



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:32 PM GMT

PDB ID : 4KRY  
Title : Structure of Aes from E. coli in covalent complex with PMS  
Authors : Schiefner, A.; Gerber, K.; Brosig, A.; Boos, W.  
Deposited on : 2013-05-17  
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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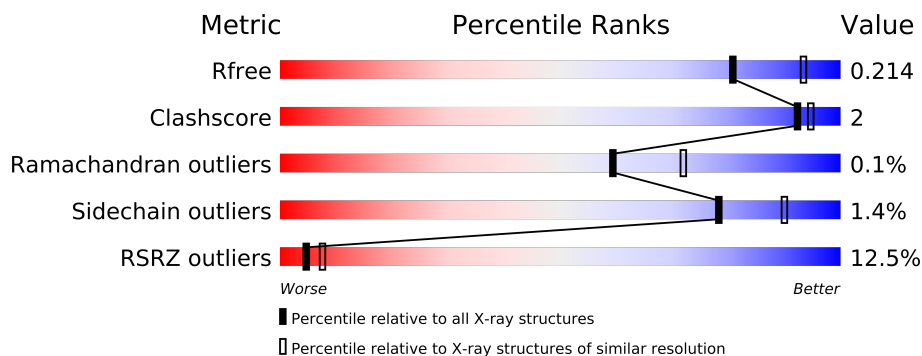
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	333	
1	B	333	
1	C	333	
1	D	333	
1	E	333	
1	F	333	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	PGE	D	402	-	X
2	PGE	F	401	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	IMD	A	403	-	X
3	IMD	D	404	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15961 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Acetyl esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2537	1621	424	474	18			
1	B	318	Total	C	N	O	S	0	1	0
			2545	1626	427	474	18			
1	C	318	Total	C	N	O	S	0	2	0
			2554	1631	428	477	18			
1	D	318	Total	C	N	O	S	0	1	0
			2545	1626	427	474	18			
1	E	329	Total	C	N	O	S	0	3	0
			2660	1695	455	490	20			
1	F	318	Total	C	N	O	S	0	0	0
			2537	1621	424	474	18			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP P23872
A	-12	ARG	-	EXPRESSION TAG	UNP P23872
A	-11	GLY	-	EXPRESSION TAG	UNP P23872
A	-10	SER	-	EXPRESSION TAG	UNP P23872
A	-9	HIS	-	EXPRESSION TAG	UNP P23872
A	-8	HIS	-	EXPRESSION TAG	UNP P23872
A	-7	HIS	-	EXPRESSION TAG	UNP P23872
A	-6	HIS	-	EXPRESSION TAG	UNP P23872
A	-5	HIS	-	EXPRESSION TAG	UNP P23872
A	-4	HIS	-	EXPRESSION TAG	UNP P23872
A	-3	THR	-	EXPRESSION TAG	UNP P23872
A	-2	ASP	-	EXPRESSION TAG	UNP P23872
A	-1	PRO	-	EXPRESSION TAG	UNP P23872
A	0	ILE	-	EXPRESSION TAG	UNP P23872
B	-13	MET	-	EXPRESSION TAG	UNP P23872
B	-12	ARG	-	EXPRESSION TAG	UNP P23872
B	-11	GLY	-	EXPRESSION TAG	UNP P23872

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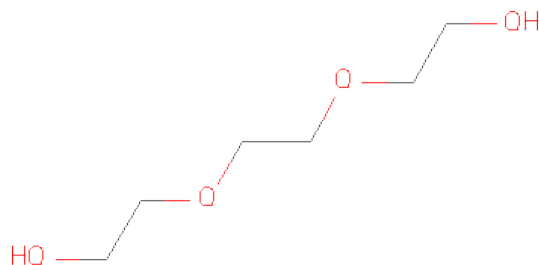
Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	SER	-	EXPRESSION TAG	UNP P23872
B	-9	HIS	-	EXPRESSION TAG	UNP P23872
B	-8	HIS	-	EXPRESSION TAG	UNP P23872
B	-7	HIS	-	EXPRESSION TAG	UNP P23872
B	-6	HIS	-	EXPRESSION TAG	UNP P23872
B	-5	HIS	-	EXPRESSION TAG	UNP P23872
B	-4	HIS	-	EXPRESSION TAG	UNP P23872
B	-3	THR	-	EXPRESSION TAG	UNP P23872
B	-2	ASP	-	EXPRESSION TAG	UNP P23872
B	-1	PRO	-	EXPRESSION TAG	UNP P23872
B	0	ILE	-	EXPRESSION TAG	UNP P23872
C	-13	MET	-	EXPRESSION TAG	UNP P23872
C	-12	ARG	-	EXPRESSION TAG	UNP P23872
C	-11	GLY	-	EXPRESSION TAG	UNP P23872
C	-10	SER	-	EXPRESSION TAG	UNP P23872
C	-9	HIS	-	EXPRESSION TAG	UNP P23872
C	-8	HIS	-	EXPRESSION TAG	UNP P23872
C	-7	HIS	-	EXPRESSION TAG	UNP P23872
C	-6	HIS	-	EXPRESSION TAG	UNP P23872
C	-5	HIS	-	EXPRESSION TAG	UNP P23872
C	-4	HIS	-	EXPRESSION TAG	UNP P23872
C	-3	THR	-	EXPRESSION TAG	UNP P23872
C	-2	ASP	-	EXPRESSION TAG	UNP P23872
C	-1	PRO	-	EXPRESSION TAG	UNP P23872
C	0	ILE	-	EXPRESSION TAG	UNP P23872
D	-13	MET	-	EXPRESSION TAG	UNP P23872
D	-12	ARG	-	EXPRESSION TAG	UNP P23872
D	-11	GLY	-	EXPRESSION TAG	UNP P23872
D	-10	SER	-	EXPRESSION TAG	UNP P23872
D	-9	HIS	-	EXPRESSION TAG	UNP P23872
D	-8	HIS	-	EXPRESSION TAG	UNP P23872
D	-7	HIS	-	EXPRESSION TAG	UNP P23872
D	-6	HIS	-	EXPRESSION TAG	UNP P23872
D	-5	HIS	-	EXPRESSION TAG	UNP P23872
D	-4	HIS	-	EXPRESSION TAG	UNP P23872
D	-3	THR	-	EXPRESSION TAG	UNP P23872
D	-2	ASP	-	EXPRESSION TAG	UNP P23872
D	-1	PRO	-	EXPRESSION TAG	UNP P23872
D	0	ILE	-	EXPRESSION TAG	UNP P23872
E	-13	MET	-	EXPRESSION TAG	UNP P23872
E	-12	ARG	-	EXPRESSION TAG	UNP P23872
E	-11	GLY	-	EXPRESSION TAG	UNP P23872

