



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 1, 2018 – 06:46 PM EST

PDB ID : 5MOI  
Title : Crystal structure of human IgE-Fc epsilon 3-4  
Authors : Dore, K.A.; Davies, A.M.; Drinkwater, N.; Beavil, A.J.; McDonnell, J.M.; Sutton, B.J.  
Deposited on : 2016-12-14  
Resolution : 2.20 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

<http://wwpdb.org/validation/2016/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  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

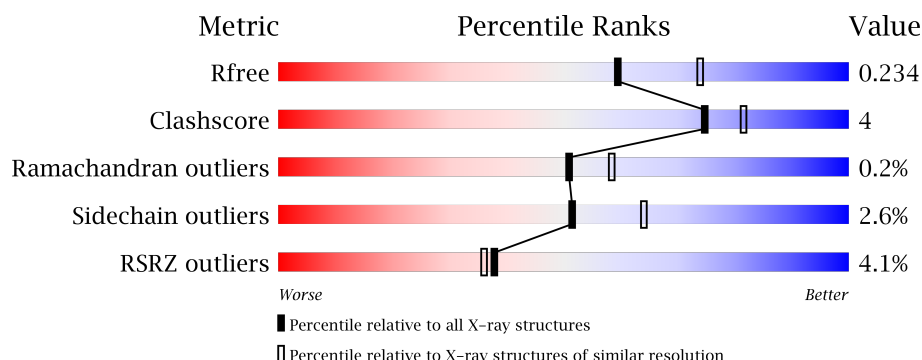
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	223	<div> <div>3%</div> <div>74%</div> <div>5%</div> <div>21%</div> </div>
1	B	223	<div> <div>4%</div> <div>74%</div> <div>11%</div> <div>14%</div> </div>
1	C	223	<div> <div>3%</div> <div>83%</div> <div>9%</div> <div>7%</div> </div>
1	D	223	<div> <div>3%</div> <div>77%</div> <div>10%</div> <div>13%</div> </div>
1	E	223	<div> <div>0%</div> <div>78%</div> <div>11%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	223	

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	NAG	E	601	-	-	-	X
4	MAN	B	605	-	-	-	X
4	MAN	D	605	-	-	-	X
5	PEG	A	605	-	-	-	X
5	PEG	A	606	-	-	-	X
5	PEG	B	606	-	-	-	X
5	PEG	B	607	-	-	-	X
5	PEG	D	608	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9364 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 Ig epsilon chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	177	Total	C	N	O	S	0	3	0
			1366	859	240	262	5			
1	B	191	Total	C	N	O	S	0	0	0
			1463	924	255	278	6			
1	C	208	Total	C	N	O	S	0	0	0
			1588	996	288	298	6			
1	D	193	Total	C	N	O	S	0	0	0
			1440	904	250	280	6			
1	E	200	Total	C	N	O	S	0	0	0
			1544	968	277	293	6			
1	F	176	Total	C	N	O	S	0	0	0
			1331	834	234	258	5			

There are 30 discrepancies between the modelled and reference sequences:

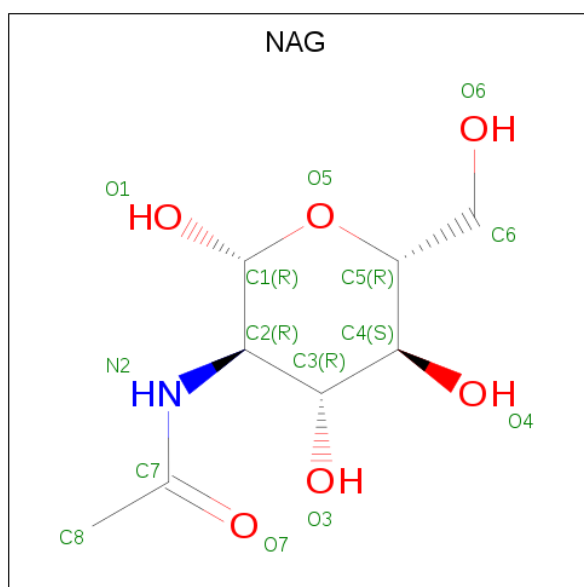
Chain	Residue	Modelled	Actual	Comment	Reference
A	325	ALA	-	expression tag	UNP P01854
A	326	ASP	-	expression tag	UNP P01854
A	327	PRO	-	expression tag	UNP P01854
A	371	GLN	ASN	conflict	UNP P01854
A	383	GLN	ASN	conflict	UNP P01854
B	325	ALA	-	expression tag	UNP P01854
B	326	ASP	-	expression tag	UNP P01854
B	327	PRO	-	expression tag	UNP P01854
B	371	GLN	ASN	conflict	UNP P01854
B	383	GLN	ASN	conflict	UNP P01854
C	325	ALA	-	expression tag	UNP P01854
C	326	ASP	-	expression tag	UNP P01854
C	327	PRO	-	expression tag	UNP P01854
C	371	GLN	ASN	conflict	UNP P01854
C	383	GLN	ASN	conflict	UNP P01854
D	325	ALA	-	expression tag	UNP P01854
D	326	ASP	-	expression tag	UNP P01854

