



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 12:33 AM UTC

PDB ID : 9NWG / pdb\_00009nwg  
Title : Crystal Structure of the Third Immunoglobulin-Like Domain of Human Muscle-Specific Kinase  
Authors : Canciani, A.; Palamini, M.; Forneris, F.  
Deposited on : 2025-03-22  
Resolution : 1.70 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)

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<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

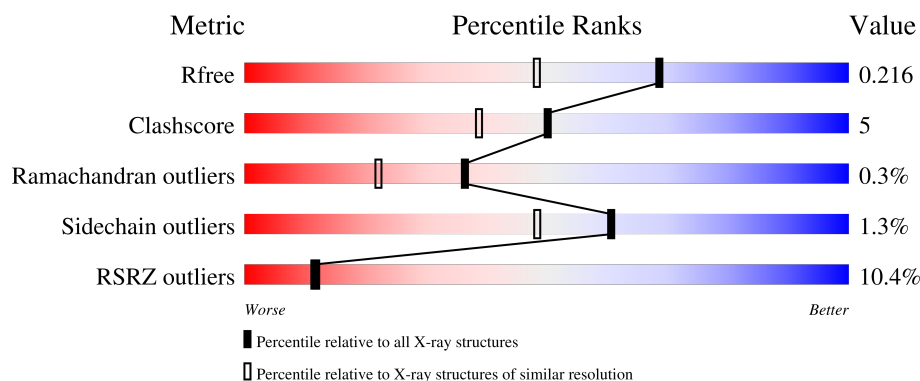
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	104	
1	B	104	
1	C	104	
1	D	104	
1	E	104	

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Mol	Chain	Length	Quality of chain
1	F	104	
1	G	104	
1	H	104	
1	I	104	
1	J	104	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BR	D	401	-	-	X	-
4	PEG	D	407	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8339 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 Muscle, skeletal receptor tyrosine-protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	99	Total	C	N	O	S	0	14	0
			794	513	132	146	3			
1	B	96	Total	C	N	O	S	0	8	0
			747	474	129	141	3			
1	C	97	Total	C	N	O	S	0	10	0
			767	488	132	144	3			
1	D	97	Total	C	N	O	S	0	14	0
			786	500	136	147	3			
1	E	97	Total	C	N	O	S	0	10	0
			760	485	128	144	3			
1	F	95	Total	C	N	O	S	0	6	0
			737	468	128	139	2			
1	G	96	Total	C	N	O	S	0	6	0
			751	474	135	139	3			
1	H	97	Total	C	N	O	S	0	4	0
			735	465	127	140	3			
1	I	98	Total	C	N	O	S	0	6	0
			753	476	129	145	3			
1	J	98	Total	C	N	O	S	0	8	0
			756	480	128	145	3			

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	204	THR	-	expression tag	UNP O15146
A	205	GLY	-	expression tag	UNP O15146
A	206	GLU	-	expression tag	UNP O15146
A	207	PHE	-	expression tag	UNP O15146
A	208	THR	-	expression tag	UNP O15146
A	209	SER	-	expression tag	UNP O15146
A	210	GLY	-	expression tag	UNP O15146
A	211	SER	-	expression tag	UNP O15146
A	305	ALA	-	expression tag	UNP O15146

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Chain	Residue	Modelled	Actual	Comment	Reference
A	306	ALA	-	expression tag	UNP O15146
A	307	ALA	-	expression tag	UNP O15146
B	204	THR	-	expression tag	UNP O15146
B	205	GLY	-	expression tag	UNP O15146
B	206	GLU	-	expression tag	UNP O15146
B	207	PHE	-	expression tag	UNP O15146
B	208	THR	-	expression tag	UNP O15146
B	209	SER	-	expression tag	UNP O15146
B	210	GLY	-	expression tag	UNP O15146
B	211	SER	-	expression tag	UNP O15146
B	305	ALA	-	expression tag	UNP O15146
B	306	ALA	-	expression tag	UNP O15146
B	307	ALA	-	expression tag	UNP O15146
C	204	THR	-	expression tag	UNP O15146
C	205	GLY	-	expression tag	UNP O15146
C	206	GLU	-	expression tag	UNP O15146
C	207	PHE	-	expression tag	UNP O15146
C	208	THR	-	expression tag	UNP O15146
C	209	SER	-	expression tag	UNP O15146
C	210	GLY	-	expression tag	UNP O15146
C	211	SER	-	expression tag	UNP O15146
C	305	ALA	-	expression tag	UNP O15146
C	306	ALA	-	expression tag	UNP O15146
C	307	ALA	-	expression tag	UNP O15146
D	204	THR	-	expression tag	UNP O15146
D	205	GLY	-	expression tag	UNP O15146
D	206	GLU	-	expression tag	UNP O15146
D	207	PHE	-	expression tag	UNP O15146
D	208	THR	-	expression tag	UNP O15146
D	209	SER	-	expression tag	UNP O15146
D	210	GLY	-	expression tag	UNP O15146
D	211	SER	-	expression tag	UNP O15146
D	305	ALA	-	expression tag	UNP O15146
D	306	ALA	-	expression tag	UNP O15146
D	307	ALA	-	expression tag	UNP O15146
E	204	THR	-	expression tag	UNP O15146
E	205	GLY	-	expression tag	UNP O15146
E	206	GLU	-	expression tag	UNP O15146
E	207	PHE	-	expression tag	UNP O15146
E	208	THR	-	expression tag	UNP O15146
E	209	SER	-	expression tag	UNP O15146
E	210	GLY	-	expression tag	UNP O15146

