



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:02 PM UTC

PDB ID : 2FA2 / pdb\_00002fa2  
Title : Crystal structure of Fus3 without a peptide from Ste5  
Authors : Bhattacharyya, R.P.; Remenyi, A.; Good, M.C.; Bashor, C.J.; Falick, A.M.;  
Lim, W.A.  
Deposited on : 2005-12-06  
Resolution : 2.85 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

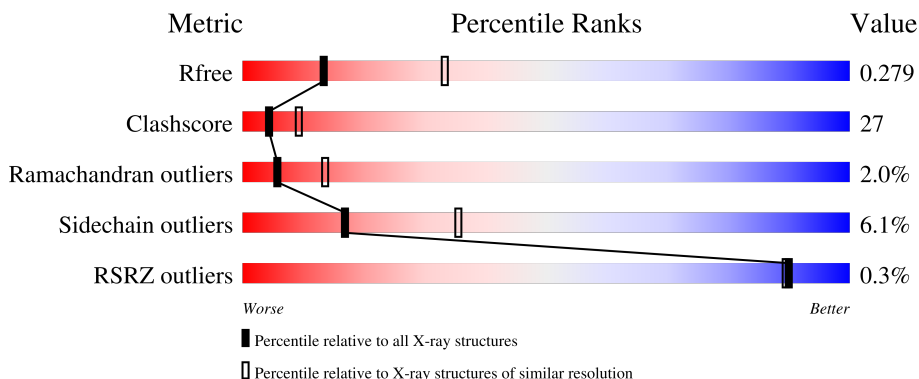
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	353	
1	B	353	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5363 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.

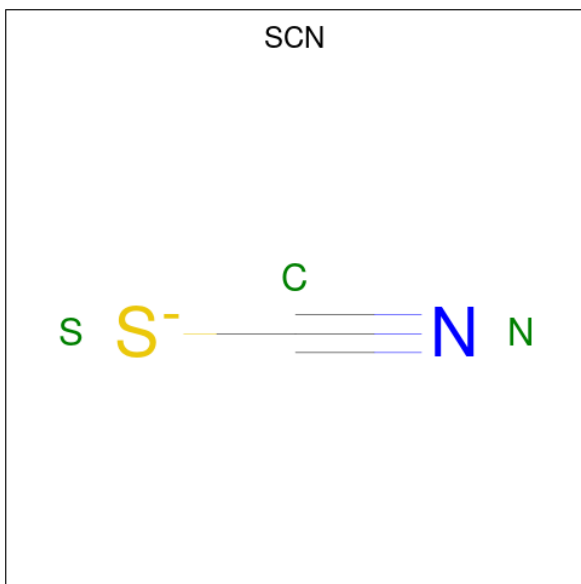
- Molecule 1 is a protein called Mitogen-activated protein kinase FUS3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	333	2671	1731	451	477	12	0	0	0
1	B	332	2647	1717	445	473	12	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	180	VAL	THR	engineered mutation	UNP P16892
A	182	PHE	TYR	engineered mutation	UNP P16892
B	180	VAL	THR	engineered mutation	UNP P16892
B	182	PHE	TYR	engineered mutation	UNP P16892

- Molecule 2 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	0
			3	1	1	1		
2	A	1	Total	C	N	S	0	0
			3	1	1	1		
2	A	1	Total	C	N	S	0	0
			3	1	1	1		
2	B	1	Total	C	N	S	0	0
			3	1	1	1		
2	B	1	Total	C	N	S	0	0
			3	1	1	1		
2	B	1	Total	C	N	S	0	0
			3	1	1	1		

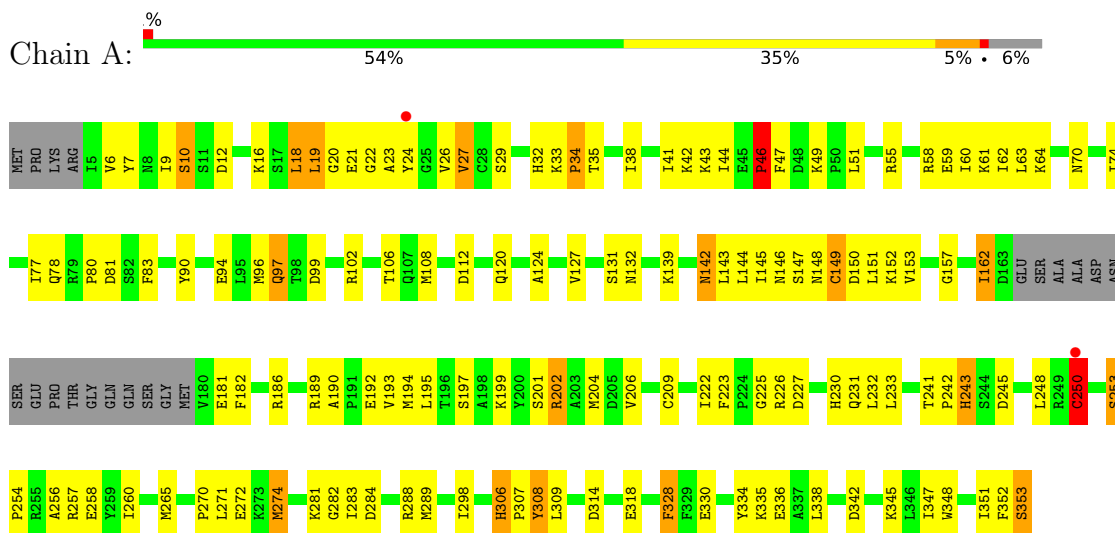
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total	O	0	0
			14	14		
3	B	13	Total	O	0	0
			13	13		