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Chain	Residue	Modelled	Actual	Comment	Reference
D	327	PRO	-	expression tag	UNP P01854
D	371	GLN	ASN	conflict	UNP P01854
D	383	GLN	ASN	conflict	UNP P01854
E	325	ALA	-	expression tag	UNP P01854
E	326	ASP	-	expression tag	UNP P01854
E	327	PRO	-	expression tag	UNP P01854
E	371	GLN	ASN	conflict	UNP P01854
E	383	GLN	ASN	conflict	UNP P01854
F	325	ALA	-	expression tag	UNP P01854
F	326	ASP	-	expression tag	UNP P01854
F	327	PRO	-	expression tag	UNP P01854
F	371	GLN	ASN	conflict	UNP P01854
F	383	GLN	ASN	conflict	UNP P01854

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



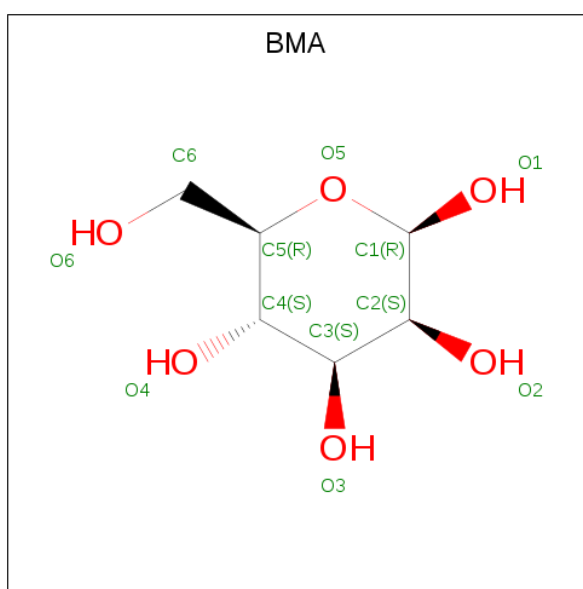
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		

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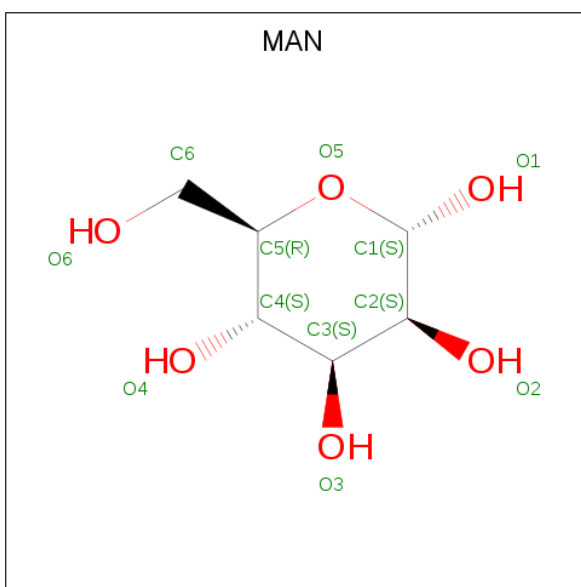
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



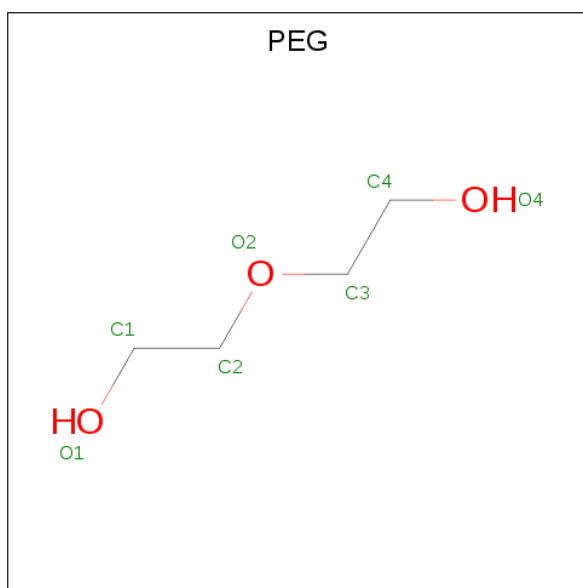
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	C	1	Total	C	O	0	0
			11	6	5		
3	D	1	Total	C	O	0	0
			11	6	5		
3	E	1	Total	C	O	0	0
			11	6	5		
3	F	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	D	1	Total	C	O	0	0
			11	6	5		
4	D	1	Total	C	O	0	0
			11	6	5		
4	D	1	Total	C	O	0	0
			11	6	5		
4	E	1	Total	C	O	0	0
			11	6	5		
4	E	1	Total	C	O	0	0
			11	6	5		
4	F	1	Total	C	O	0	0
			11	6	5		
4	F	1	Total	C	O	0	0
			11	6	5		