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Chain	Residue	Modelled	Actual	Comment	Reference
E	211	SER	-	expression tag	UNP O15146
E	305	ALA	-	expression tag	UNP O15146
E	306	ALA	-	expression tag	UNP O15146
E	307	ALA	-	expression tag	UNP O15146
F	204	THR	-	expression tag	UNP O15146
F	205	GLY	-	expression tag	UNP O15146
F	206	GLU	-	expression tag	UNP O15146
F	207	PHE	-	expression tag	UNP O15146
F	208	THR	-	expression tag	UNP O15146
F	209	SER	-	expression tag	UNP O15146
F	210	GLY	-	expression tag	UNP O15146
F	211	SER	-	expression tag	UNP O15146
F	305	ALA	-	expression tag	UNP O15146
F	306	ALA	-	expression tag	UNP O15146
F	307	ALA	-	expression tag	UNP O15146
G	204	THR	-	expression tag	UNP O15146
G	205	GLY	-	expression tag	UNP O15146
G	206	GLU	-	expression tag	UNP O15146
G	207	PHE	-	expression tag	UNP O15146
G	208	THR	-	expression tag	UNP O15146
G	209	SER	-	expression tag	UNP O15146
G	210	GLY	-	expression tag	UNP O15146
G	211	SER	-	expression tag	UNP O15146
G	305	ALA	-	expression tag	UNP O15146
G	306	ALA	-	expression tag	UNP O15146
G	307	ALA	-	expression tag	UNP O15146
H	204	THR	-	expression tag	UNP O15146
H	205	GLY	-	expression tag	UNP O15146
H	206	GLU	-	expression tag	UNP O15146
H	207	PHE	-	expression tag	UNP O15146
H	208	THR	-	expression tag	UNP O15146
H	209	SER	-	expression tag	UNP O15146
H	210	GLY	-	expression tag	UNP O15146
H	211	SER	-	expression tag	UNP O15146
H	305	ALA	-	expression tag	UNP O15146
H	306	ALA	-	expression tag	UNP O15146
H	307	ALA	-	expression tag	UNP O15146
I	204	THR	-	expression tag	UNP O15146
I	205	GLY	-	expression tag	UNP O15146
I	206	GLU	-	expression tag	UNP O15146
I	207	PHE	-	expression tag	UNP O15146
I	208	THR	-	expression tag	UNP O15146

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Chain	Residue	Modelled	Actual	Comment	Reference
I	209	SER	-	expression tag	UNP O15146
I	210	GLY	-	expression tag	UNP O15146
I	211	SER	-	expression tag	UNP O15146
I	305	ALA	-	expression tag	UNP O15146
I	306	ALA	-	expression tag	UNP O15146
I	307	ALA	-	expression tag	UNP O15146
J	204	THR	-	expression tag	UNP O15146
J	205	GLY	-	expression tag	UNP O15146
J	206	GLU	-	expression tag	UNP O15146
J	207	PHE	-	expression tag	UNP O15146
J	208	THR	-	expression tag	UNP O15146
J	209	SER	-	expression tag	UNP O15146
J	210	GLY	-	expression tag	UNP O15146
J	211	SER	-	expression tag	UNP O15146
J	305	ALA	-	expression tag	UNP O15146
J	306	ALA	-	expression tag	UNP O15146
J	307	ALA	-	expression tag	UNP O15146

- Molecule 2 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Br 1 1	0	0
2	D	2	Total Br 2 2	0	0
2	H	1	Total Br 1 1	0	0

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

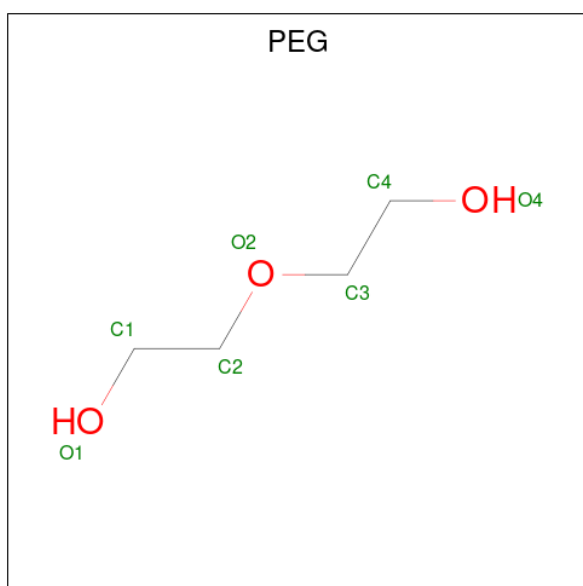
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total K 5 5	0	0
3	B	2	Total K 2 2	0	0
3	C	3	Total K 3 3	0	0
3	D	2	Total K 2 2	0	0
3	E	3	Total K 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total K 1 1	0	0
3	G	3	Total K 3 3	0	0
3	H	2	Total K 2 2	0	0
3	I	3	Total K 3 3	0	0
3	J	2	Total K 2 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 7 4 3	0	0
4	D	1	Total C O 7 4 3	0	0
4	D	1	Total C O 7 4 3	0	0
4	D	1	Total C O 7 4 3	0	0
4	I	1	Total C O 7 4 3	0	0
4	I	1	Total C O 7 4 3	0	0