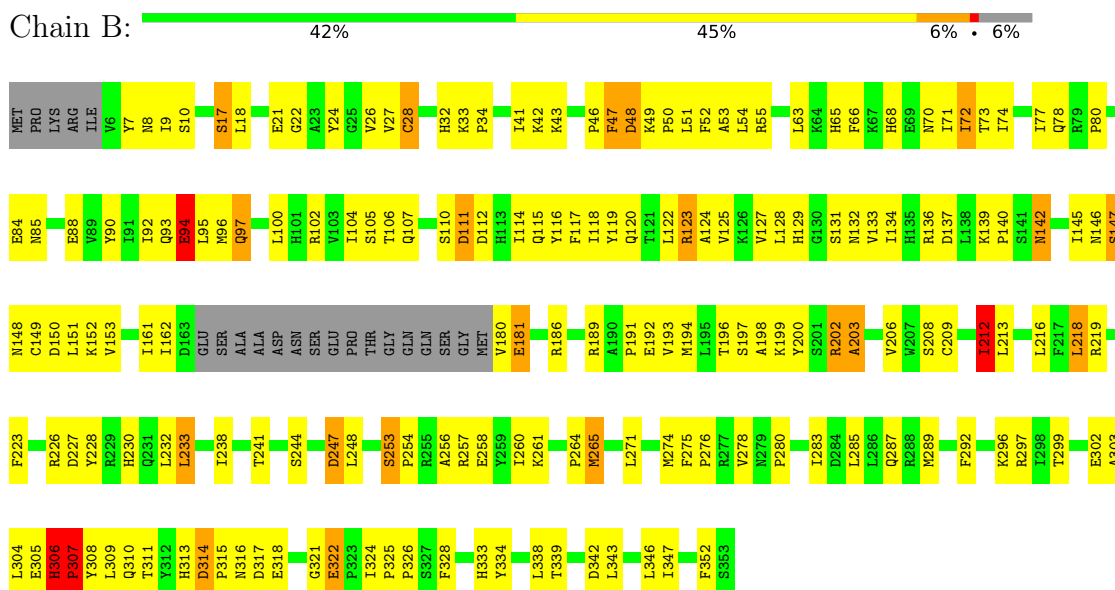
### 3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Mitogen-activated protein kinase FUS3



- Molecule 1: Mitogen-activated protein kinase FUS3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.14Å 94.47Å 113.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.85 20.00 – 2.86	Depositor EDS
% Data completeness (in resolution range)	93.3 (20.00-2.85) 93.5 (20.00-2.86)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.61 (at 2.86Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.209 , 0.285 0.209 , 0.279	Depositor DCC
$R_{free}$ test set	1880 reflections (9.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.4	Xtrriage
Anisotropy	0.695	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5363	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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: SCN

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	0.66	0/2741	1.10	21/3723 (0.6%)
1	B	0.63	0/2716	1.12	21/3692 (0.6%)
All	All	0.65	0/5457	1.11	42/7415 (0.6%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	PHE	N-CA-C	-8.80	102.53	113.18
1	A	47	PHE	N-CA-C	8.06	122.68	113.01
1	A	108	MET	N-CA-C	-7.79	96.98	109.76
1	B	253	SER	N-CA-C	7.60	119.80	109.24
1	B	247	ASP	N-CA-C	-7.17	103.08	111.03
1	B	202	ARG	N-CA-C	-7.11	103.57	111.82
1	B	306	HIS	CA-C-N	6.91	128.47	119.84
1	B	306	HIS	C-N-CA	6.91	128.47	119.84
1	B	47	PHE	N-CA-C	6.62	121.21	113.20
1	A	306	HIS	CA-C-N	6.55	128.02	119.84
1	A	306	HIS	C-N-CA	6.55	128.02	119.84
1	B	212	ILE	N-CA-C	-6.37	104.54	110.53
1	A	318	GLU	CA-C-N	6.22	127.61	119.84
1	A	318	GLU	C-N-CA	6.22	127.61	119.84
1	A	282	GLY	N-CA-C	-6.12	105.40	112.50
1	B	241	THR	CA-C-N	-6.08	113.42	119.99
1	B	241	THR	C-N-CA	-6.08	113.42	119.99
1	B	253	SER	CA-C-N	6.02	125.23	118.97
1	B	253	SER	C-N-CA	6.02	125.23	118.97
1	B	328	PHE	N-CA-C	-6.01	104.79	111.71
1	A	314	ASP	CA-C-N	5.80	125.50	119.82
1	A	314	ASP	C-N-CA	5.80	125.50	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	181	GLU	N-CA-C	5.68	118.13	109.95
1	A	142	ASN	N-CA-C	-5.58	106.64	113.50
1	A	49	LYS	CA-C-N	5.55	126.78	119.84
1	A	49	LYS	C-N-CA	5.55	126.78	119.84
1	B	111	ASP	N-CA-C	-5.50	105.67	112.38
1	A	258	GLU	N-CA-C	-5.47	104.96	111.03
1	B	17	SER	N-CA-C	5.46	117.48	109.24
1	B	142	ASN	N-CA-C	-5.42	106.25	112.92
1	B	94	GLU	N-CA-C	5.42	117.30	108.63
1	A	202	ARG	N-CA-C	-5.41	105.46	111.36
1	A	250	CYS	N-CA-C	-5.34	106.26	114.16
1	A	43	LYS	N-CA-C	-5.31	100.52	109.07
1	B	95	LEU	N-CA-C	5.24	117.69	110.35
1	A	23	ALA	N-CA-C	-5.24	106.39	112.89
1	A	253	SER	CA-C-N	5.22	124.54	118.85
1	A	253	SER	C-N-CA	5.22	124.54	118.85
1	B	203	ALA	N-CA-C	5.21	117.63	111.33
1	B	48	ASP	N-CA-C	-5.20	106.34	113.30
1	B	28	CYS	N-CA-C	5.16	116.92	109.07
1	A	328	PHE	N-CA-C	-5.11	104.98	111.11