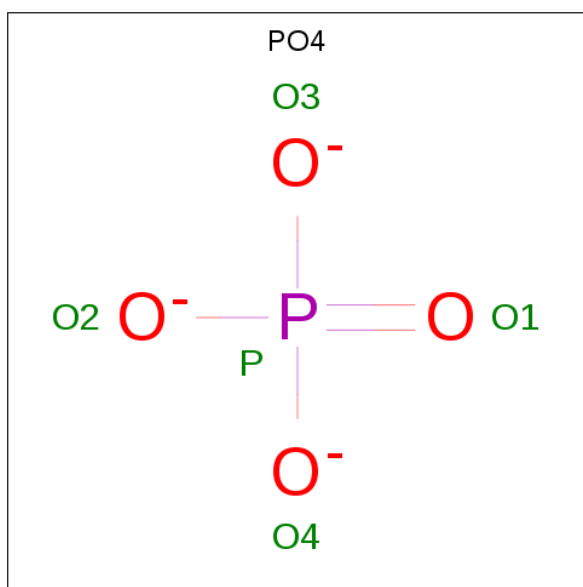
- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			6	4	2		
5	D	1	Total	C	O	0	0
			5	3	2		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		
6	D	1	Total	O	P	0	0
			5	4	1		
6	E	1	Total	O	P	0	0
			5	4	1		
6	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			4	2	2		

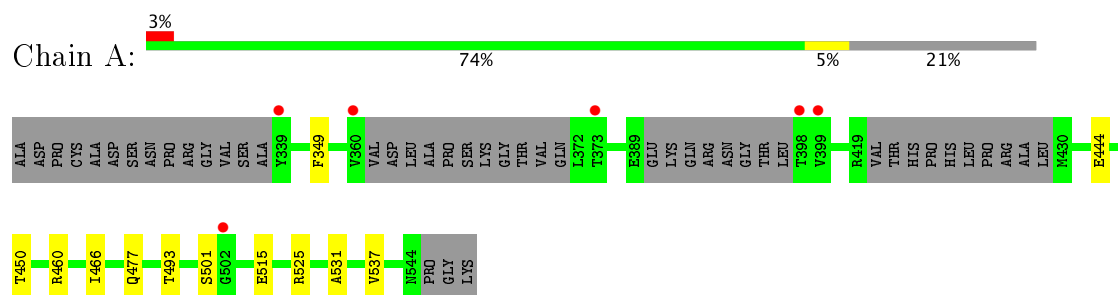
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	52	Total	O	0	0
			52	52		
8	B	51	Total	O	0	0
			51	51		
8	C	37	Total	O	0	0
			37	37		
8	D	11	Total	O	0	0
			11	11		
8	E	46	Total	O	0	0
			46	46		
8	F	16	Total	O	0	0
			16	16		

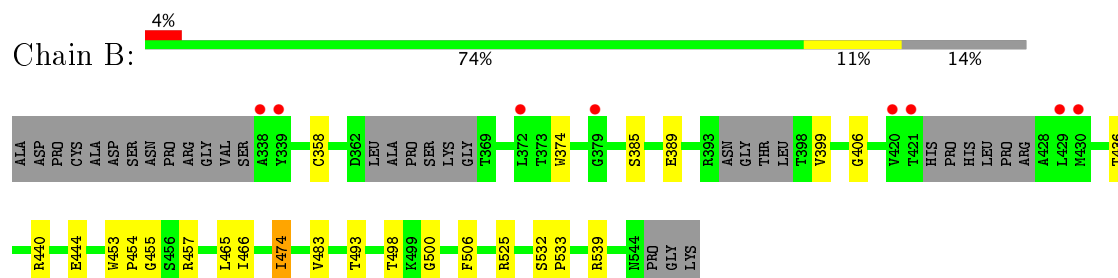
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