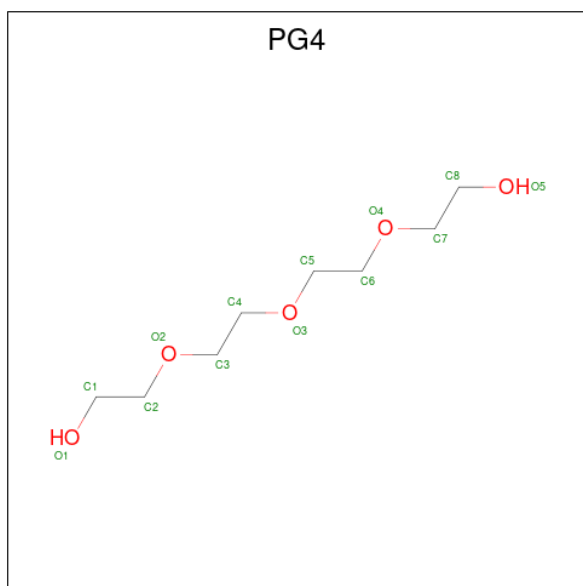
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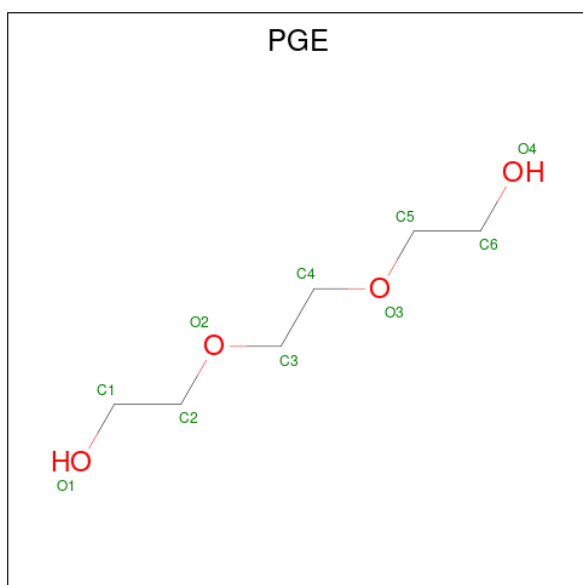
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	J	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total C O 10 6 4	0	0
6	I	1	Total C O 10 6 4	0	0
6	J	1	Total C O 10 6 4	0	0
6	J	1	Total C O 10 6 4	0	0

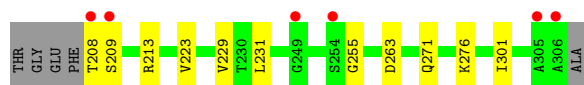
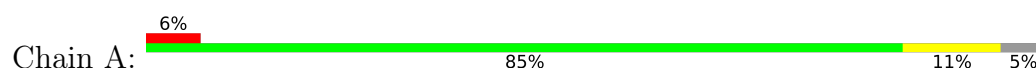
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	70	Total O 70 70	0	0
7	B	56	Total O 56 56	0	0
7	C	51	Total O 51 51	0	0
7	D	83	Total O 83 83	0	0
7	E	60	Total O 60 60	0	0
7	F	36	Total O 36 36	0	0
7	G	49	Total O 49 49	0	0
7	H	64	Total O 64 64	0	0
7	I	58	Total O 58 58	0	0
7	J	94	Total O 94 94	0	0

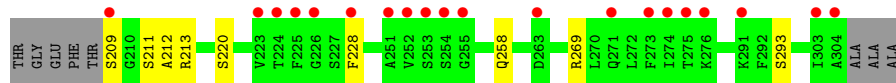
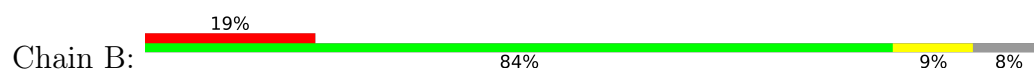
### 3 Residue-property plots

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.

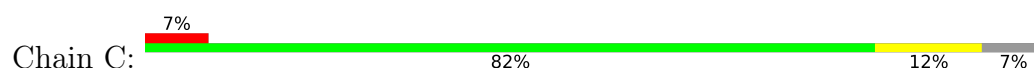
- Molecule 1: Muscle, skeletal receptor tyrosine-protein kinase



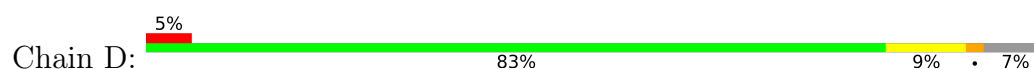
- Molecule 1: Muscle, skeletal receptor tyrosine-protein kinase