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	2671	0	2641	113	0
1	B	2647	0	2606	174	0
2	A	9	0	0	1	0
2	B	9	0	0	1	0
3	A	14	0	0	2	0
3	B	13	0	0	2	0
All	All	5363	0	5247	284	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 27.

All (284) 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:97:GLN:HE21	1:A:147:SER:HB2	1.16	1.10
1:B:104:ILE:HD11	1:B:216:LEU:HD23	1.28	1.10
1:B:24:TYR:HB3	1:B:52:PHE:CZ	1.96	1.00
1:B:114:ILE:HD12	1:B:216:LEU:HB3	1.44	0.99
1:B:226:ARG:H	1:B:230:HIS:CD2	1.85	0.93
1:B:196:THR:HG22	1:B:198:ALA:H	1.34	0.91
1:B:226:ARG:H	1:B:230:HIS:HD2	1.01	0.91
1:B:285:LEU:HG	1:B:289:MET:HE2	1.51	0.90
1:B:196:THR:HG22	1:B:197:SER:H	1.38	0.88
1:B:196:THR:CG2	1:B:197:SER:H	1.87	0.88
1:B:97:GLN:HG2	1:B:146:ASN:HA	1.55	0.88
1:B:104:ILE:HD11	1:B:216:LEU:CD2	2.04	0.87
1:A:19:LEU:HD21	1:A:29:SER:HB3	1.59	0.84
1:A:139:LYS:H	1:A:142:ASN:HD22	1.24	0.83
1:A:120:GLN:NE2	1:A:151:LEU:H	1.76	0.83
1:B:111:ASP:O	1:B:115:GLN:HG3	1.79	0.83
1:B:196:THR:HG22	1:B:197:SER:N	1.94	0.81
1:B:33:LYS:HB2	1:B:34:PRO:HD3	1.64	0.80
1:A:186:ARG:HD3	1:A:194:MET:HE3	1.61	0.80
1:A:352:PHE:O	1:A:353:SER:HB3	1.81	0.79
1:B:104:ILE:CD1	1:B:216:LEU:HD23	2.12	0.79
1:B:274:MET:HE3	1:B:275:PHE:CE2	2.18	0.78
1:B:226:ARG:N	1:B:230:HIS:HD2	1.81	0.78
1:A:97:GLN:NE2	1:A:147:SER:HB2	1.99	0.77
1:B:233:LEU:HD11	1:B:264:PRO:HD2	1.66	0.77
1:A:21:GLU:HG3	1:A:26:VAL:HG12	1.67	0.77
1:B:218:LEU:HD13	1:B:275:PHE:CE1	2.20	0.76
1:B:213:LEU:CD2	1:B:289:MET:HE1	2.16	0.76
1:B:24:TYR:HB3	1:B:52:PHE:CE1	2.21	0.75
1:B:118:ILE:HG12	1:B:213:LEU:HD13	1.67	0.75
1:B:146:ASN:ND2	1:B:150:ASP:HB2	2.01	0.75
1:A:226:ARG:H	1:A:230:HIS:HD2	1.35	0.74
1:A:139:LYS:HG2	1:A:142:ASN:HD21	1.51	0.74
1:B:42:LYS:HE3	1:B:93:GLN:OE1	1.87	0.74
1:B:21:GLU:HG2	1:B:26:VAL:HG12	1.68	0.74
1:B:180:VAL:HG12	1:B:181:GLU:N	2.04	0.72
1:A:270:PRO:O	1:A:274:MET:HG2	1.90	0.72
1:B:196:THR:CG2	1:B:197:SER:N	2.52	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:GLY:HA3	1:A:24:TYR:CZ	2.26	0.71
1:B:134:ILE:HD13	1:B:162:ILE:HD11	1.73	0.71
1:A:44:ILE:O	1:A:46:PRO:HD3	1.90	0.71
1:B:314:ASP:O	1:B:316:ASN:N	2.24	0.71
1:A:33:LYS:HB2	1:A:34:PRO:HD3	1.73	0.70
1:B:147:SER:O	1:B:149:CYS:N	2.20	0.70
1:B:271:LEU:CD1	1:B:287:GLN:HG3	2.22	0.69
1:B:120:GLN:O	1:B:123:ARG:HB3	1.93	0.69
1:B:309:LEU:O	1:B:313:HIS:HB2	1.94	0.68
1:B:17:SER:O	1:B:28:CYS:HB2	1.95	0.67
1:A:102:ARG:O	1:A:106:THR:HG23	1.94	0.67
1:A:124:ALA:O	1:A:127:VAL:HG12	1.92	0.67
1:B:146:ASN:CG	1:B:150:ASP:HB2	2.19	0.67
1:A:18:LEU:HD23	1:A:20:GLY:H	1.59	0.67
1:A:32:HIS:HD2	1:A:35:THR:OG1	1.77	0.67
1:B:146:ASN:HD21	1:B:150:ASP:HB2	1.57	0.67
1:B:72:ILE:HD11	1:B:96:MET:HE2	1.76	0.66
1:B:18:LEU:HA	1:B:28:CYS:HB3	1.78	0.66
1:A:139:LYS:H	1:A:142:ASN:ND2	1.93	0.65
1:B:213:LEU:HD22	1:B:289:MET:HE1	1.78	0.65
1:A:148:ASN:O	1:A:149:CYS:HB2	1.97	0.65
1:B:314:ASP:C	1:B:316:ASN:H	2.05	0.65
1:B:146:ASN:OD1	1:B:150:ASP:HB2	1.97	0.64
1:B:213:LEU:HD23	1:B:289:MET:HE1	1.79	0.64
1:B:314:ASP:OD1	1:B:316:ASN:HB2	1.98	0.64
1:B:102:ARG:HB2	1:B:102:ARG:HH11	1.63	0.64
1:A:226:ARG:N	1:A:230:HIS:HD2	1.96	0.63
1:A:206:VAL:HG11	1:A:298:ILE:O	1.99	0.63
1:B:129:HIS:CE1	1:B:202:ARG:HB3	2.34	0.63