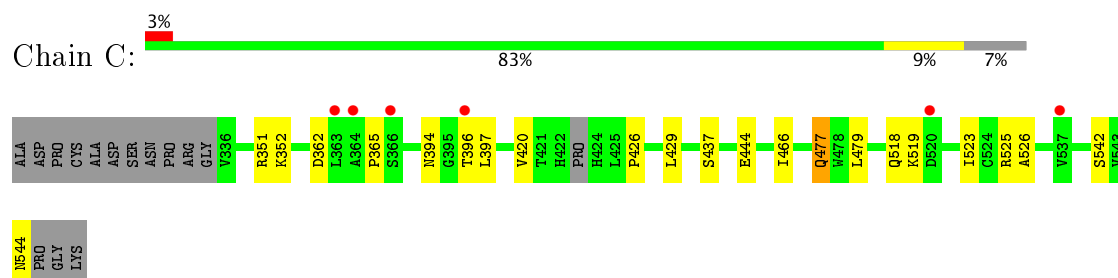
- Molecule 1: Ig epsilon chain C region



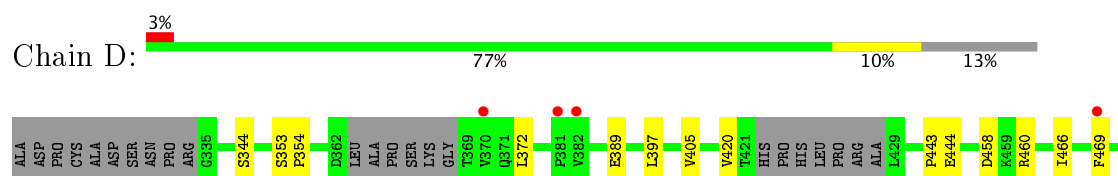
- Molecule 1: Ig epsilon chain C region

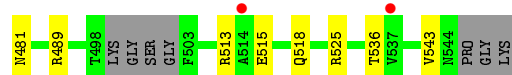


- Molecule 1: Ig epsilon chain C region

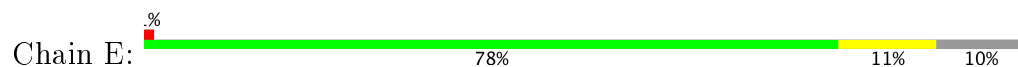


- Molecule 1: Ig epsilon chain C region

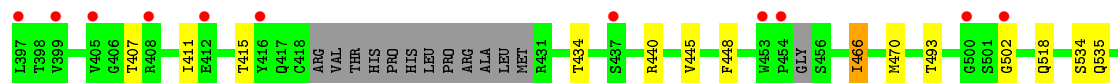
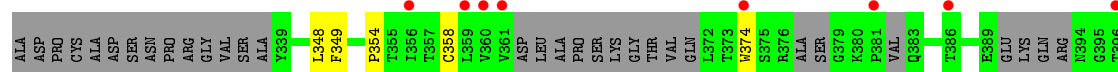




- Molecule 1: Ig epsilon chain C region



- Molecule 1: Ig epsilon chain C region



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.67Å 90.30Å 92.91Å 114.41° 90.63° 96.10°	Depositor
Resolution (Å)	42.22 – 2.20 76.83 – 2.20	Depositor EDS
% Data completeness (in resolution range)	84.5 (42.22-2.20) 84.6 (76.83-2.20)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.213 , 0.234 0.213 , 0.234	Depositor DCC
$R_{free}$ test set	2992 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.6	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 46.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9364	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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: BMA, NAG, PO4, EDO, PEG, MAN

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	0.25	0/1408	0.46	0/1920
1	B	0.26	0/1497	0.46	0/2044
1	C	0.25	0/1625	0.45	0/2217
1	D	0.24	0/1470	0.44	0/2010
1	E	0.25	0/1577	0.46	0/2147
1	F	0.24	0/1359	0.44	0/1851
All	All	0.25	0/8936	0.45	0/12189

There are no bond length outliers.

There are no bond angle outliers.

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	1366	0	1279	8	0
1	B	1463	0	1367	16	0
1	C	1588	0	1516	11	0
1	D	1440	0	1299	11	0
1	E	1544	0	1468	16	0
1	F	1331	0	1213	11	0
2	A	14	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	28	0	24	0	0
2	C	28	0	24	0	0
2	D	28	0	24	0	0
2	E	28	0	24	0	0
3	A	11	0	8	0	0
3	B	11	0	9	0	0
3	C	11	0	8	0	0
3	D	11	0	8	0	0
3	E	11	0	8	0	0
3	F	11	0	8	0	0
4	A	22	0	20	0	0
4	B	22	0	19	2	0
4	C	22	0	20	0	0
4	D	44	0	38	0	0
4	E	22	0	20	0	0
4	F	22	0	20	0	0
5	A	14	0	20	2	0
5	B	20	0	27	2	0
5	D	5	0	5	0	0
6	B	5	0	0	0	0
6	C	10	0	0	0	0
6	D	5	0	0	0	0
6	E	5	0	0	0	0
6	F	5	0	0	0	0
7	C	4	0	6	0	0
8	A	52	0	0	0	0
8	B	51	0	0	1	0
8	C	37	0	0	0	0
8	D	11	0	0	0	0
8	E	46	0	0	1	0
8	F	16	0	0	0	0
All	All	9364	0	8494	65	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 4.