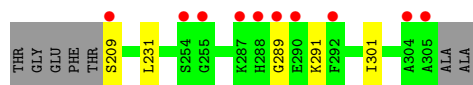
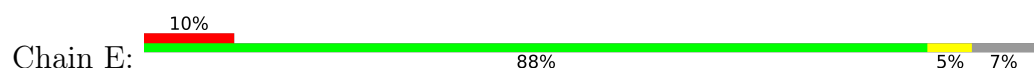
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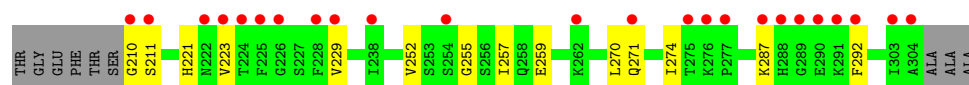
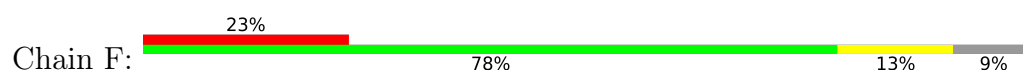
- Molecule 1: Muscle, skeletal receptor tyrosine-protein kinase



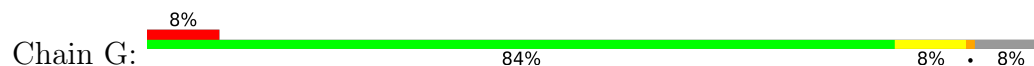
- Molecule 1: Muscle, skeletal receptor tyrosine-protein kinase



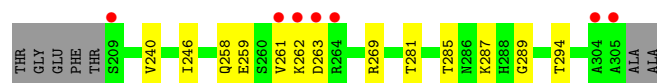
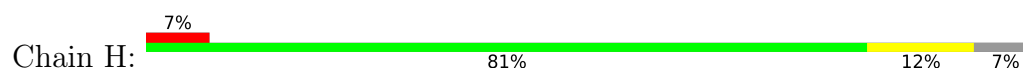
- Molecule 1: Muscle, skeletal receptor tyrosine-protein kinase



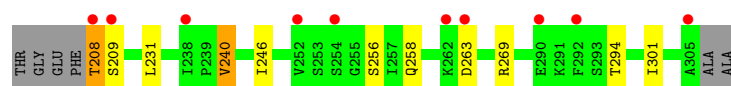
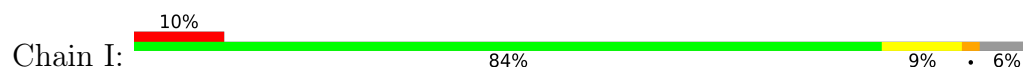
- Molecule 1: Muscle, skeletal receptor tyrosine-protein kinase



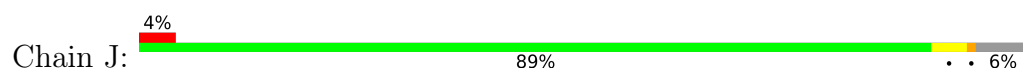
- Molecule 1: Muscle, skeletal receptor tyrosine-protein kinase



- Molecule 1: Muscle, skeletal receptor tyrosine-protein kinase



- Molecule 1: Muscle, skeletal receptor tyrosine-protein kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.15Å 49.43Å 143.42Å 90.00° 92.10° 90.00°	Depositor
Resolution (Å)	46.73 – 1.70 46.73 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.73-1.70) 99.9 (46.73-1.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 1.70Å)	Xtriage
Refinement program	PHENIX (1.20_4459: ???)	Depositor
R, $R_{free}$	0.199 , 0.216 0.198 , 0.216	Depositor DCC
$R_{free}$ test set	6232 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.7	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8339	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.20% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, PEG, PG4, PGE, BR

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	0/849	0.58	0/1153
1	B	0.34	0/784	0.59	0/1064
1	C	0.29	0/810	0.55	0/1100
1	D	0.35	0/841	0.58	0/1141
1	E	0.36	0/803	0.61	0/1092
1	F	0.28	0/769	0.57	0/1047
1	G	0.29	0/782	0.55	0/1060
1	H	0.32	0/760	0.56	0/1034
1	I	0.33	0/784	0.57	1/1066 (0.1%)
1	J	0.38	0/793	0.64	0/1079
All	All	0.33	0/7975	0.58	1/10836 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	209	SER	N-CA-C	-5.44	106.14	112.89

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	213	ARG	Sidechain

## 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	794	0	866	7	0
1	B	747	0	781	7	0
1	C	767	0	811	13	0
1	D	786	0	839	8	0
1	E	760	0	804	3	0
1	F	737	0	762	12	0
1	G	751	0	779	7	0
1	H	735	0	755	8	0
1	I	753	0	773	6	0
1	J	756	0	789	5	0
2	A	1	0	0	0	0
2	D	2	0	0	8	0
2	H	1	0	0	0	0
3	A	5	0	0	0	0
3	B	2	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0
3	E	3	0	0	0	0
3	F	1	0	0	0	0
3	G	3	0	0	0	0
3	H	2	0	0	0	0
3	I	3	0	0	0	0
3	J	2	0	0	0	0
4	C	7	0	10	0	0
4	D	21	0	30	8	0
4	I	14	0	20	0	0
4	J	7	0	10	1	0
5	D	13	0	18	1	0
6	H	10	0	14	3	0
6	I	10	0	14	1	0
6	J	20	0	28	4	0
7	A	70	0	0	2	1
7	B	56	0	0	2	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	51	0	0	3	0
7	D	83	0	0	3	2
7	E	60	0	0	1	0
7	F	36	0	0	4	0
7	G	49	0	0	2	0
7	H	64	0	0	3	0
7	I	58	0	0	0	0
7	J	94	0	0	2	2
All	All	8339	0	8103	84	3

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 5.