1:B:70:ASN:HD21	1:B:120:GLN:HE21	1.46	0.62
1:B:102:ARG:HB2	1:B:102:ARG:NH1	2.14	0.62
1:B:70:ASN:OD1	1:B:123:ARG:HG2	1.99	0.62
1:B:136:ARG:O	1:B:189:ARG:NH1	2.32	0.62
1:B:254:PRO:O	1:B:258:GLU:HG2	2.00	0.62
1:B:48:ASP:OD2	1:B:49:LYS:HD3	2.00	0.61
1:B:218:LEU:HD13	1:B:275:PHE:HE1	1.64	0.61
1:A:201:SER:O	1:A:204:MET:HG2	2.00	0.61
1:B:71:ILE:HD13	1:B:128:LEU:HD21	1.82	0.61
1:A:9:ILE:O	1:A:10:SER:O	2.18	0.61
1:A:120:GLN:HE22	1:A:151:LEU:H	1.45	0.60
1:A:226:ARG:H	1:A:230:HIS:CD2	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ALA:HB3	1:B:343:LEU:HD13	1.83	0.60
1:A:253:SER:HB3	1:A:256:ALA:HB3	1.85	0.59
1:A:306:HIS:CG	1:A:307:PRO:HD2	2.37	0.59
1:A:139:LYS:N	1:A:142:ASN:HD22	1.99	0.59
1:B:133:VAL:HG22	1:B:161:ILE:CD1	2.33	0.59
1:B:72:ILE:CD1	1:B:152:LYS:HB2	2.33	0.59
1:B:208:SER:O	1:B:212:ILE:HD12	2.03	0.59
1:A:120:GLN:HE22	1:A:150:ASP:HA	1.68	0.58
1:A:18:LEU:HD23	1:A:20:GLY:N	2.18	0.58
1:A:9:ILE:HA	1:A:78:GLN:HE22	1.69	0.58
1:B:306:HIS:CE1	1:B:308:TYR:H	2.22	0.58
1:B:299:THR:OG1	1:B:302:GLU:HG3	2.05	0.57
1:B:72:ILE:HD13	1:B:152:LYS:HB2	1.88	0.56
1:B:244:SER:O	1:B:247:ASP:HB2	2.06	0.56
1:A:194:MET:HE1	1:A:231:GLN:HB3	1.88	0.56
1:A:209:CYS:HB3	1:A:289:MET:HE1	1.88	0.56
1:B:307:PRO:O	1:B:310:GLN:HG2	2.05	0.56
1:A:243:HIS:HB3	1:A:265:MET:SD	2.45	0.56
1:A:139:LYS:N	1:A:142:ASN:ND2	2.52	0.56
1:B:100:LEU:HD21	1:B:216:LEU:HD21	1.88	0.55
1:A:222:ILE:HG23	1:A:223:PHE:CD2	2.41	0.55
1:B:85:ASN:N	1:B:85:ASN:HD22	2.04	0.55
1:A:131:SER:O	1:A:132:ASN:HB2	2.07	0.55
1:B:129:HIS:HB3	1:B:202:ARG:HD3	1.88	0.54
1:A:352:PHE:O	1:A:353:SER:CB	2.53	0.54
1:B:51:LEU:O	1:B:51:LEU:HD23	2.07	0.54
1:B:74:ILE:HD11	1:B:77:ILE:CG1	2.38	0.54
1:A:242:PRO:HG2	1:A:260:ILE:HD13	1.90	0.53
1:B:134:ILE:HD13	1:B:200:TYR:O	2.09	0.53
1:A:19:LEU:HD21	1:A:29:SER:CB	2.35	0.53
1:A:80:PRO:HG2	1:A:348:TRP:CZ3	2.43	0.53
1:A:139:LYS:HG2	1:A:142:ASN:ND2	2.21	0.53
1:B:202:ARG:HG3	1:B:202:ARG:HH11	1.74	0.52
1:A:42:LYS:O	1:A:90:TYR:HA	2.10	0.52
1:A:186:ARG:CD	1:A:194:MET:HE3	2.37	0.52
1:B:333:HIS:C	1:B:334:TYR:HD1	2.18	0.52
1:B:271:LEU:HD22	1:B:274:MET:CE	2.39	0.52
1:B:102:ARG:HA	1:B:105:SER:HB3	1.92	0.52
1:A:70:ASN:HD21	1:A:120:GLN:HG2	1.75	0.52
1:A:194:MET:HG2	2:A:504:SCN:S	2.51	0.51
1:B:305:GLU:O	1:B:306:HIS:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:HIS:C	1:B:306:HIS:ND1	2.67	0.51
1:B:68:HIS:CE1	1:B:70:ASN:HB2	2.45	0.51
1:B:72:ILE:CD1	1:B:96:MET:HE2	2.39	0.51
1:A:59:GLU:OE2	1:A:63:LEU:HD11	2.11	0.51
1:B:49:LYS:C	2:B:502:SCN:N	2.68	0.51
1:A:189:ARG:HD3	3:A:519:HOH:O	2.09	0.51
1:B:196:THR:HG22	1:B:198:ALA:N	2.14	0.51
1:B:129:HIS:ND1	1:B:202:ARG:HB3	2.26	0.50
1:A:143:LEU:HD22	1:A:151:LEU:HD21	1.93	0.50
1:A:347:ILE:O	1:A:351:ILE:HG13	2.11	0.50
1:B:115:GLN:HA	1:B:118:ILE:HG22	1.93	0.50
1:B:146:ASN:HD21	1:B:150:ASP:CB	2.25	0.50
1:A:7:TYR:OH	1:A:26:VAL:HG23	2.12	0.50
1:A:16:LYS:NZ	1:A:38:ILE:HD13	2.27	0.50
1:B:274:MET:HE3	1:B:275:PHE:HE2	1.72	0.50
1:B:275:PHE:HB2	1:B:283:ILE:CD1	2.42	0.50
1:A:19:LEU:HD12	1:A:27:VAL:HG22	1.93	0.49
1:A:242:PRO:HB2	1:A:248:LEU:HD23	1.94	0.49
1:B:84:GLU:C	1:B:85:ASN:HD22	2.20	0.49
1:B:271:LEU:HD23	1:B:271:LEU:N	2.26	0.49