All (65) 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:B:436:THR:O	1:B:440:ARG:NH2	2.22	0.69
1:E:448:PHE:CZ	1:F:448:PHE:HB3	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:479:LEU:HB2	1:C:523:ILE:HB	1.79	0.64
1:D:481:ASN:OD1	1:D:518:GLN:NE2	2.24	0.61
1:C:466:ILE:HD13	1:C:526:ALA:HB2	1.83	0.59
1:B:455:GLY:H	1:C:437:SER:HB2	1.66	0.58
1:D:372:LEU:HD22	1:D:420:VAL:HG22	1.85	0.58
1:C:420:VAL:HB	1:C:429:LEU:HB2	1.87	0.57
1:A:525[B]:ARG:HH12	5:A:606:PEG:H12	1.68	0.57
1:B:389:GLU:HG2	1:B:399:VAL:HG22	1.88	0.55
1:C:365:PRO:HB3	1:C:397:LEU:HB2	1.89	0.55
1:E:487:ASP:OD1	8:E:701:HOH:O	2.18	0.55
1:D:444:GLU:O	1:D:466:ILE:HA	2.07	0.54
1:E:446:TYR:HE2	1:E:448:PHE:CE2	2.25	0.54
1:E:347:ASP:HA	1:E:351:ARG:HB2	1.90	0.54
1:C:352:LYS:HG3	1:E:378:SER:HB3	1.92	0.51
1:A:450:THR:O	1:A:460[A]:ARG:NH1	2.44	0.50
1:B:498:THR:HG23	1:B:500:GLY:N	2.26	0.49
1:F:538:GLN:O	1:F:539:ARG:NE	2.45	0.49
1:B:453:TRP:CG	1:B:454:PRO:HD2	2.48	0.49
1:E:440:ARG:HB2	1:E:530:ALA:HB2	1.95	0.49
1:A:349:PHE:HE1	1:E:533:PRO:HG3	1.78	0.49
1:B:385:SER:H	5:B:608:PEG:H41	1.77	0.49
1:F:348:LEU:HD23	1:F:349:PHE:CZ	2.47	0.49
1:C:477:GLN:HE22	1:C:525:ARG:HE	1.61	0.48
1:E:448:PHE:CE2	1:F:448:PHE:HB3	2.49	0.47
1:C:362:ASP:O	1:C:396:THR:HG23	2.14	0.47
1:E:474:ILE:HD11	1:E:526:ALA:HB1	1.97	0.46
1:D:525:ARG:HG3	1:D:536:THR:HG23	1.98	0.46
1:E:498:THR:HG22	1:E:504:PHE:HD2	1.80	0.46
1:E:475:SER:HB2	1:E:527:VAL:HB	1.98	0.46
1:E:389:GLU:HG2	1:E:399:VAL:HG22	1.97	0.46
1:E:446:TYR:HE2	1:E:448:PHE:CZ	2.35	0.45
1:E:493:THR:HG21	1:F:493:THR:HG21	1.98	0.44
1:B:406:GLY:HA2	5:B:607:PEG:H22	2.00	0.44
1:D:466:ILE:HG22	1:D:469:PHE:CE2	2.52	0.44
1:F:445:VAL:HG22	1:F:466:ILE:HG23	1.99	0.44
1:F:407:THR:O	1:F:411:ILE:HG12	2.18	0.44
1:A:349:PHE:CE1	1:E:533:PRO:HG3	2.52	0.43
1:B:532:SER:HA	1:B:533:PRO:HA	1.70	0.43
1:B:498:THR:HG23	1:B:500:GLY:H	1.84	0.43
1:B:454:PRO:HA	1:C:437:SER:CB	2.47	0.43
1:A:493:THR:HG21	1:B:493:THR:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:470:MET:HG2	1:F:502:GLY:HA2	2.00	0.43
1:D:354:PRO:HG2	1:D:405:VAL:HG23	2.01	0.43
1:A:515:GLU:OE2	5:A:605:PEG:H21	2.19	0.43
1:D:443:PRO:HB2	1:D:466:ILE:HG23	2.01	0.43
1:D:460:ARG:HG2	1:D:543:VAL:HG13	2.01	0.43
1:B:525:ARG:NH2	8:B:704:HOH:O	2.39	0.43
1:D:458:ASP:OD1	1:D:513:ARG:NE	2.50	0.43
1:F:348:LEU:HD12	1:F:354:PRO:HB3	2.01	0.42
4:B:604:MAN:H62	4:B:605:MAN:H2	1.74	0.42
1:B:444:GLU:O	1:B:466:ILE:HA	2.19	0.42
1:F:415:THR:HA	1:F:434:THR:HB	2.01	0.42
1:E:499:LYS:HA	1:E:499:LYS:HD3	1.71	0.42
1:A:531:ALA:HB1	1:A:537:VAL:HG23	2.01	0.42
1:B:465:LEU:HD13	1:B:506:PHE:CE1	2.55	0.42
1:B:474:ILE:O	4:B:605:MAN:H62	2.18	0.42
1:D:489:ARG:NH1	1:D:515:GLU:OE1	2.43	0.42
1:C:394:ASN:OD1	1:C:396:THR:HB	2.20	0.41
1:D:389:GLU:HG2	1:D:397:LEU:HD11	2.02	0.41
1:C:444:GLU:O	1:C:466:ILE:HA	2.20	0.41
1:F:358:CYS:HB2	1:F:374:TRP:CH2	2.56	0.41
1:A:444:GLU:O	1:A:466:ILE:HA	2.22	0.40
1:B:358:CYS:HB2	1:B:374:TRP:CH2	2.56	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	172/223 (77%)	171 (99%)	1 (1%)	0	100	100
1	B	183/223 (82%)	178 (97%)	5 (3%)	0	100	100
1	C	204/223 (92%)	200 (98%)	3 (2%)	1 (0%)	32	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	185/223 (83%)	183 (99%)	2 (1%)	0	100	100
1	E	192/223 (86%)	188 (98%)	3 (2%)	1 (0%)	32	34
1	F	162/223 (73%)	157 (97%)	5 (3%)	0	100	100
All	All	1098/1338 (82%)	1077 (98%)	19 (2%)	2 (0%)	51	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	426	PRO
1	E	426	PRO

### 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	145/195 (74%)	143 (99%)	2 (1%)	71	84
1	B	152/195 (78%)	148 (97%)	4 (3%)	51	64
1	C	167/195 (86%)	161 (96%)	6 (4%)	40	50
1	D	145/195 (74%)	143 (99%)	2 (1%)	71	84
1	E	165/195 (85%)	160 (97%)	5 (3%)	46	58
1	F	137/195 (70%)	132 (96%)	5 (4%)	40	50
All	All	911/1170 (78%)	887 (97%)	24 (3%)	51	64