All (84) 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)
2:D:401:BR:BR	4:D:407:PEG:H11	1.89	1.27
2:D:401:BR:BR	4:D:407:PEG:H32	1.92	1.25
1:B:258:GLN:OE1	1:B:269:ARG:NH2	2.15	0.80
1:B:209:SER:N	7:B:502:HOH:O	2.17	0.76
1:F:221:HIS:O	7:F:501:HOH:O	2.07	0.71
1:C:259:GLU:OE2	7:C:501:HOH:O	2.09	0.69
1:G:230:THR:HG21	1:G:269[B]:ARG:HE	1.57	0.69
1:E:209:SER:OG	7:E:501:HOH:O	2.10	0.68
1:C:288:HIS:ND1	7:C:502:HOH:O	2.26	0.67
6:H:404:PGE:O4	7:H:501:HOH:O	2.13	0.67
1:D:296:LYS:NZ	7:D:505:HOH:O	2.26	0.67
1:G:253:SER:O	7:G:501:HOH:O	2.13	0.67
2:D:402:BR:BR	7:D:560:HOH:O	2.67	0.66
1:I:258:GLN:OE1	1:I:269:ARG:NH2	2.29	0.65
1:H:259:GLU:HG3	7:H:506:HOH:O	1.96	0.65
2:D:401:BR:BR	4:D:408:PEG:H32	2.54	0.63
1:D:246:ILE:HD13	1:D:283:ILE:HD12	1.81	0.62
1:D:290[A]:GLU:H	1:D:290[A]:GLU:CD	2.08	0.62
1:B:213:ARG:NH1	7:B:503:HOH:O	2.32	0.62
2:D:401:BR:BR	4:D:407:PEG:C3	2.86	0.61
1:I:240:VAL:HG22	1:I:263:ASP:O	2.01	0.60
1:H:294[B]:THR:HG23	7:H:507:HOH:O	2.01	0.60
1:A:208:THR:OG1	1:A:209:SER:N	2.35	0.59
1:J:240:VAL:HG23	7:J:559:HOH:O	2.03	0.58
1:C:238:ILE:O	1:C:288:HIS:NE2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:GLN:HB3	7:A:525:HOH:O	2.03	0.57
1:I:231:LEU:HD21	1:I:301[B]:ILE:HD11	1.86	0.56
1:D:256:SER:HB2	4:D:407:PEG:H41	1.87	0.56
1:J:296:LYS:NZ	7:J:503:HOH:O	2.37	0.55
1:D:247:GLU:HB2	1:D:252:VAL:HG22	1.87	0.55
1:C:274:ILE:HG22	1:C:303[B]:ILE:HD11	1.89	0.55
1:I:208:THR:HA	6:J:404:PGE:H62	1.89	0.54
1:D:258:GLN:OE1	1:D:269:ARG:NH2	2.38	0.54
1:H:246[A]:ILE:CG1	1:H:281:THR:HB	2.38	0.53
1:C:252[B]:VAL:HG21	1:C:270:LEU:HD11	1.91	0.53
1:F:274:ILE:HA	7:F:502:HOH:O	2.08	0.53
1:F:255:GLY:HA3	1:F:271:GLN:O	2.10	0.52
1:F:211:SER:O	7:F:503:HOH:O	2.18	0.52
1:H:285:THR:HG21	6:H:404:PGE:H3	1.91	0.51
1:F:252:VAL:HG11	1:F:270:LEU:HD11	1.93	0.50
1:F:287:LYS:HE2	1:F:292:PHE:HE1	1.76	0.49
1:I:256:SER:HB2	6:I:404:PGE:H32	1.95	0.49
1:F:287:LYS:HG2	1:F:292:PHE:CD1	2.48	0.49
1:D:283:ILE:HG21	5:D:406:PG4:H62	1.94	0.49
1:A:223:VAL:HG11	1:A:229:VAL:HG21	1.96	0.48
1:A:276:LYS:NZ	7:A:501:HOH:O	2.32	0.48
1:F:287:LYS:HG2	1:F:292:PHE:HD1	1.79	0.47
1:H:262:LYS:HE3	1:H:262:LYS:HB2	1.67	0.47
1:F:287:LYS:HE2	1:F:292:PHE:CE1	2.50	0.47
1:C:252[A]:VAL:HG11	1:C:270:LEU:HD11	1.95	0.47
2:D:401:BR:BR	4:D:408:PEG:O1	2.85	0.46
1:B:220[A]:SER:CB	1:C:258[A]:GLN:HE21	2.27	0.46
1:E:289:GLY:C	1:E:291:LYS:H	2.24	0.46
1:G:264[A]:ARG:NH1	7:G:504:HOH:O	2.49	0.46
1:I:294:THR:HB	1:J:259:GLU:CG	2.45	0.46
6:J:404:PGE:H42	6:J:404:PGE:H22	1.69	0.46
1:E:231:LEU:HD21	1:E:301[B]:ILE:HD11	1.99	0.45
6:H:404:PGE:H5	6:H:404:PGE:H32	1.77	0.45
1:A:255:GLY:HA3	1:A:271:GLN:O	2.17	0.45
1:C:259:GLU:CD	7:C:501:HOH:O	2.60	0.44
1:G:291:LYS:HB2	1:G:291:LYS:HE3	1.84	0.44
1:B:211:SER:HB2	1:B:293[A]:SER:OG	2.17	0.44
1:G:228:PHE:CZ	1:G:271:GLN:HB3	2.52	0.43
1:G:234:THR:HG23	1:G:267[B]:ASP:OD1	2.18	0.43
1:J:208:THR:O	1:J:208:THR:OG1	2.33	0.43
1:A:231:LEU:HD21	1:A:301[B]:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258[A]:GLN:NE2	1:C:271:GLN:NE2	2.66	0.43
1:F:210:GLY:N	7:F:505:HOH:O	2.51	0.43
1:J:294[A]:THR:HG21	6:J:403:PGE:H4	2.02	0.42
1:G:230:THR:CG2	1:G:269[B]:ARG:HE	2.28	0.41
1:D:250:ASN:OD1	7:D:502:HOH:O	2.22	0.41
6:J:404:PGE:O4	4:J:405:PEG:H31	2.21	0.41
1:C:240:VAL:HG21	1:C:261:VAL:HG13	2.02	0.41
1:A:223:VAL:HG11	1:A:229:VAL:CG2	2.51	0.41
1:B:212:ALA:O	1:C:262[A]:LYS:HE2	2.21	0.41
2:D:401:BR:BR	4:D:407:PEG:C1	2.86	0.41
1:H:285:THR:OG1	1:H:294[B]:THR:HG22	2.21	0.41
1:F:257:ILE:HG22	1:F:259:GLU:HG3	2.03	0.41
1:H:287:LYS:HE2	1:H:289:GLY:O	2.20	0.41
2:D:401:BR:BR	4:D:408:PEG:C3	3.24	0.40
1:B:213:ARG:HG2	1:C:262[A]:LYS:HE3	2.02	0.40
1:F:223:VAL:HG11	1:F:229:VAL:HG21	2.04	0.40
1:H:240:VAL:HG21	1:H:261:VAL:HG13	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:549:HOH:O	7:D:562:HOH:O[2_656]	1.96	0.24
7:D:573:HOH:O	7:J:575:HOH:O[2_557]	2.05	0.15
7:A:554:HOH:O	7:J:530:HOH:O[1_654]	2.16	0.04