1:B:321:GLY:C	1:B:322:GLU:HG2	2.38	0.49
1:A:145:ILE:HA	1:A:150:ASP:O	2.13	0.49
1:B:133:VAL:HG22	1:B:161:ILE:HD13	1.94	0.49
1:B:41:ILE:HG12	1:B:92:ILE:HG13	1.95	0.49
1:B:147:SER:C	1:B:149:CYS:H	2.16	0.49
1:B:27:VAL:HG22	1:B:42:LYS:HG2	1.95	0.49
1:B:223:PHE:HE1	1:B:238:ILE:HD12	1.78	0.49
1:B:309:LEU:HA	3:B:516:HOH:O	2.13	0.49
1:A:248:LEU:C	1:A:250:CYS:H	2.21	0.48
1:B:118:ILE:CG1	1:B:213:LEU:HD13	2.42	0.48
1:A:225:GLY:HA2	1:A:230:HIS:CD2	2.48	0.48
1:A:342:ASP:OD2	1:B:186:ARG:NH2	2.47	0.48
1:B:63:LEU:HD22	1:B:72:ILE:O	2.13	0.48
1:A:307:PRO:O	1:A:309:LEU:N	2.46	0.48
1:A:21:GLU:HG3	1:A:26:VAL:CG1	2.40	0.48
1:A:335:LYS:O	1:A:336:GLU:C	2.55	0.48
1:B:106:THR:C	1:B:107:GLN:HG2	2.38	0.48
1:B:80:PRO:HD2	1:B:352:PHE:CZ	2.48	0.47
1:A:248:LEU:HD12	1:A:257:ARG:NH2	2.30	0.47
1:B:193:VAL:HG22	1:B:199:LYS:HA	1.96	0.47
1:B:248:LEU:HD22	1:B:260:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:LYS:HE2	1:B:142:ASN:HD21	1.80	0.47
1:B:180:VAL:HG12	1:B:181:GLU:H	1.76	0.47
1:B:218:LEU:O	1:B:219:ARG:HB2	2.13	0.47
1:B:116:TYR:CE2	1:B:149:CYS:O	2.67	0.47
1:B:124:ALA:O	1:B:127:VAL:HG12	2.15	0.47
1:A:189:ARG:HD3	1:A:189:ARG:HA	1.75	0.47
1:A:22:GLY:HA3	1:A:24:TYR:CE2	2.50	0.47
1:A:32:HIS:O	1:A:33:LYS:C	2.57	0.47
1:B:85:ASN:N	1:B:85:ASN:ND2	2.61	0.47
1:B:313:HIS:O	1:B:314:ASP:HB2	2.15	0.47
1:A:190:ALA:HB1	1:A:192:GLU:OE1	2.15	0.46
1:B:194:MET:HE2	1:B:232:LEU:HD21	1.97	0.46
1:B:271:LEU:HD11	1:B:287:GLN:HG3	1.94	0.46
1:B:147:SER:C	1:B:149:CYS:N	2.73	0.46
1:B:137:ASP:O	1:B:142:ASN:ND2	2.48	0.46
1:A:99:ASP:HA	1:A:144:LEU:HA	1.97	0.46
1:B:206:VAL:O	1:B:209:CYS:HB2	2.15	0.46
1:A:186:ARG:HD3	1:A:194:MET:CE	2.42	0.46
1:B:33:LYS:CB	1:B:34:PRO:HD3	2.41	0.46
1:B:253:SER:HA	1:B:254:PRO:HD3	1.76	0.46
1:A:51:LEU:HD12	1:A:51:LEU:HA	1.70	0.46
1:A:330:GLU:HG3	1:A:334:TYR:CE2	2.51	0.46
1:A:193:VAL:O	1:A:199:LYS:NZ	2.46	0.45
1:A:281:LYS:HB3	1:A:308:TYR:HB2	1.98	0.45
1:B:63:LEU:HD13	1:B:72:ILE:HG22	1.97	0.45
1:B:124:ALA:O	1:B:125:VAL:C	2.59	0.45
1:B:265:MET:O	1:B:265:MET:HG3	2.13	0.45
1:A:44:ILE:C	1:A:46:PRO:HD3	2.41	0.45
1:A:284:ASP:OD2	1:A:288:ARG:NE	2.33	0.45
1:A:272:GLU:HA	1:A:283:ILE:HD13	1.97	0.45
1:A:193:VAL:HG13	1:A:199:LYS:HG2	1.98	0.45
1:A:241:THR:HB	1:A:265:MET:HG3	1.98	0.45
1:A:195:LEU:HD21	1:A:232:LEU:HD13	1.97	0.45
1:B:43:LYS:HG3	1:B:90:TYR:CE1	2.52	0.45
1:B:80:PRO:HD2	1:B:352:PHE:CE2	2.52	0.45
1:B:265:MET:O	1:B:265:MET:CG	2.65	0.45
1:A:6:VAL:HG12	1:A:7:TYR:N	2.31	0.45
1:B:119:TYR:CE1	1:B:304:LEU:HD22	2.52	0.45
1:B:275:PHE:O	1:B:278:VAL:HB	2.17	0.45
1:B:276:PRO:C	1:B:278:VAL:H	2.25	0.45
1:B:271:LEU:HA	1:B:274:MET:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LEU:HD23	1:A:18:LEU:C	2.42	0.45
1:A:243:HIS:CD2	1:A:265:MET:SD	3.10	0.45
1:B:73:THR:O	1:B:94:GLU:HG2	2.17	0.45
1:A:61:LYS:HB3	1:A:328:PHE:CZ	2.51	0.44
1:B:339:THR:N	1:B:342:ASP:OD2	2.46	0.44
1:B:9:ILE:HA	1:B:78:GLN:NE2	2.32	0.44
1:A:97:GLN:HG2	1:A:146:ASN:HA	1.99	0.44
1:B:116:TYR:HE2	1:B:149:CYS:O	2.01	0.44
1:B:51:LEU:CD2	1:B:55:ARG:NE	2.80	0.44
1:B:203:ALA:HB1	1:B:297:ARG:NH1	2.32	0.44
1:B:32:HIS:O	1:B:33:LYS:C	2.61	0.44
1:A:306:HIS:ND1	1:A:307:PRO:HD2	2.33	0.44