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	477	GLN
1	A	501	SER
1	B	457	ARG
1	B	474	ILE
1	B	483	VAL
1	B	539	ARG

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Mol	Chain	Res	Type
1	C	351	ARG
1	C	477	GLN
1	C	518	GLN
1	C	519	LYS
1	C	542	SER
1	C	544	ASN
1	D	344	SER
1	D	353	SER
1	E	361	VAL
1	E	362	ASP
1	E	430	MET
1	E	477	GLN
1	E	518	GLN
1	F	440	ARG
1	F	466	ILE
1	F	518	GLN
1	F	534	SER
1	F	535	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

42 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	NAG	A	601	3	14,14,15	0.22	0	15,19,21	0.45	0
3	BMA	A	602	2,4	11,11,12	0.62	0	13,15,17	0.86	0
4	MAN	A	603	3	11,11,12	0.65	0	13,15,17	1.10	2 (15%)
4	MAN	A	604	3	11,11,12	0.67	0	13,15,17	1.01	1 (7%)
5	PEG	A	605	-	6,6,6	0.83	0	5,5,5	0.23	0
5	PEG	A	606	-	6,6,6	0.84	0	5,5,5	0.21	0
2	NAG	B	601	2	14,14,15	0.22	0	15,19,21	0.44	0
2	NAG	B	602	3,2	14,14,15	0.29	0	15,19,21	0.45	0
3	BMA	B	603	2,4	11,11,12	0.70	0	13,15,17	0.90	0
4	MAN	B	604	3,4	11,11,12	0.70	0	13,15,17	1.16	2 (15%)
4	MAN	B	605	4	11,11,12	0.64	0	13,15,17	1.12	2 (15%)
5	PEG	B	606	-	6,6,6	0.85	0	5,5,5	0.28	0
5	PEG	B	607	-	6,6,6	0.84	0	5,5,5	0.26	0
5	PEG	B	608	-	5,5,6	0.85	0	4,4,5	0.28	0
6	PO4	B	609	-	4,4,4	0.80	0	6,6,6	0.35	0
2	NAG	C	601	1,2	14,14,15	0.23	0	15,19,21	0.48	0
2	NAG	C	602	3,2	14,14,15	0.24	0	15,19,21	0.46	0
3	BMA	C	603	2,4	11,11,12	0.49	0	13,15,17	0.91	0
4	MAN	C	604	3	11,11,12	0.74	0	13,15,17	0.92	1 (7%)
4	MAN	C	605	3	11,11,12	0.60	0	13,15,17	1.18	2 (15%)
7	EDO	C	606	-	3,3,3	0.46	0	2,2,2	0.36	0
6	PO4	C	607	-	4,4,4	0.76	0	6,6,6	0.38	0
6	PO4	C	608	-	4,4,4	0.83	0	6,6,6	0.39	0
2	NAG	D	601	1,2	14,14,15	0.21	0	15,19,21	0.54	0
2	NAG	D	602	3,2	14,14,15	0.24	0	15,19,21	0.52	0
3	BMA	D	603	2,4	11,11,12	0.61	0	13,15,17	1.25	1 (7%)
4	MAN	D	604	3,4	11,11,12	0.71	0	13,15,17	1.21	2 (15%)
4	MAN	D	605	4	11,11,12	0.58	0	13,15,17	1.17	2 (15%)
4	MAN	D	606	4	11,11,12	0.71	0	13,15,17	1.30	2 (15%)
4	MAN	D	607	3	11,11,12	0.64	0	13,15,17	1.18	2 (15%)
5	PEG	D	608	-	4,4,6	0.82	0	3,3,5	0.23	0
6	PO4	D	609	-	4,4,4	0.76	0	6,6,6	0.40	0
2	NAG	E	601	1,2	14,14,15	0.14	0	15,19,21	0.47	0
2	NAG	E	602	3,2	14,14,15	0.16	0	15,19,21	0.51	0
3	BMA	E	603	2,4	11,11,12	0.73	0	13,15,17	1.30	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MAN	E	604	3	11,11,12	0.59	0	13,15,17	1.03	2 (15%)
4	MAN	E	605	3	11,11,12	0.78	0	13,15,17	1.70	2 (15%)
6	PO4	E	606	-	4,4,4	0.80	0	6,6,6	0.43	0
3	BMA	F	601	4	11,11,12	0.76	0	13,15,17	0.89	0
4	MAN	F	602	3	11,11,12	0.69	0	13,15,17	1.01	2 (15%)
4	MAN	F	603	3	11,11,12	0.76	0	13,15,17	0.96	1 (7%)
6	PO4	F	604	-	4,4,4	0.78	0	6,6,6	0.39	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
2	NAG	A	601	3	-	0/6/23/26	0/1/1/1
3	BMA	A	602	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	603	3	-	0/2/19/22	0/1/1/1
4	MAN	A	604	3	-	0/2/19/22	0/1/1/1
5	PEG	A	605	-	-	0/4/4/4	0/0/0/0
5	PEG	A	606	-	-	0/4/4/4	0/0/0/0
2	NAG	B	601	2	-	0/6/23/26	0/1/1/1
2	NAG	B	602	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	603	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	604	3,4	-	0/2/19/22	0/1/1/1