## 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	111/104 (107%)	110 (99%)	0	1 (1%)	14 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	102/104 (98%)	102 (100%)	0	0	100	100
1	C	105/104 (101%)	105 (100%)	0	0	100	100
1	D	109/104 (105%)	108 (99%)	0	1 (1%)	14	4
1	E	105/104 (101%)	104 (99%)	1 (1%)	0	100	100
1	F	99/104 (95%)	94 (95%)	5 (5%)	0	100	100
1	G	100/104 (96%)	99 (99%)	1 (1%)	0	100	100
1	H	99/104 (95%)	98 (99%)	0	1 (1%)	12	3
1	I	102/104 (98%)	102 (100%)	0	0	100	100
1	J	104/104 (100%)	103 (99%)	1 (1%)	0	100	100
All	All	1036/1040 (100%)	1025 (99%)	8 (1%)	3 (0%)	36	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	263	ASP
1	H	263	ASP
1	A	263	ASP

### 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	94/83 (113%)	94 (100%)	0	100	100
1	B	87/83 (105%)	86 (99%)	1 (1%)	65	54
1	C	90/83 (108%)	90 (100%)	0	100	100
1	D	93/83 (112%)	90 (97%)	3 (3%)	34	17
1	E	89/83 (107%)	89 (100%)	0	100	100
1	F	84/83 (101%)	84 (100%)	0	100	100
1	G	85/83 (102%)	84 (99%)	1 (1%)	63	51
1	H	83/83 (100%)	81 (98%)	2 (2%)	43	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	86/83 (104%)	83 (96%)	3 (4%)	32	15
1	J	88/83 (106%)	87 (99%)	1 (1%)	65	54
All	All	879/830 (106%)	868 (99%)	11 (1%)	61	48