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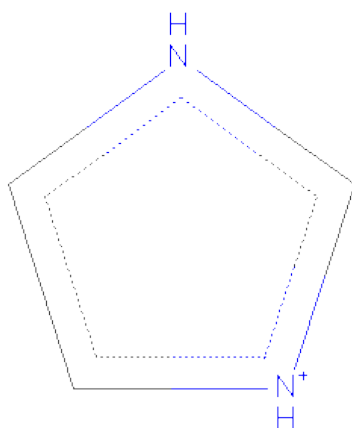
Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	SER	-	EXPRESSION TAG	UNP P23872
E	-9	HIS	-	EXPRESSION TAG	UNP P23872
E	-8	HIS	-	EXPRESSION TAG	UNP P23872
E	-7	HIS	-	EXPRESSION TAG	UNP P23872
E	-6	HIS	-	EXPRESSION TAG	UNP P23872
E	-5	HIS	-	EXPRESSION TAG	UNP P23872
E	-4	HIS	-	EXPRESSION TAG	UNP P23872
E	-3	THR	-	EXPRESSION TAG	UNP P23872
E	-2	ASP	-	EXPRESSION TAG	UNP P23872
E	-1	PRO	-	EXPRESSION TAG	UNP P23872
E	0	ILE	-	EXPRESSION TAG	UNP P23872
F	-13	MET	-	EXPRESSION TAG	UNP P23872
F	-12	ARG	-	EXPRESSION TAG	UNP P23872
F	-11	GLY	-	EXPRESSION TAG	UNP P23872
F	-10	SER	-	EXPRESSION TAG	UNP P23872
F	-9	HIS	-	EXPRESSION TAG	UNP P23872
F	-8	HIS	-	EXPRESSION TAG	UNP P23872
F	-7	HIS	-	EXPRESSION TAG	UNP P23872
F	-6	HIS	-	EXPRESSION TAG	UNP P23872
F	-5	HIS	-	EXPRESSION TAG	UNP P23872
F	-4	HIS	-	EXPRESSION TAG	UNP P23872
F	-3	THR	-	EXPRESSION TAG	UNP P23872
F	-2	ASP	-	EXPRESSION TAG	UNP P23872
F	-1	PRO	-	EXPRESSION TAG	UNP P23872
F	0	ILE	-	EXPRESSION TAG	UNP P23872

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



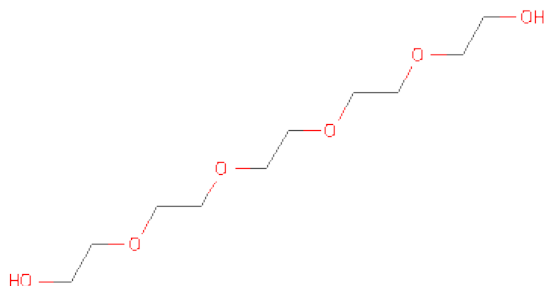
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		
2	A	1	Total	C	O	0	0
			10	6	4		
2	B	1	Total	C	O	0	0
			10	6	4		
2	C	1	Total	C	O	0	0
			10	6	4		
2	D	1	Total	C	O	0	0
			10	6	4		
2	D	1	Total	C	O	0	0
			10	6	4		
2	E	1	Total	C	O	0	0
			10	6	4		
2	F	1	Total	C	O	0	0
			10	6	4		