4	MAN	B	605	4	-	0/2/19/22	0/1/1/1
5	PEG	B	606	-	-	0/4/4/4	0/0/0/0
5	PEG	B	607	-	-	0/4/4/4	0/0/0/0
5	PEG	B	608	-	-	0/3/3/4	0/0/0/0
6	PO4	B	609	-	-	0/0/0/0	0/0/0/0
2	NAG	C	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	602	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	603	2,4	-	0/2/19/22	0/1/1/1
4	MAN	C	604	3	-	0/2/19/22	0/1/1/1
4	MAN	C	605	3	-	0/2/19/22	0/1/1/1
7	EDO	C	606	-	-	0/1/1/1	0/0/0/0
6	PO4	C	607	-	-	0/0/0/0	0/0/0/0
6	PO4	C	608	-	-	0/0/0/0	0/0/0/0
2	NAG	D	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	602	3,2	-	0/6/23/26	0/1/1/1
3	BMA	D	603	2,4	-	0/2/19/22	0/1/1/1
4	MAN	D	604	3,4	-	0/2/19/22	0/1/1/1
4	MAN	D	605	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	D	606	4	-	0/2/19/22	0/1/1/1
4	MAN	D	607	3	-	0/2/19/22	0/1/1/1
5	PEG	D	608	-	-	0/2/2/4	0/0/0/0
6	PO4	D	609	-	-	0/0/0/0	0/0/0/0
2	NAG	E	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	602	3,2	-	0/6/23/26	0/1/1/1
3	BMA	E	603	2,4	-	0/2/19/22	0/1/1/1
4	MAN	E	604	3	-	0/2/19/22	0/1/1/1
4	MAN	E	605	3	-	0/2/19/22	0/1/1/1
6	PO4	E	606	-	-	0/0/0/0	0/0/0/0
3	BMA	F	601	4	-	0/2/19/22	0/1/1/1
4	MAN	F	602	3	-	0/2/19/22	0/1/1/1
4	MAN	F	603	3	-	0/2/19/22	0/1/1/1
6	PO4	F	604	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	605	MAN	O2-C2-C3	-2.38	105.50	110.17
4	D	605	MAN	O2-C2-C3	-2.35	105.56	110.17
4	D	604	MAN	O2-C2-C3	-2.34	105.58	110.17
4	C	605	MAN	O2-C2-C3	-2.31	105.64	110.17
4	D	606	MAN	O2-C2-C3	-2.31	105.64	110.17
4	E	604	MAN	O2-C2-C3	-2.28	105.70	110.17
4	A	604	MAN	O2-C2-C3	-2.27	105.71	110.17
4	E	605	MAN	O2-C2-C3	-2.27	105.71	110.17
4	A	603	MAN	O2-C2-C3	-2.25	105.75	110.17
4	B	604	MAN	O2-C2-C3	-2.24	105.77	110.17
4	C	604	MAN	O2-C2-C3	-2.21	105.83	110.17
4	D	607	MAN	O2-C2-C3	-2.17	105.91	110.17
4	F	602	MAN	O2-C2-C3	-2.14	105.98	110.17
4	F	603	MAN	O2-C2-C3	-2.13	106.00	110.17
4	F	602	MAN	C1-O5-C5	2.20	115.20	112.17
4	E	604	MAN	C1-O5-C5	2.42	115.51	112.17
4	D	604	MAN	C1-O5-C5	2.47	115.57	112.17
4	A	603	MAN	C1-O5-C5	2.58	115.72	112.17
3	D	603	BMA	C1-C2-C3	2.64	113.00	109.65
4	B	605	MAN	C1-O5-C5	2.66	115.84	112.17
3	E	603	BMA	C1-C2-C3	2.77	113.16	109.65
4	D	605	MAN	C1-O5-C5	2.87	116.12	112.17
4	D	607	MAN	C1-O5-C5	2.87	116.12	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	604	MAN	C1-O5-C5	2.92	116.18	112.17
4	C	605	MAN	C1-O5-C5	3.04	116.35	112.17
4	D	606	MAN	C1-O5-C5	3.39	116.84	112.17
4	E	605	MAN	C1-O5-C5	5.24	119.39	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	605	PEG	1	0
5	A	606	PEG	1	0
4	B	604	MAN	1	0
4	B	605	MAN	2	0
5	B	607	PEG	1	0
5	B	608	PEG	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	177/223 (79%)	0.07	6 (3%)	46	43	24, 54, 104, 119	0
1	B	191/223 (85%)	0.05	8 (4%)	37	35	25, 54, 103, 130	0
1	C	208/223 (93%)	0.06	6 (2%)	52	50	36, 63, 113, 155	0
1	D	193/223 (86%)	0.33	6 (3%)	49	47	49, 79, 114, 133	0
1	E	200/223 (89%)	0.14	2 (1%)	82	81	32, 64, 112, 160	0
1	F	176/223 (78%)	0.58	19 (10%)	6	6	41, 77, 142, 157	0
All	All	1145/1338 (85%)	0.20	47 (4%)	38	36	24, 65, 118, 160	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	374	TRP	6.9