1:A:245:ASP:HA	1:A:257:ARG:HH22	1.82	0.44
1:B:110:SER:C	1:B:112:ASP:N	2.73	0.44
1:B:120:GLN:NE2	1:B:151:LEU:H	2.16	0.44
1:B:66:PHE:CZ	1:B:128:LEU:HD23	2.53	0.44
1:B:324:ILE:CG2	1:B:325:PRO:HD2	2.48	0.44
1:A:9:ILE:O	1:A:10:SER:C	2.60	0.44
1:A:288:ARG:O	1:A:298:ILE:HG22	2.18	0.44
1:B:123:ARG:HG2	1:B:123:ARG:HH11	1.83	0.44
1:A:227:ASP:OD1	1:A:227:ASP:C	2.60	0.43
1:B:191:PRO:HB2	1:B:292:PHE:HE1	1.83	0.43
1:B:74:ILE:HD11	1:B:77:ILE:HG12	2.00	0.43
1:A:162:ILE:HD12	1:A:202:ARG:NH1	2.33	0.43
1:B:324:ILE:HG23	1:B:325:PRO:HD2	2.00	0.43
1:A:55:ARG:HG2	1:A:157:GLY:HA3	2.01	0.43
1:B:202:ARG:HG3	1:B:202:ARG:NH1	2.33	0.43
1:B:111:ASP:O	1:B:115:GLN:CG	2.58	0.43
1:A:32:HIS:CD2	1:A:35:THR:OG1	2.63	0.43
1:A:336:GLU:HG2	1:B:228:TYR:CE1	2.54	0.43
1:A:58:ARG:HH11	1:A:58:ARG:HG2	1.84	0.43
1:A:62:ILE:O	1:A:63:LEU:C	2.61	0.43
1:A:64:LYS:HB3	1:A:64:LYS:HE2	1.79	0.43
1:A:7:TYR:HE2	1:A:41:ILE:HG22	1.83	0.43
1:B:117:PHE:CE1	1:B:145:ILE:HD13	2.54	0.43
1:B:227:ASP:O	1:B:228:TYR:C	2.62	0.43
1:B:192:GLU:OE1	1:B:192:GLU:N	2.46	0.42
1:B:325:PRO:HA	1:B:326:PRO:HD3	1.96	0.42
1:B:134:ILE:CG2	1:B:162:ILE:HD11	2.49	0.42
1:B:271:LEU:HD12	1:B:287:GLN:HG3	1.97	0.42
1:B:78:GLN:HB2	1:B:90:TYR:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:SER:HB3	1:B:256:ALA:HB3	2.01	0.42
1:B:43:LYS:HE2	1:B:88:GLU:HG2	2.01	0.42
1:B:70:ASN:HD21	1:B:120:GLN:NE2	2.15	0.42
1:B:65:HIS:ND1	1:B:65:HIS:C	2.76	0.42
1:A:94:GLU:OE1	1:A:152:LYS:NZ	2.48	0.42
1:A:209:CYS:CB	1:A:289:MET:HE1	2.49	0.42
1:A:44:ILE:HG22	1:A:46:PRO:HD3	2.01	0.42
1:A:143:LEU:CD2	1:A:153:VAL:HG22	2.50	0.42
1:B:71:ILE:CD1	1:B:128:LEU:HD21	2.49	0.42
1:B:120:GLN:CD	1:B:151:LEU:H	2.27	0.42
1:B:131:SER:O	1:B:132:ASN:HB2	2.19	0.42
1:B:304:LEU:HD13	1:B:318:GLU:CD	2.45	0.42
1:A:99:ASP:OD1	1:A:99:ASP:C	2.62	0.41
1:B:47:PHE:HE1	1:B:347:ILE:HD12	1.85	0.41
1:B:151:LEU:C	1:B:151:LEU:HD23	2.45	0.41
1:A:181:GLU:HG3	1:A:182:PHE:N	2.35	0.41
1:A:253:SER:HA	1:A:254:PRO:HD3	1.79	0.41
1:B:311:THR:HB	3:B:516:HOH:O	2.19	0.41
1:A:139:LYS:CG	1:A:142:ASN:ND2	2.83	0.41
1:B:317:ASP:O	1:B:318:GLU:HG3	2.21	0.41
1:B:196:THR:HG23	1:B:197:SER:H	1.79	0.41
1:A:189:ARG:NE	3:A:519:HOH:O	2.54	0.41
1:A:60:ILE:HD13	1:A:77:ILE:HD13	2.03	0.41
1:A:96:MET:HE2	1:A:152:LYS:HB2	2.03	0.41
1:A:271:LEU:HD23	1:A:271:LEU:HA	1.76	0.41
1:B:213:LEU:HD23	1:B:289:MET:CE	2.47	0.41
1:B:307:PRO:C	1:B:309:LEU:N	2.77	0.41
1:B:296:LYS:O	1:B:297:ARG:C	2.64	0.41
1:A:182:PHE:CG	1:B:50:PRO:HB3	2.56	0.40
1:A:248:LEU:HB2	1:A:257:ARG:CZ	2.51	0.40
1:B:127:VAL:HG13	1:B:128:LEU:N	2.36	0.40
1:B:194:MET:HE1	1:B:232:LEU:HG	2.03	0.40
1:B:203:ALA:HB1	1:B:297:ARG:HH11	1.86	0.40
1:B:122:LEU:HD13	1:B:303:ALA:HB1	2.02	0.40
1:B:47:PHE:CE1	1:B:347:ILE:HD12	2.57	0.40
1:B:72:ILE:HD12	1:B:72:ILE:HA	1.79	0.40
1:B:248:LEU:HD11	1:B:261:LYS:HE3	2.04	0.40
1:B:7:TYR:OH	1:B:41:ILE:O	2.34	0.40
1:A:63:LEU:HD12	1:A:74:ILE:HG13	2.04	0.40
1:A:197:SER:O	1:A:199:LYS:N	2.54	0.40
1:B:21:GLU:HB3	1:B:22:GLY:H	1.67	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	329/353 (93%)	287 (87%)	36 (11%)	6 (2%)	6	15
1	B	328/353 (93%)	284 (87%)	37 (11%)	7 (2%)	5	13
All	All	657/706 (93%)	571 (87%)	73 (11%)	13 (2%)	6	13