- Molecule 3 is IMIDAZOLE (three-letter code: IMD) (formula:  $C_3H_5N_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			5	3	2		
3	B	1	Total	C	N	0	0
			5	3	2		
3	D	1	Total	C	N	0	0
			5	3	2		
3	D	1	Total	C	N	0	0
			5	3	2		

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			16	10	6		
4	E	1	Total	C	O	0	0
			16	10	6		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	72	Total	O	0	0
			72	72		
5	B	82	Total	O	0	1
			83	83		
5	C	45	Total	O	0	0
			45	45		
5	D	98	Total	O	0	0
			98	98		
5	E	116	Total	O	0	1
			117	117		
5	F	36	Total	O	0	0
			36	36		

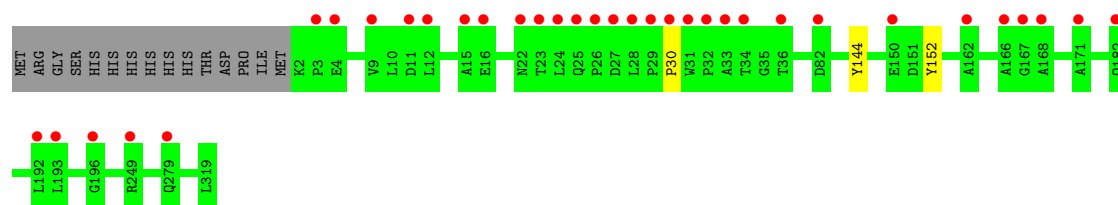


### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

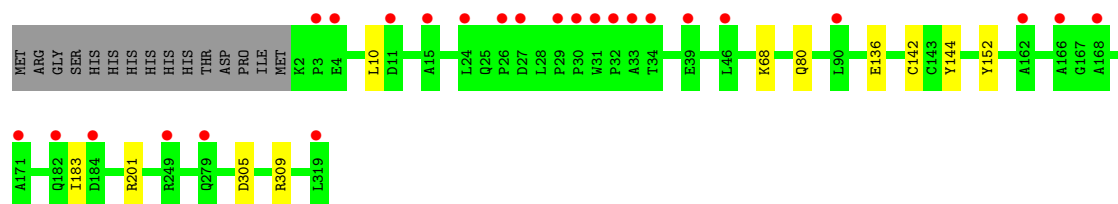
- Molecule 1: Acetyl esterase

Chain A: 



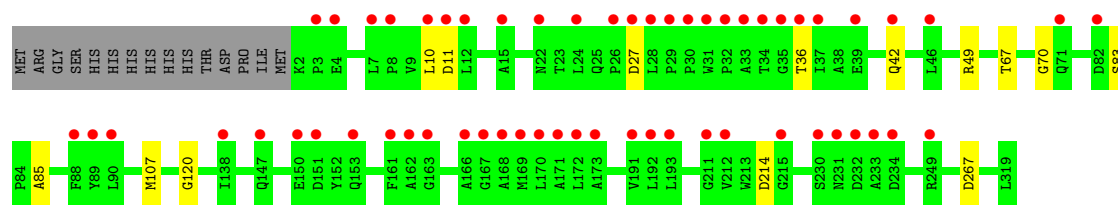
- Molecule 1: Acetyl esterase

Chain B: 



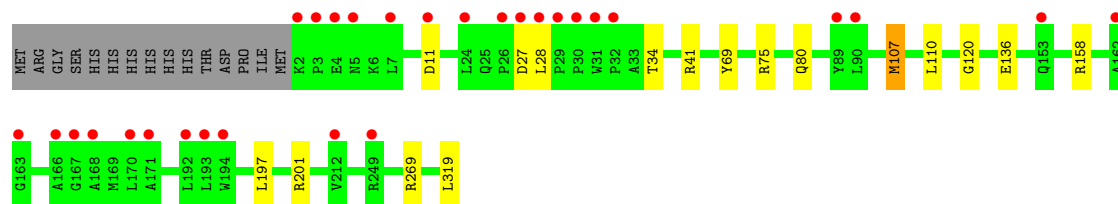
- Molecule 1: Acetyl esterase

Chain C: 



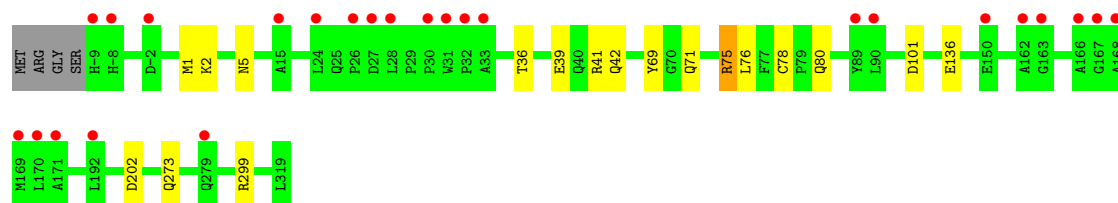
- Molecule 1: Acetyl esterase

Chain D: 