1	B	429	LEU	5.0
1	C	396	THR	4.7
1	C	363	LEU	4.7
1	F	397	LEU	4.1
1	A	398	THR	4.1
1	F	500	GLY	4.0
1	D	381	PRO	3.5
1	F	361	VAL	3.5
1	F	412	GLU	3.3
1	F	399	VAL	3.2
1	F	408	ARG	3.1
1	A	339	TYR	2.9
1	D	537	VAL	2.9
1	C	364	ALA	2.9
1	F	356	ILE	2.9
1	A	360	VAL	2.8
1	D	382	VAL	2.8
1	F	453	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	502	GLY	2.7
1	B	372	LEU	2.7
1	C	537	VAL	2.6
1	F	416	TYR	2.6
1	F	386	THR	2.6
1	C	366	SER	2.5
1	D	370	VAL	2.5
1	D	469	PHE	2.5
1	B	379	GLY	2.4
1	D	514	ALA	2.4
1	B	338	ALA	2.4
1	B	421	THR	2.4
1	F	381	PRO	2.4
1	F	396	THR	2.4
1	F	405	VAL	2.3
1	F	360	VAL	2.3
1	F	359	LEU	2.3
1	F	454	PRO	2.3
1	B	430	MET	2.2
1	E	382	VAL	2.2
1	A	502	GLY	2.2
1	E	372	LEU	2.2
1	B	420	VAL	2.1
1	C	520	ASP	2.1
1	B	339	TYR	2.1
1	A	373	THR	2.1
1	F	437	SER	2.1
1	A	399	VAL	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 carbohydrates 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	PEG	B	606	7/7	0.83	0.28	9.69	69,71,80,82	0
5	PEG	B	607	7/7	0.73	0.26	8.23	91,97,99,99	0
5	PEG	D	608	5/7	0.71	0.27	7.42	68,70,72,74	0
5	PEG	A	606	7/7	0.86	0.30	7.14	71,76,81,81	0
4	MAN	D	605	11/12	0.80	0.27	7.01	91,95,96,97	0
5	PEG	A	605	7/7	0.78	0.29	5.67	56,57,61,61	0
4	MAN	B	605	11/12	0.61	0.31	3.62	86,93,98,99	0
2	NAG	E	601	14/15	0.90	0.21	3.05	75,85,92,96	0
6	PO4	F	604	5/5	0.89	0.16	0.79	99,102,103,104	0
6	PO4	D	609	5/5	0.74	0.18	-0.07	114,115,115,116	0
5	PEG	B	608	6/7	0.81	0.16	-0.30	81,82,83,84	0
2	NAG	C	602	14/15	0.91	0.14	-0.30	65,75,79,81	0
6	PO4	B	609	5/5	0.97	0.13	-0.35	47,54,56,66	0
2	NAG	D	602	14/15	0.90	0.12	-0.75	65,69,77,79	0
6	PO4	E	606	5/5	0.94	0.14	-0.79	64,65,74,77	0
4	MAN	A	603	11/12	0.86	0.12	-	90,94,96,98	0
3	BMA	B	603	11/12	0.78	0.14	-	98,105,108,109	0
4	MAN	F	603	11/12	0.77	0.25	-	124,126,127,128	0
4	MAN	F	602	11/12	0.51	0.25	-	127,129,130,131	0
4	MAN	B	604	11/12	0.75	0.17	-	88,96,98,100	0
2	NAG	D	601	14/15	0.89	0.13	-	51,64,76,79	0
3	BMA	F	601	11/12	0.83	0.24	-	124,126,129,130	0
3	BMA	C	603	11/12	0.90	0.12	-	85,91,94,94	0
4	MAN	A	604	11/12	0.84	0.12	-	99,102,103,103	0
2	NAG	A	601	14/15	0.78	0.23	-	104,106,107,108	0
4	MAN	C	604	11/12	0.72	0.18	-	87,94,99,101	0
4	MAN	D	604	11/12	0.79	0.15	-	76,83,92,95	0
4	MAN	E	604	11/12	0.83	0.18	-	90,91,97,101	0
2	NAG	E	602	14/15	0.89	0.14	-	82,88,91,91	0
4	MAN	E	605	11/12	0.83	0.15	-	84,91,92,96	0
2	NAG	B	602	14/15	0.86	0.32	-	111,115,117,117	0
6	PO4	C	607	5/5	0.85	0.15	-	109,110,111,113	0
4	MAN	D	606	11/12	0.84	0.14	-	91,94,98,101	0
4	MAN	D	607	11/12	0.86	0.27	-	83,87,90,90	0
3	BMA	A	602	11/12	0.83	0.13	-	97,100,103,103	0
7	EDO	C	606	4/4	0.76	0.17	-	77,78,78,80	0
2	NAG	B	601	14/15	0.61	0.38	-	113,120,122,123	0
3	BMA	E	603	11/12	0.90	0.10	-	84,87,89,91	0
3	BMA	D	603	11/12	0.89	0.13	-	65,68,75,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	C	601	14/15	0.86	0.30	-	67,78,83,84	0
6	PO4	C	608	5/5	0.97	0.13	-	76,77,78,78	0
4	MAN	C	605	11/12	0.81	0.22	-	96,99,101,101	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.