



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 10:15 AM EDT

PDB ID : 1EF0  
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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
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) : 2.23.2

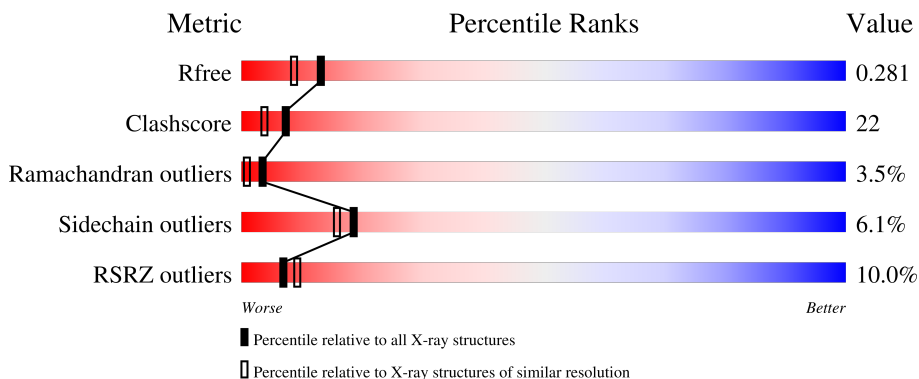
# 1 Overall quality at a glance

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))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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  $\geq 3$ , 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	
1	B	462	

## 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
			Total	C	N	O	S			
1	A	425	3369	2124	584	647	14	0	4	0
1	B	394	3106	1965	534	594	13	0	0	0

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 (three-letter code: ZN) (formula: Zn).

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

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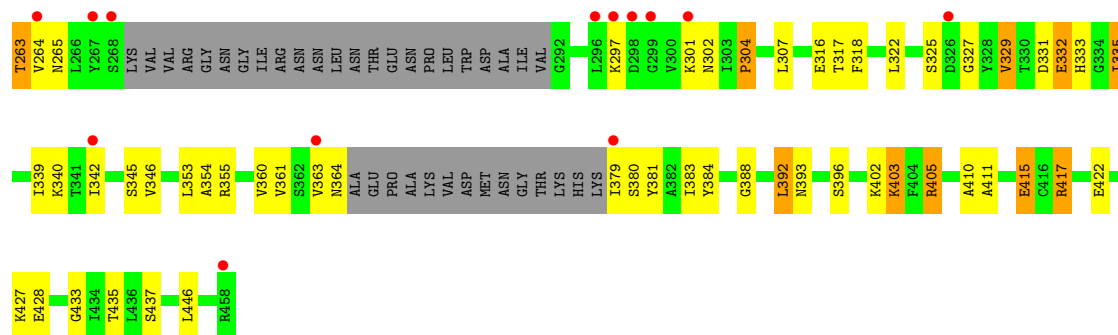
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.00Å 101.68Å 86.77Å 90.00° 93.51° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 19.93 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.3 (20.00-2.10) 88.3 (19.93-2.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 2.09Å)	Xtrriage
Refinement program	CNS, XTALVIEW	Depositor
R, $R_{free}$	0.231 , 0.281 0.231 , 0.281	Depositor DCC
$R_{free}$ test set	5333 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.2	Xtrriage
Anisotropy	0.130	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6887	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.34	0/3430	0.61	0/4626
1	B	0.35	0/3157	0.60	1/4251 (0.0%)
All	All	0.34	0/6587	0.61	1/8877 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	700	GLY	N-CA-C	-5.61	99.08	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	149	0
1	B	3106	0	3097	149	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	288	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 22.