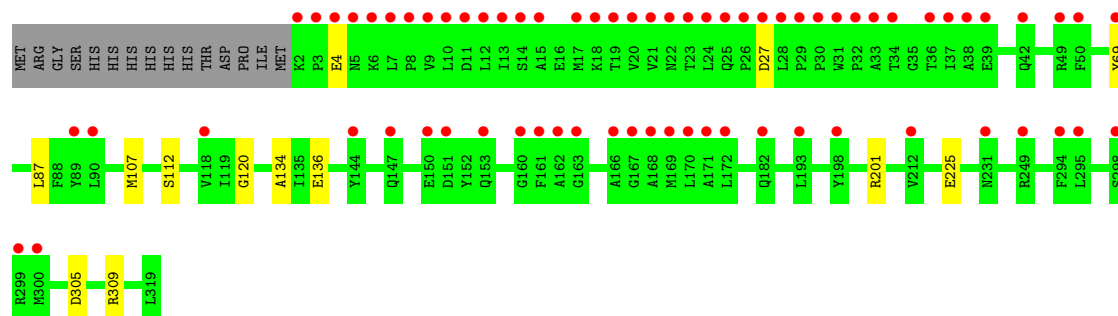
- Molecule 1: Acetyl esterase

Chain E: 



- Molecule 1: Acetyl esterase

Chain F: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.40Å 111.40Å 282.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.37 – 2.30 29.35 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.37-2.30) 99.8 (29.35-2.30)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.40 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.179 , 0.209 0.185 , 0.214	Depositor DCC
$R_{free}$ test set	7572 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.8	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 42.3	EDS
Estimated twinning fraction	0.068 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 151348 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15961	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, 1PE, SEB, IMD

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	0.57	0/2586	0.70	0/3516
1	B	0.61	0/2597	0.76	1/3530 (0.0%)
1	C	0.49	0/2606	0.64	0/3542
1	D	0.68	0/2597	0.81	4/3530 (0.1%)
1	E	0.64	0/2719	0.79	5/3697 (0.1%)
1	F	0.50	0/2586	0.67	1/3516 (0.0%)
All	All	0.59	0/15691	0.73	11/21331 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	41	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	E	101	ASP	CB-CG-OD1	6.16	123.84	118.30
1	E	41	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	E	202	ASP	CB-CG-OD1	5.46	123.22	118.30
1	D	269	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	E	75	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	D	41	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	D	201	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	B	201	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	F	87	LEU	CA-CB-CG	5.02	126.85	115.30
1	D	107	MET	CG-SD-CE	-5.01	92.18	100.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2537	0	0	1	0
1	B	2545	0	0	3	0
1	C	2554	0	0	3	0
1	D	2545	0	0	5	0
1	E	2660	0	0	9	0
1	F	2537	0	0	5	0
2	A	20	0	28	0	0
2	B	10	0	14	0	0
2	C	10	0	14	0	0
2	D	20	0	28	2	0
2	E	10	0	14	0	0
2	F	10	0	14	0	0
3	A	5	0	5	0	0
3	B	5	0	5	0	0
3	D	10	0	10	0	0
4	D	16	0	22	0	0
4	E	16	0	22	0	0
5	A	72	0	0	0	0
5	B	83	0	0	0	0
5	C	45	0	0	0	0
5	D	98	0	0	3	0
5	E	117	0	0	4	0
5	F	36	0	0	1	0
All	All	15961	0	176	28	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (28) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:76:LEU:CD2	1:E:78[A]:CYS:SG	2.68	0.81
1:F:305:ASP:OD2	1:F:309:ARG:NH1	2.34	0.60
1:F:107:MET:CE	1:F:120:GLY:CA	2.81	0.59
1:D:107:MET:CE	1:D:120:GLY:CA	2.80	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:144:TYR:OH	1:A:152:TYR:OH	2.24	0.55
1:B:144:TYR:OH	1:B:152:TYR:OH	2.24	0.55
2:D:402:PGE:H12	5:D:566:HOH:O	2.07	0.54
1:D:69:TYR:OH	1:D:136:GLU:OE1	2.26	0.54
1:C:67:THR:OG1	1:C:70:GLY:O	2.30	0.50
1:F:134:ALA:N	5:F:506:HOH:O	2.45	0.49
1:C:83:SER:OG	1:C:85:ALA:O	2.30	0.49
1:F:201:ARG:NH2	1:F:225:GLU:OE2	2.46	0.49
1:E:299[A]:ARG:CG	1:E:299[A]:ARG:NH1	2.76	0.47
1:E:2:LYS:O	1:E:5:ASN:N	2.48	0.47
1:E:36:THR:OG1	1:E:39:GLU:OE1	2.31	0.47
2:D:402:PGE:C1	5:D:566:HOH:O	2.62	0.47
1:D:75:ARG:NH1	5:D:536:HOH:O	2.47	0.46
1:E:71:GLN:NE2	5:E:587:HOH:O	2.48	0.46
1:E:273:GLN:NE2	5:E:596:HOH:O	2.49	0.46
1:C:107:MET:CE	1:C:120:GLY:CA	2.95	0.45
1:B:68:LYS:NZ	1:B:136:GLU:OE2	2.51	0.44
1:E:69:TYR:OH	1:E:136:GLU:OE1	2.37	0.43
1:F:69:TYR:OH	1:F:136:GLU:OE1	2.37	0.42
1:E:75:ARG:NH1	5:E:539:HOH:O	2.51	0.42
1:E:42:GLN:NE2	5:E:578:HOH:O	2.53	0.42
1:D:158:ARG:NH1	1:D:319:LEU:O	2.53	0.42
1:D:107:MET:CE	1:D:120:GLY:N	2.84	0.41
1:B:305:ASP:OD2	1:B:309:ARG:NE	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	315/333 (95%)	306 (97%)	9 (3%)	0	100	100
1	B	316/333 (95%)	302 (96%)	14 (4%)	0	100	100
1	C	317/333 (95%)	302 (95%)	15 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	316/333 (95%)	302 (96%)	14 (4%)	0	100	100
1	E	329/333 (99%)	317 (96%)	11 (3%)	1 (0%)	50	60
1	F	315/333 (95%)	303 (96%)	11 (4%)	1 (0%)	50	60
All	All	1908/1998 (96%)	1832 (96%)	74 (4%)	2 (0%)	59	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	1	MET
1	F	4	GLU