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	228	PHE
1	D	246	ILE
1	D	290[A]	GLU
1	D	290[B]	GLU
1	G	253	SER
1	H	258	GLN
1	H	269	ARG
1	I	208	THR
1	I	240	VAL
1	I	246	ILE
1	J	296	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	ASN
1	C	271	GLN
1	D	271	GLN
1	G	222	ASN
1	H	232	HIS
1	H	258	GLN
1	I	222	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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 30 are monoatomic - leaving 12 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	$\# Z  > 2$
4	PEG	I	405	3	6,6,6	0.18	0	5,5,5	0.19	0
4	PEG	D	408	-	6,6,6	0.11	0	5,5,5	0.12	0
6	PGE	J	403	-	9,9,9	0.33	0	8,8,8	0.32	0
6	PGE	J	404	-	9,9,9	0.31	0	8,8,8	0.53	0
6	PGE	I	404	3	9,9,9	0.31	0	8,8,8	0.42	0
4	PEG	D	407	-	6,6,6	0.08	0	5,5,5	0.10	0
4	PEG	I	406	-	6,6,6	0.14	0	5,5,5	0.12	0
6	PGE	H	404	-	9,9,9	0.31	0	8,8,8	0.37	0
4	PEG	D	405	-	6,6,6	0.07	0	5,5,5	0.32	0
4	PEG	C	404	-	6,6,6	0.11	0	5,5,5	0.12	0
4	PEG	J	405	-	6,6,6	0.17	0	5,5,5	0.11	0
5	PG4	D	406	-	12,12,12	0.14	0	11,11,11	0.62	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	I	405	3	-	3/4/4/4	-
4	PEG	D	408	-	-	1/4/4/4	-
6	PGE	J	403	-	-	3/7/7/7	-
6	PGE	J	404	-	-	6/7/7/7	-
6	PGE	I	404	3	-	3/7/7/7	-
4	PEG	D	407	-	-	3/4/4/4	-
4	PEG	I	406	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PGE	H	404	-	-	2/7/7/7	-
4	PEG	D	405	-	-	0/4/4/4	-
4	PEG	C	404	-	-	1/4/4/4	-
4	PEG	J	405	-	-	2/4/4/4	-
5	PG4	D	406	-	-	4/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	J	404	PGE	C4-C3-O2-C2
5	D	406	PG4	O4-C7-C8-O5
6	I	404	PGE	O3-C5-C6-O4
4	C	404	PEG	O2-C3-C4-O4
6	I	404	PGE	O1-C1-C2-O2
6	J	403	PGE	O1-C1-C2-O2
4	D	407	PEG	O1-C1-C2-O2
4	J	405	PEG	O1-C1-C2-O2
6	J	404	PGE	O3-C5-C6-O4
4	I	406	PEG	O2-C3-C4-O4
4	I	405	PEG	O1-C1-C2-O2
4	D	407	PEG	O2-C3-C4-O4
6	J	404	PGE	O1-C1-C2-O2
5	D	406	PG4	C5-C6-O4-C7
6	J	403	PGE	O2-C3-C4-O3
4	I	405	PEG	C4-C3-O2-C2
5	D	406	PG4	O2-C3-C4-O3
4	D	408	PEG	C1-C2-O2-C3
6	H	404	PGE	C3-C4-O3-C5
4	I	405	PEG	O2-C3-C4-O4
6	J	404	PGE	C1-C2-O2-C3
6	J	404	PGE	C3-C4-O3-C5
6	H	404	PGE	O1-C1-C2-O2
4	J	405	PEG	O2-C3-C4-O4
6	J	403	PGE	C3-C4-O3-C5
5	D	406	PG4	C4-C3-O2-C2
6	J	404	PGE	O2-C3-C4-O3
4	D	407	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
6	I	404	PGE	C1-C2-O2-C3

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	408	PEG	3	0
6	J	403	PGE	1	0
6	J	404	PGE	3	0
6	I	404	PGE	1	0
4	D	407	PEG	5	0
6	H	404	PGE	3	0
4	J	405	PEG	1	0
5	D	406	PG4	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

### 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	99/104 (95%)	0.24	6 (6%) 27 29	12, 25, 43, 64	14 (14%)
1	B	96/104 (92%)	0.72	20 (20%) 2 2	12, 30, 66, 74	8 (8%)
1	C	97/104 (93%)	0.49	7 (7%) 21 23	15, 31, 55, 74	10 (10%)
1	D	97/104 (93%)	0.21	5 (5%) 33 36	12, 25, 48, 58	14 (14%)
1	E	97/104 (93%)	0.44	10 (10%) 12 12	12, 24, 62, 86	10 (10%)
1	F	95/104 (91%)	1.34	24 (25%) 1 1	14, 41, 76, 87	6 (6%)
1	G	96/104 (92%)	0.59	8 (8%) 17 18	18, 33, 58, 78	6 (6%)
1	H	97/104 (93%)	0.37	7 (7%) 21 23	16, 30, 61, 72	4 (4%)
1	I	98/104 (94%)	0.63	10 (10%) 12 12	16, 33, 56, 72	6 (6%)
1	J	98/104 (94%)	0.02	4 (4%) 41 45	12, 22, 41, 66	8 (8%)
All	All	970/1040 (93%)	0.50	101 (10%) 11 12	12, 30, 60, 87	86 (8%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	304	ALA	6.9
1	B	228	PHE	6.1
1	A	305	ALA	5.8
1	F	303	ILE	5.8
1	F	288[A]	HIS	5.5
1	F	290	GLU	5.4
1	E	254	SER	5.3
1	D	253	SER	4.9
1	E	289	GLY	4.8
1	B	254	SER	4.7
1	E	292	PHE	4.7
1	I	208	THR	4.7
1	B	253	SER	4.6