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	308	TYR
1	A	34	PRO
1	B	148	ASN
1	A	149	CYS
1	B	8	ASN
1	B	147	SER
1	B	315	PRO
1	A	12	ASP
1	B	306	HIS
1	A	46	PRO
1	B	314	ASP
1	B	307	PRO

### 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	290/319 (91%)	275 (95%)	15 (5%)	21	43
1	B	285/319 (89%)	265 (93%)	20 (7%)	14	29
All	All	575/638 (90%)	540 (94%)	35 (6%)	17	35

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	19	LEU
1	A	27	VAL
1	A	46	PRO
1	A	81	ASP
1	A	97	GLN
1	A	112	ASP
1	A	162	ILE
1	A	233	LEU
1	A	243	HIS
1	A	250	CYS
1	A	274	MET
1	A	338	LEU
1	A	345	LYS
1	A	353	SER
1	B	10	SER
1	B	46	PRO
1	B	54	LEU
1	B	72	ILE
1	B	94	GLU
1	B	97	GLN
1	B	123	ARG
1	B	140	PRO
1	B	153	VAL
1	B	212	ILE
1	B	218	LEU
1	B	233	LEU
1	B	257	ARG
1	B	265	MET
1	B	280	PRO
1	B	306	HIS
1	B	307	PRO
1	B	322	GLU
1	B	338	LEU
1	B	346	LEU