### 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	264/278 (95%)	263 (100%)	1 (0%)	95	98
1	B	265/278 (95%)	261 (98%)	4 (2%)	76	89
1	C	266/278 (96%)	258 (97%)	8 (3%)	53	70
1	D	265/278 (95%)	258 (97%)	7 (3%)	59	76
1	E	278/278 (100%)	277 (100%)	1 (0%)	95	98
1	F	264/278 (95%)	262 (99%)	2 (1%)	89	96
All	All	1602/1668 (96%)	1579 (99%)	23 (1%)	78	90

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	PRO
1	B	10	LEU
1	B	80	GLN
1	B	142	CYS
1	B	183	ILE
1	C	10	LEU
1	C	11	ASP
1	C	27	ASP

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Mol	Chain	Res	Type
1	C	36	THR
1	C	42	GLN
1	C	49	ARG
1	C	214	ASP
1	C	267	ASP
1	D	11	ASP
1	D	27	ASP
1	D	28	LEU
1	D	34	THR
1	D	80	GLN
1	D	110	LEU
1	D	197	LEU
1	E	80	GLN
1	F	27	ASP
1	F	112	SER

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 chains in this entry.

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

6 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	SEB	A	165	1	16,16,17	5.87	3 (18%)	19,21,23	2.37	3 (15%)
1	SEB	B	165	1	16,16,17	5.70	3 (18%)	19,21,23	1.72	3 (15%)
1	SEB	C	165	1	16,16,17	5.31	3 (18%)	19,21,23	1.55	3 (15%)
1	SEB	D	165	1	16,16,17	4.72	3 (18%)	19,21,23	1.38	4 (21%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	SEB	E	165	1	16,16,17	5.09	3 (18%)	19,21,23	1.70	5 (26%)
1	SEB	F	165	1	16,16,17	5.45	3 (18%)	19,21,23	1.88	4 (21%)

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
1	SEB	A	165	1	-	0/11/13/15	0/1/1/1
1	SEB	B	165	1	-	0/11/13/15	0/1/1/1
1	SEB	C	165	1	-	0/11/13/15	0/1/1/1
1	SEB	D	165	1	-	0/11/13/15	0/1/1/1
1	SEB	E	165	1	-	0/11/13/15	0/1/1/1
1	SEB	F	165	1	-	0/11/13/15	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	SEB	O-C	20.16	1.25	1.11
1	B	165	SEB	O-C	19.23	1.24	1.11
1	E	165	SEB	O-C	18.11	1.23	1.11
1	F	165	SEB	O-C	17.27	1.23	1.11
1	C	165	SEB	O-C	16.55	1.22	1.11
1	D	165	SEB	O-C	16.45	1.22	1.11
1	F	165	SEB	CE-SD	-12.67	1.68	1.78
1	C	165	SEB	CE-SD	-12.53	1.68	1.78
1	B	165	SEB	CE-SD	-11.52	1.69	1.78
1	A	165	SEB	CE-SD	-10.67	1.70	1.78
1	E	165	SEB	CE-SD	-8.60	1.71	1.78
1	D	165	SEB	CE-SD	-8.31	1.71	1.78
1	A	165	SEB	CA-C	5.02	1.58	1.48
1	C	165	SEB	CA-C	4.20	1.56	1.48
1	B	165	SEB	CA-C	3.85	1.55	1.48
1	F	165	SEB	CA-C	3.56	1.55	1.48
1	D	165	SEB	CA-C	3.45	1.54	1.48
1	E	165	SEB	CA-C	2.62	1.53	1.48