All (288) 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:A:130:TYR:HB2	1:A:138:ARG:HD2	1.59	0.84
1:B:415:GLU:CD	1:B:415:GLU:H	1.82	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
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:HZ1	1.49	0.77
1:A:340:LYS:HZ3	1:A:340:LYS:HB3	1.48	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: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:28:MET:HE3	1:B:28:MET:HA	1.68	0.73
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:113:LYS:HB2	1:B:113:LYS:HZ2	1.63	0.63
1:A:148:LYS:HB2	1:A:148:LYS:HZ2	1.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:415:GLU:CD	1:B:415:GLU:N	2.55	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:53:LYS:HE2	1:B:422:GLU:OE2	2.06	0.56
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
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:B:38:ILE:HD11	1:B:437:SER:HA	1.89	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:B:379:ILE:HG12	1:B:380:SER:N	2.23	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: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:A:323:ILE:CG1	1:A:339:ILE:HD11	2.40	0.52
1:A:29:GLY:C	1:A:31:ASP:N	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:363:VAL:HG22	1:B:364:ASN:N	2.26	0.51
1:A:1:ALA:HB1	1:A:432:TYR:C	2.31	0.51
1:A:11:ALA:HA	1:A:28:MET:HE2	1.93	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: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:B:206:LYS:O	1:B:317:THR:HG21	2.11	0.50
1:B:102:PHE:CE2	1:B:132:ILE:HG23	2.47	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: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:A:257:GLU:O	1:A:258:PRO:C	2.50	0.49
1:B:427:LYS:NZ	1:B:428:GLU:HB3	2.27	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:O	1:A:122:LEU:HD12	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: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:B:302:ASN:O	1:B:304:PRO:HD3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:GLU:N	1:B:415:GLU:OE1	2.45	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: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
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:B:39:LYS:C	1:B:41:PRO:HD3	2.34	0.48
1:A:301:LYS:O	1:A:302:ASN:HB3	2.14	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:29:GLY:C	1:A:31:ASP:H	2.18	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:112:LYS:HD3	1:B:112:LYS:C	2.34	0.47
1:B:101:TYR:HD2	1:B:131:PRO:N	2.13	0.47
1:B:28:MET:HA	1:B:28:MET:CE	2.43	0.46
1:A:231:ARG:NH2	1:A:260:VAL:HG13	2.17	0.46
1:A:115:PRO:C	1:A:117:GLY:H	2.19	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:B:166:LEU:N	1:B:166:LEU:HD22	2.29	0.46
1:A:227:SER:HB3	1:A:256:LYS:HZ3	1.79	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:B:76:ASN:C	1:B:76:ASN:HD22	2.20	0.45
1:A:39:LYS:HB3	1:A:435:THR:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:ASP:O	1:B:332:GLU:C	2.54	0.45
1:A:264:VAL:HG12	1:A:266:LEU:HD12	1.99	0.45
1:A:215:TRP:CD1	1:A:215:TRP:C	2.88	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
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:A:122:LEU:HD12	1:A:122:LEU:C	2.36	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:139:ALA:C	1:A:141:GLU:H	2.21	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: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:340:LYS:NZ	1:A:380:SER:OG	2.48	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:PHE:CD1	1:A:306:PHE:C	2.92	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: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:B:100:GLU:OE2	1:B:132:ILE:HD12	2.20	0.42
1:A:138:ARG:NE	1:A:138:ARG:C	2.73	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:427:LYS:HD3	1:B:427:LYS:C	2.39	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:220:LEU:HD12	1:A:220:LEU:HA	1.89	0.41
1:A:56:HIS:C	1:A:57:ARG:HG3	2.41	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:192:TYR:CD1	1:B:192:TYR:C	2.94	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:148:LYS:HB2	1:A:148:LYS:HZ3	1.85	0.40
1:A:187:ASP:HA	3:A:760:HOH:O	2.20	0.40

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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	0.40
1:B:207:VAL:HG13	1:B:242:TYR:CD2	2.56	0.40
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%)	4	1
1	B	382/462 (83%)	346 (91%)	21 (6%)	15 (4%)	3	1
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

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Mol	Chain	Res	Type
1	B	232	ASP
1	B	255	ARG
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 [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	367/396 (93%)	341 (93%)	26 (7%)	14	11
1	B	337/396 (85%)	320 (95%)	17 (5%)	24	23
All	All	704/792 (89%)	661 (94%)	43 (6%)	18	16

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	21	ILE
1	A	55	GLN
1	A	66	GLU
1	A	129	SER
1	A	137	GLU
1	A	138	ARG
1	A	148	LYS