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Mol	Chain	Res	Type	RSRZ
1	J	208	THR	4.5
1	A	306	ALA	4.4
1	C	208	THR	4.4
1	E	305	ALA	4.2
1	F	292	PHE	4.1
1	F	225	PHE	4.0
1	E	288	HIS	3.9
1	H	263	ASP	3.9
1	E	304	ALA	3.8
1	A	208	THR	3.6
1	I	305	ALA	3.6
1	G	304	ALA	3.6
1	E	290	GLU	3.5
1	B	304	ALA	3.4
1	C	254[A]	SER	3.4
1	F	211	SER	3.4
1	F	289	GLY	3.4
1	H	261	VAL	3.3
1	G	252	VAL	3.3
1	B	226	GLY	3.2
1	F	275	THR	3.2
1	I	209	SER	3.2
1	F	238	ILE	3.2
1	C	304	ALA	3.1
1	J	209	SER	3.1
1	F	276	LYS	3.1
1	B	252	VAL	3.1
1	E	209	SER	3.1
1	I	254	SER	3.0
1	D	263	ASP	3.0
1	H	305	ALA	3.0
1	D	305	ALA	2.9
1	E	255	GLY	2.9
1	F	229	VAL	2.9
1	F	223	VAL	2.8
1	F	287	LYS	2.8
1	A	209	SER	2.8
1	B	209	SER	2.8
1	B	303	ILE	2.8
1	A	249	GLY	2.8
1	F	210	GLY	2.8
1	A	254[A]	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	263	ASP	2.7
1	B	224	THR	2.6
1	F	271	GLN	2.6
1	C	209	SER	2.6
1	C	276	LYS	2.5
1	G	209	SER	2.5
1	D	304	ALA	2.5
1	H	304	ALA	2.5
1	B	273	PHE	2.5
1	G	292	PHE	2.5
1	C	255	GLY	2.5
1	I	262	LYS	2.4
1	F	224	THR	2.4
1	F	291	LYS	2.4
1	H	264	ARG	2.4
1	F	254	SER	2.4
1	B	225	PHE	2.4
1	I	252	VAL	2.4
1	F	226	GLY	2.3
1	I	238	ILE	2.3
1	B	251	ALA	2.3
1	J	305	ALA	2.3
1	F	228	PHE	2.3
1	F	222	ASN	2.3
1	B	255	GLY	2.3
1	B	263	ASP	2.3
1	B	274	ILE	2.3
1	G	303	ILE	2.3
1	B	276	LYS	2.2
1	I	292	PHE	2.2
1	I	290	GLU	2.2
1	B	275	THR	2.2
1	G	253	SER	2.2
1	G	276	LYS	2.2
1	E	287	LYS	2.1
1	B	223	VAL	2.1
1	C	290	GLU	2.1
1	H	262	LYS	2.1
1	H	209	SER	2.1
1	J	264	ARG	2.1
1	B	291	LYS	2.1
1	B	271	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	275	THR	2.0
1	F	277	PRO	2.0
1	D	252	VAL	2.0
1	F	262	LYS	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, 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
6	PGE	J	404	10/10	0.64	0.24	39,54,73,75	0
4	PEG	J	405	7/7	0.71	0.21	46,53,69,73	0
6	PGE	I	404	10/10	0.72	0.20	40,51,56,67	0
4	PEG	I	405	7/7	0.75	0.17	45,55,60,74	0
4	PEG	D	405	7/7	0.75	0.17	48,66,76,77	0
3	K	C	402	1/1	0.76	0.20	74,74,74,74	0
6	PGE	H	404	10/10	0.77	0.16	49,59,64,64	0
4	PEG	C	404	7/7	0.78	0.18	44,59,75,79	0
6	PGE	J	403	10/10	0.81	0.15	45,53,55,62	0
4	PEG	D	408	7/7	0.81	0.16	46,51,52,59	0
4	PEG	I	406	7/7	0.84	0.16	54,58,62,67	0
4	PEG	D	407	7/7	0.85	0.14	37,41,50,50	0
5	PG4	D	406	13/13	0.87	0.14	38,48,60,65	0
3	K	G	403	1/1	0.89	0.28	60,60,60,60	0
3	K	B	402	1/1	0.93	0.19	48,48,48,48	0
3	K	A	404	1/1	0.94	0.15	52,52,52,52	0
2	BR	H	401	1/1	0.94	0.12	48,48,48,48	0
3	K	I	403	1/1	0.94	0.25	41,41,41,41	0
2	BR	D	401	1/1	0.95	0.15	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	K	E	403	1/1	0.95	0.14	55,55,55,55	0
3	K	G	401	1/1	0.96	0.13	59,59,59,59	0
3	K	C	403	1/1	0.96	0.20	41,41,41,41	0
3	K	H	403	1/1	0.96	0.11	51,51,51,51	0
3	K	A	405	1/1	0.96	0.23	49,49,49,49	0
3	K	A	406	1/1	0.97	0.19	39,39,39,39	0
2	BR	D	402	1/1	0.97	0.19	50,50,50,50	0
3	K	I	401	1/1	0.97	0.08	41,41,41,41	0
3	K	A	403	1/1	0.97	0.07	32,32,32,32	0
3	K	D	404	1/1	0.98	0.09	42,42,42,42	0
3	K	H	402	1/1	0.98	0.07	32,32,32,32	0
3	K	E	401	1/1	0.98	0.06	29,29,29,29	0
3	K	B	401	1/1	0.98	0.05	26,26,26,26	0
3	K	I	402	1/1	0.98	0.06	35,35,35,35	1
2	BR	A	401	1/1	0.98	0.15	58,58,58,58	0
3	K	J	401	1/1	0.99	0.12	32,32,32,32	0
3	K	J	402	1/1	0.99	0.13	39,39,39,39	0
3	K	C	401	1/1	0.99	0.06	36,36,36,36	0
3	K	F	401	1/1	0.99	0.09	34,34,34,34	0
3	K	D	403	1/1	0.99	0.05	27,27,27,27	0
3	K	G	402	1/1	0.99	0.04	20,20,20,20	0
3	K	E	402	1/1	0.99	0.14	41,41,41,41	0
3	K	A	402	1/1	1.00	0.03	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.