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	SEB	CZ-CE-SD	6.95	120.08	112.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	SEB	OD1-SD-CE	5.93	114.82	107.36
1	F	165	SEB	CZ-CE-SD	5.10	118.06	112.52
1	B	165	SEB	CZ-CE-SD	4.86	117.80	112.52
1	C	165	SEB	CZ-CE-SD	4.48	117.39	112.52
1	E	165	SEB	CZ-CE-SD	4.33	117.23	112.52
1	B	165	SEB	OD1-SD-CE	3.96	112.35	107.36
1	F	165	SEB	OD1-SD-CE	3.96	112.34	107.36
1	F	165	SEB	OG-CB-CA	3.61	113.39	107.37
1	E	165	SEB	OG-CB-CA	3.47	113.16	107.37
1	B	165	SEB	OG-CB-CA	3.33	112.93	107.37
1	A	165	SEB	OG-CB-CA	3.29	112.86	107.37
1	D	165	SEB	C-CA-N	-2.79	111.05	113.83
1	F	165	SEB	OG-SD-CE	2.76	111.54	103.64
1	D	165	SEB	CZ-CE-SD	2.75	115.51	112.52
1	E	165	SEB	C-CA-N	-2.57	111.26	113.83
1	E	165	SEB	OD2-SD-CE	2.43	110.42	107.36
1	C	165	SEB	OG-CB-CA	2.40	111.37	107.37
1	D	165	SEB	OD2-SD-CE	2.13	110.04	107.36
1	E	165	SEB	OD1-SD-CE	2.11	110.02	107.36
1	C	165	SEB	OD1-SD-CE	2.08	109.98	107.36
1	D	165	SEB	CB-OG-SD	2.03	123.78	119.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

14 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	PGE	A	401	-	9,9,9	0.54	0	8,8,8	0.24	0
2	PGE	A	402	-	9,9,9	0.74	0	8,8,8	0.54	0
3	IMD	A	403	-	5,5,5	1.32	1 (20%)	5,5,5	0.20	0
2	PGE	B	401	-	9,9,9	0.50	0	8,8,8	0.40	0
3	IMD	B	402	-	5,5,5	1.44	1 (20%)	5,5,5	0.87	0
2	PGE	C	401	-	9,9,9	0.40	0	8,8,8	0.23	0
2	PGE	D	401	-	9,9,9	0.71	0	8,8,8	0.58	0
2	PGE	D	402	-	9,9,9	0.56	0	8,8,8	0.47	0
4	1PE	D	403	-	15,15,15	0.57	0	14,14,14	0.39	0
3	IMD	D	404	-	5,5,5	1.48	2 (40%)	5,5,5	0.19	0
3	IMD	D	405	-	5,5,5	1.85	2 (40%)	5,5,5	0.54	0
2	PGE	E	401	-	9,9,9	0.64	0	8,8,8	0.52	0
4	1PE	E	402	-	15,15,15	0.76	0	14,14,14	0.89	0
2	PGE	F	401	-	9,9,9	0.49	0	8,8,8	0.82	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	PGE	A	401	-	-	0/7/7/7	0/0/0/0
2	PGE	A	402	-	-	0/7/7/7	0/0/0/0
3	IMD	A	403	-	-	0/0/0/0	0/1/1/1
2	PGE	B	401	-	-	0/7/7/7	0/0/0/0
3	IMD	B	402	-	-	0/0/0/0	0/1/1/1
2	PGE	C	401	-	-	0/7/7/7	0/0/0/0
2	PGE	D	401	-	-	0/7/7/7	0/0/0/0
2	PGE	D	402	-	-	0/7/7/7	0/0/0/0
4	1PE	D	403	-	-	0/13/13/13	0/0/0/0
3	IMD	D	404	-	-	0/0/0/0	0/1/1/1
3	IMD	D	405	-	-	0/0/0/0	0/1/1/1
2	PGE	E	401	-	-	0/7/7/7	0/0/0/0
4	1PE	E	402	-	-	0/13/13/13	0/0/0/0
2	PGE	F	401	-	-	0/7/7/7	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	405	IMD	C2-N3	3.11	1.37	1.31
3	D	405	IMD	C2-N1	2.56	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	IMD	C2-N3	2.44	1.36	1.31
3	D	404	IMD	C2-N3	2.29	1.36	1.31
3	D	404	IMD	C2-N1	2.24	1.36	1.31
3	A	403	IMD	C2-N3	2.06	1.35	1.31

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	318/333 (95%)	0.42	34 (10%) 6 10	25, 39, 88, 113	0
1	B	318/333 (95%)	0.30	25 (7%) 13 19	27, 37, 74, 115	0
1	C	318/333 (95%)	0.78	58 (18%) 2 3	32, 53, 95, 134	0
1	D	318/333 (95%)	0.34	29 (9%) 9 15	24, 31, 83, 128	0
1	E	329/333 (98%)	0.21	25 (7%) 14 20	24, 32, 52, 107	0
1	F	318/333 (95%)	1.00	70 (22%) 1 2	33, 51, 122, 144	0
All	All	1919/1998 (96%)	0.51	241 (12%) 5 7	24, 39, 91, 144	0