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	32	HIS
1	A	78	GLN
1	A	85	ASN
1	A	93	GLN
1	A	97	GLN
1	A	113	HIS
1	A	120	GLN
1	A	142	ASN
1	A	230	HIS
1	B	32	HIS
1	B	85	ASN
1	B	115	GLN
1	B	120	GLN
1	B	142	ASN
1	B	230	HIS
1	B	310	GLN
1	B	333	HIS

### 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](#)

6 ligands are modelled in this entry.

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
2	SCN	B	506	-	1,2,2	3.05	1 (100%)	0,1,1	-	-
2	SCN	A	505	-	1,2,2	2.76	1 (100%)	0,1,1	-	-
2	SCN	B	503	-	1,2,2	3.03	1 (100%)	0,1,1	-	-
2	SCN	A	504	-	1,2,2	3.21	1 (100%)	0,1,1	-	-
2	SCN	B	502	-	1,2,2	2.38	1 (100%)	0,1,1	-	-
2	SCN	A	501	-	1,2,2	2.67	1 (100%)	0,1,1	-	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	504	SCN	C-N	3.21	1.26	1.15
2	B	506	SCN	C-N	3.05	1.26	1.15
2	B	503	SCN	C-N	3.03	1.25	1.15
2	A	505	SCN	C-N	2.76	1.25	1.15
2	A	501	SCN	C-N	2.67	1.24	1.15
2	B	502	SCN	C-N	2.38	1.23	1.15

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	504	SCN	1	0
2	B	502	SCN	1	0

## 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 [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, 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	333/353 (94%)	-0.37	2 (0%) 85 82	20, 38, 79, 94	0
1	B	332/353 (94%)	-0.16	0 100 100	26, 49, 75, 88	0
All	All	665/706 (94%)	-0.27	2 (0%) 90 89	20, 43, 77, 94	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250	CYS	2.2
1	A	24	TYR	2.1

### 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, 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	SCN	A	505	3/3	0.76	0.17	75,75,75,77	0
2	SCN	B	502	3/3	0.87	0.14	56,56,56,60	0
2	SCN	A	501	3/3	0.91	0.13	77,77,78,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SCN	B	506	3/3	0.92	0.10	68,68,70,72	0
2	SCN	A	504	3/3	0.97	0.12	42,42,44,44	0
2	SCN	B	503	3/3	0.98	0.06	57,57,58,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.