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Mol	Chain	Res	Type
1	A	157	TRP
1	A	173	LYS
1	A	191	ASP
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	310	ASP
1	A	319	LEU
1	A	322	LEU
1	A	331	ASP
1	A	340	LYS
1	A	345	SER
1	A	350	LEU
1	A	376	LYS
1	B	699	GLU
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	156	GLU
1	B	157	TRP
1	B	187	ASP
1	B	329	VAL
1	B	335	ILE
1	B	392	LEU
1	B	403	LYS
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 (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	79	HIS
1	A	140	ASN

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Mol	Chain	Res	Type
1	A	177	GLN
1	A	259	GLN
1	A	302	ASN
1	A	311	ASN
1	B	25	ASN
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	343	HIS
1	B	424	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 monosaccharides 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	425/462 (91%)	0.42	36 (8%) 10 13	13, 28, 62, 81	4 (0%)
1	B	394/462 (85%)	0.57	46 (11%) 4 6	14, 30, 73, 92	0
All	All	819/924 (88%)	0.50	82 (10%) 7 9	13, 29, 68, 92	4 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	58	ALA	9.6
1	B	258	PRO	8.4
1	A	61	SER	7.8
1	A	59	HIS	6.5
1	B	259	GLN	6.2
1	A	257	GLU	6.1
1	A	136	PRO	6.1
1	B	267	TYR	5.7
1	B	257	GLU	5.5
1	A	133	SER	5.5
1	A	438	ASP	5.3
1	B	255	ARG	4.6
1	B	233	THR	4.5
1	B	250	ALA	4.5
1	A	130	TYR	4.5
1	A	132	ILE	4.5
1	A	374	GLY	4.4
1	A	57	ARG	4.4
1	A	60	LYS	4.2
1	B	190	PHE	4.2
1	B	249	CYS	4.2
1	B	222	ASP	4.1
1	B	342	ILE	4.0
1	B	268	SER	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	299	GLY	3.9
1	B	226	PHE	3.9
1	A	258	PRO	3.9
1	B	247	ASN	3.8
1	A	439	ASP	3.8
1	B	256	LYS	3.8
1	B	251	GLU	3.7
1	B	298	ASP	3.6
1	A	151	ASN	3.5
1	B	296	LEU	3.5
1	A	371	ASP	3.5
1	B	264	VAL	3.5
1	B	228	VAL	3.4
1	A	131	PRO	3.4
1	B	214	LEU	3.4
1	A	256	LYS	3.3
1	B	326	ASP	3.2
1	A	267	TYR	3.2
1	A	135	GLY	3.1
1	B	137	GLU	3.1
1	A	249	CYS	3.0
1	A	259	GLN	2.9
1	B	135	GLY	2.9
1	A	283	GLU	2.9
1	A	129	SER	2.8
1	B	191	ASP	2.8
1	A	138	ARG	2.8
1	B	187	ASP	2.8
1	B	220	LEU	2.8
1	B	231	ARG	2.8
1	B	143	VAL	2.7
1	A	119	ILE	2.7
1	A	142	LEU	2.6
1	A	297	LYS	2.5
1	B	260	VAL	2.5
1	B	458	ARG	2.5
1	B	54	SER	2.5
1	A	137	GLU	2.5
1	A	197	LYS	2.5
1	B	297	LYS	2.5
1	B	379	ILE	2.4
1	B	363	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	455[A]	CYS	2.3
1	B	219	GLY	2.2
1	B	138	ARG	2.2
1	A	260	VAL	2.2
1	B	193	MET	2.2
1	B	253	LYS	2.2
1	B	131	PRO	2.1
1	B	252	TYR	2.1
1	A	369	LYS	2.1
1	A	202	ILE	2.1
1	B	94	ARG	2.1
1	A	114	ALA	2.1
1	B	218	ASP	2.1
1	B	254	ASP	2.1
1	B	301	LYS	2.1
1	A	370	VAL	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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	ZN	A	701[A]	1/1	0.98	0.10	13,13,13,13	1
2	ZN	A	701[B]	1/1	0.98	0.10	42,42,42,42	1
2	ZN	B	701	1/1	1.00	0.08	18,18,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.