All (241) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	PRO	11.4
1	F	30	PRO	9.4
1	F	3	PRO	9.2
1	B	33	ALA	9.0
1	C	3	PRO	8.6
1	C	34	THR	8.3
1	F	34	THR	7.9
1	C	29	PRO	7.7
1	F	28	LEU	7.6
1	F	26	PRO	7.3
1	D	26	PRO	7.1
1	F	12	LEU	7.1
1	C	33	ALA	6.8
1	F	33	ALA	6.7
1	F	27	ASP	6.7
1	A	34	THR	6.5
1	C	30	PRO	6.5
1	F	11	ASP	6.5
1	F	17	MET	6.3

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Mol	Chain	Res	Type	RSRZ
1	F	2	LYS	6.3
1	F	24	LEU	6.2
1	E	-9	HIS	6.1
1	E	26	PRO	6.0
1	B	34	THR	6.0
1	C	28	LEU	5.9
1	C	26	PRO	5.9
1	F	21	VAL	5.7
1	F	31	TRP	5.7
1	A	30	PRO	5.4
1	A	33	ALA	5.3
1	D	30	PRO	5.3
1	F	15	ALA	5.3
1	A	24	LEU	5.3
1	F	29	PRO	5.2
1	F	7	LEU	5.2
1	C	32	PRO	5.2
1	C	171	ALA	5.0
1	D	32	PRO	4.9
1	C	24	LEU	4.9
1	F	32	PRO	4.9
1	B	26	PRO	4.9
1	F	212	VAL	4.8
1	F	20	VAL	4.8
1	B	30	PRO	4.8
1	C	150	GLU	4.7
1	C	90	LEU	4.7
1	A	26	PRO	4.6
1	C	27	ASP	4.6
1	C	31	TRP	4.5
1	D	212	VAL	4.4
1	E	31	TRP	4.4
1	C	230	SER	4.4
1	B	32	PRO	4.4
1	B	31	TRP	4.4
1	D	31	TRP	4.3
1	F	8	PRO	4.2
1	C	147	GLN	4.2
1	A	15	ALA	4.2
1	D	4	GLU	4.2
1	F	25	GLN	4.1
1	A	32	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	19	THR	4.1
1	A	31	TRP	4.1
1	A	27	ASP	4.0
1	F	23	THR	4.0
1	F	37	ILE	4.0
1	E	-8	HIS	3.9
1	F	4	GLU	3.9
1	D	2	LYS	3.9
1	F	162	ALA	3.9
1	A	3	PRO	3.9
1	F	90	LEU	3.9
1	F	9	VAL	3.8
1	F	300	MET	3.8
1	D	90	LEU	3.8
1	A	28	LEU	3.8
1	F	171	ALA	3.7
1	E	24	LEU	3.7
1	F	22	ASN	3.7
1	C	151	ASP	3.7
1	C	4	GLU	3.6
1	C	170	LEU	3.6
1	D	5	ASN	3.6
1	D	163	GLY	3.5
1	B	15	ALA	3.5
1	E	33	ALA	3.5
1	B	4	GLU	3.5
1	C	37	ILE	3.5
1	A	12	LEU	3.4
1	A	29	PRO	3.4
1	F	5	ASN	3.4
1	F	299	ARG	3.3
1	D	171	ALA	3.3
1	D	162	ALA	3.3
1	E	162	ALA	3.3
1	F	168	ALA	3.3
1	B	171	ALA	3.2
1	F	182	GLN	3.2
1	A	9	VAL	3.2
1	C	192	LEU	3.2
1	A	182	GLN	3.2
1	A	4	GLU	3.2
1	D	24	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	29	PRO	3.2
1	F	298	SER	3.2
1	F	13	ILE	3.2
1	C	8	PRO	3.1
1	C	162	ALA	3.1
1	E	168	ALA	3.1
1	D	170	LEU	3.1
1	B	168	ALA	3.1
1	C	249	ARG	3.1
1	E	30	PRO	3.1
1	F	42	GLN	3.1
1	E	279	GLN	3.1
1	F	151	ASP	3.1
1	C	231	ASN	3.1
1	F	36	THR	3.1
1	F	170	LEU	3.0
1	F	193	LEU	3.0
1	A	162	ALA	3.0
1	C	193	LEU	3.0
1	C	88	PHE	3.0
1	E	166	ALA	3.0
1	B	27	ASP	3.0
1	C	172	LEU	3.0
1	C	11	ASP	3.0
1	E	32	PRO	2.9
1	F	18	LYS	2.9
1	E	15	ALA	2.9
1	C	167	GLY	2.9
1	A	249	ARG	2.9
1	A	168	ALA	2.9
1	B	24	LEU	2.9
1	E	170	LEU	2.9
1	F	39	GLU	2.9
1	A	11	ASP	2.9
1	D	192	LEU	2.9
1	D	249	ARG	2.9
1	C	36	THR	2.9
1	C	163	GLY	2.9
1	E	90	LEU	2.8
1	E	89	TYR	2.8
1	F	172	LEU	2.8
1	F	231	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	163	GLY	2.8
1	C	161	PHE	2.8
1	C	10	LEU	2.7
1	C	89	TYR	2.7
1	A	171	ALA	2.7
1	F	14	SER	2.7
1	C	233	ALA	2.7
1	F	89	TYR	2.7
1	D	89	TYR	2.7
1	A	36	THR	2.7
1	F	147	GLN	2.6
1	F	295	LEU	2.6
1	B	279	GLN	2.6
1	C	42	GLN	2.6
1	F	163	GLY	2.6
1	E	-2	ASP	2.6
1	F	166	ALA	2.6
1	D	27	ASP	2.6
1	B	90	LEU	2.6
1	C	71	GLN	2.6
1	B	184	ASP	2.6
1	E	171	ALA	2.6
1	C	12	LEU	2.5
1	B	3	PRO	2.5
1	F	50	PHE	2.5
1	B	29	PRO	2.5
1	F	6	LYS	2.5
1	C	215	GLY	2.5
1	D	193	LEU	2.5
1	C	82	ASP	2.5
1	C	211	GLY	2.4
1	F	150	GLU	2.4
1	A	22	ASN	2.4
1	C	168	ALA	2.4
1	C	39	GLU	2.4
1	A	167	GLY	2.4
1	E	28	LEU	2.4
1	B	162	ALA	2.4
1	F	161	PHE	2.4
1	A	82	ASP	2.4
1	B	166	ALA	2.4
1	D	11	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	10	LEU	2.4
1	F	167	GLY	2.4
1	A	23	THR	2.4
1	B	182	GLN	2.4
1	C	35	GLY	2.3
1	E	27	ASP	2.3
1	E	192	LEU	2.3
1	F	160	GLY	2.3
1	A	166	ALA	2.3
1	C	212	VAL	2.3
1	F	38	ALA	2.3
1	C	153	GLN	2.3
1	C	232	ASP	2.3
1	C	166	ALA	2.3
1	D	168	ALA	2.3
1	F	153	GLN	2.3
1	A	193	LEU	2.3
1	D	167	GLY	2.3
1	C	15	ALA	2.3
1	A	150	GLU	2.2
1	A	25	GLN	2.2
1	A	192	LEU	2.2
1	D	28	LEU	2.2
1	F	198	TYR	2.2
1	B	11	ASP	2.2
1	A	196	GLY	2.2
1	E	167	GLY	2.2
1	F	169	MET	2.2
1	F	49	ARG	2.2
1	F	144	TYR	2.2
1	E	150	GLU	2.1
1	C	46	LEU	2.1
1	C	169	MET	2.1
1	D	7	LEU	2.1
1	F	118	VAL	2.1
1	C	173	ALA	2.1
1	B	46	LEU	2.1
1	C	7	LEU	2.1
1	F	69	TYR	2.1
1	A	279	GLN	2.1
1	B	319	LEU	2.1
1	C	234	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	249	ARG	2.1
1	C	22	ASN	2.1
1	D	166	ALA	2.1
1	B	249	ARG	2.1
1	F	294	PHE	2.1
1	E	169	MET	2.0
1	A	16	GLU	2.0
1	D	194	TRP	2.0
1	C	138	ILE	2.0
1	C	191	VAL	2.0
1	D	153	GLN	2.0
1	B	39	GLU	2.0

