B	135	GLY	3.7
1	A	260	VAL	3.7
1	A	258	PRO	3.6
1	B	189	PHE	3.5
1	A	256	LYS	3.4
1	A	133	SER	3.3
1	B	255	ARG	3.3
1	A	255	ARG	3.3
1	A	60	LYS	3.2
1	B	190	PHE	3.2
1	B	256	LYS	3.2
1	A	371	ASP	3.1
1	A	130	TYR	3.1
1	B	299	GLY	3.0
1	B	251	GLU	3.0
1	B	262	LYS	3.0
1	B	216	ILE	2.9
1	B	342	ILE	2.9
1	A	253	LYS	2.9
1	B	187	ASP	2.9
1	A	250	ALA	2.9
1	B	224	ALA	2.9
1	B	233	THR	2.8
1	A	136	PRO	2.8
1	B	300	VAL	2.8
1	A	267	TYR	2.8
1	B	239	VAL	2.8
1	B	326	ASP	2.7
1	B	263	THR	2.7
1	A	129	SER	2.7
1	B	228	VAL	2.7
1	B	363	VAL	2.7
1	A	157	TRP	2.7
1	B	260	VAL	2.6
1	B	226	PHE	2.6
1	B	266	LEU	2.6
1	B	92	LEU	2.6
1	B	234	SER	2.6
1	B	297	LYS	2.6
1	B	264	VAL	2.5
1	B	221	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	370	VAL	2.5
1	B	267	TYR	2.5
1	A	439	ASP	2.5
1	A	137	GLU	2.5
1	A	104	VAL	2.4
1	A	131	PRO	2.4
1	B	261	ALA	2.4
1	B	257	GLU	2.4
1	B	157	TRP	2.4
1	B	222	ASP	2.4
1	B	138	ARG	2.4
1	B	139	ALA	2.4
1	B	293	LEU	2.4
1	B	303	ILE	2.4
1	B	295	PHE	2.3
1	B	268	SER	2.3
1	A	259	GLN	2.3
1	B	192	TYR	2.3
1	B	364	ASN	2.3
1	A	228	VAL	2.3
1	A	138	ARG	2.3
1	A	114	ALA	2.3
1	B	217	GLY	2.2
1	A	40	LEU	2.2
1	B	259	GLN	2.2
1	B	149	ALA	2.2
1	B	301	LYS	2.2
1	B	191	ASP	2.2
1	A	244	GLU	2.2
1	A	215	TRP	2.2
1	A	151	ASN	2.1
1	A	440	SER	2.1
1	B	214	LEU	2.1
1	A	31	ASP	2.1
1	A	254	ASP	2.1
1	B	131	PRO	2.1
1	B	698	LEU	2.1
1	A	252	TYR	2.1
1	A	119	ILE	2.1
1	B	137	GLU	2.0
1	B	458	ARG	2.0
1	B	254	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	130	TYR	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(Å ²)	Q<0.9
2	ZN	A	701[A]	1/1	0.96	0.13	13,13,13,13	1
2	ZN	A	701[B]	1/1	0.96	0.13	42,42,42,42	1
2	ZN	B	701	1/1	1.00	0.02	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.