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

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	SEB	C	165	16/17	0.15	-0.55	41,59,67,68	0
1	SEB	F	165	16/17	0.15	-0.59	39,54,64,64	0
1	SEB	E	165	16/17	0.14	-0.62	28,36,38,38	0
1	SEB	D	165	16/17	0.14	-0.75	26,32,35,35	0
1	SEB	A	165	16/17	0.14	-0.80	33,44,48,48	0
1	SEB	B	165	16/17	0.13	-0.85	33,43,48,49	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	IMD	A	403	5/5	0.21	7.35	85,88,91,93	0
3	IMD	D	404	5/5	0.25	4.74	62,63,64,65	0
2	PGE	D	402	10/10	0.18	2.31	40,43,55,56	0
2	PGE	F	401	10/10	0.28	2.15	47,57,73,75	0
4	1PE	E	402	16/16	0.16	1.65	48,71,86,87	0
2	PGE	A	402	10/10	0.18	1.50	53,61,64,65	0
2	PGE	D	401	10/10	0.18	0.90	44,46,64,64	0
2	PGE	A	401	10/10	0.20	0.75	55,61,77,78	0
2	PGE	E	401	10/10	0.18	0.75	34,42,56,58	0
2	PGE	B	401	10/10	0.19	0.59	42,53,73,76	0
2	PGE	C	401	10/10	0.16	0.29	44,53,66,70	0
4	1PE	D	403	16/16	0.14	0.13	48,61,64,64	0
3	IMD	B	402	5/5	0.11	-0.58	47,49,50,52	0
3	IMD	D	405	5/5	0.11	-1.32	43,45,48,48	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.