



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2016 – 12:10 AM EST

PDB ID : 5HZN  
Title : Structure of NVP-AEW541 in complex with IGF-1R kinase  
Authors : Cowan-Jacob, S.W.  
Deposited on : 2016-02-02  
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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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-20028442

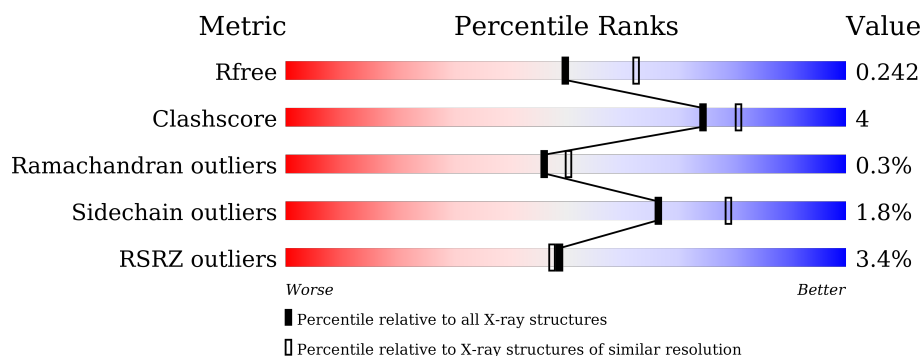
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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	304	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>88%</span> <span>9%</span> <span>.</span> </div> </div>
1	B	304	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>7%</span> <span>83%</span> <span>13%</span> <span>..</span> </div> </div>
1	C	304	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>6%</span> <span>87%</span> <span>10%</span> <span>..</span> </div> </div>
1	D	304	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>2%</span> <span>88%</span> <span>11%</span> <span>.</span> </div> </div>
1	E	304	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>87%</span> <span>10%</span> <span>.</span> </div> </div>
1	F	304	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>5%</span> <span>84%</span> <span>12%</span> <span>..</span> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	304	<div><div></div><div>5%</div><div>87%</div><div>10%</div><div>• •</div></div>
1	H	304	<div><div></div><div>89%</div><div>11%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19906 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 Insulin-like growth factor 1 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2359	1499	394	444	22			
1	B	296	Total	C	N	O	S	0	0	0
			2359	1499	394	444	22			
1	C	296	Total	C	N	O	S	0	0	0
			2359	1499	394	444	22			
1	D	304	Total	C	N	O	S	0	0	0
			2415	1534	404	454	23			
1	E	296	Total	C	N	O	S	0	0	0
			2359	1499	394	444	22			
1	F	296	Total	C	N	O	S	0	0	0
			2359	1499	394	444	22			
1	G	296	Total	C	N	O	S	0	0	0
			2359	1499	394	444	22			
1	H	303	Total	C	N	O	S	0	0	0
			2406	1528	402	453	23			

There are 16 discrepancies between the modelled and reference sequences:

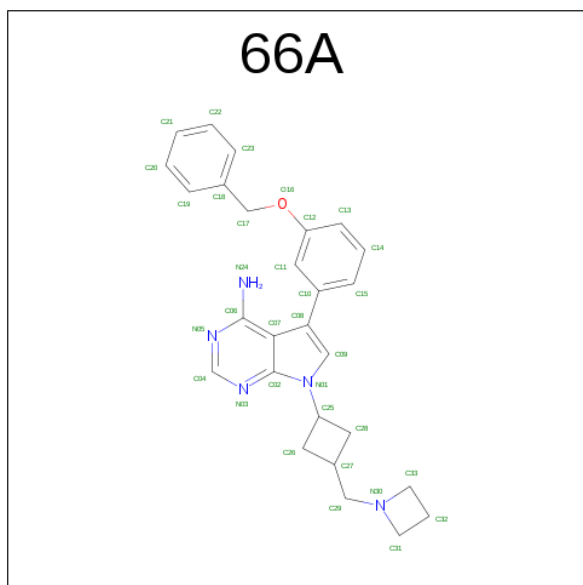
Chain	Residue	Modelled	Actual	Comment	Reference
A	1094	ALA	GLU	engineered mutation	UNP P08069
A	1096	ALA	GLU	engineered mutation	UNP P08069
B	1094	ALA	GLU	engineered mutation	UNP P08069
B	1096	ALA	GLU	engineered mutation	UNP P08069
C	1094	ALA	GLU	engineered mutation	UNP P08069
C	1096	ALA	GLU	engineered mutation	UNP P08069
D	1094	ALA	GLU	engineered mutation	UNP P08069
D	1096	ALA	GLU	engineered mutation	UNP P08069
E	1094	ALA	GLU	engineered mutation	UNP P08069
E	1096	ALA	GLU	engineered mutation	UNP P08069
F	1094	ALA	GLU	engineered mutation	UNP P08069
F	1096	ALA	GLU	engineered mutation	UNP P08069
G	1094	ALA	GLU	engineered mutation	UNP P08069

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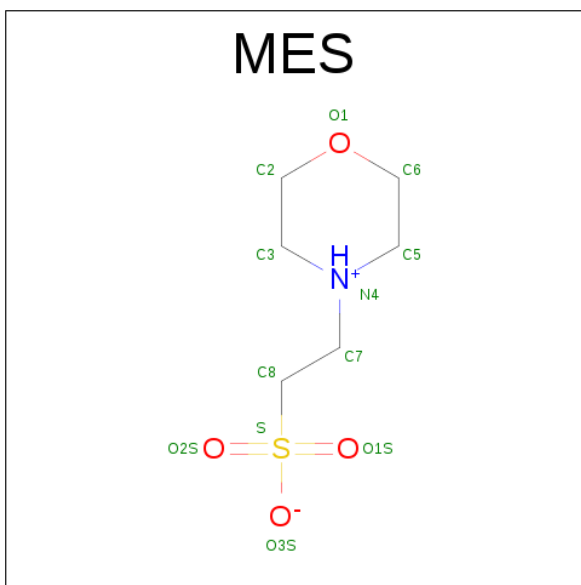
Chain	Residue	Modelled	Actual	Comment	Reference
G	1096	ALA	GLU	engineered mutation	UNP P08069
H	1094	ALA	GLU	engineered mutation	UNP P08069
H	1096	ALA	GLU	engineered mutation	UNP P08069

- Molecule 2 is 7-[cis-3-(azetidin-1-ylmethyl)cyclobutyl]-5-[3-(benzyloxy)phenyl]-7H-pyrrolo[2,3-d]pyrimidin-4-amine (three-letter code: 66A) (formula: C<sub>27</sub>H<sub>29</sub>N<sub>5</sub>O).



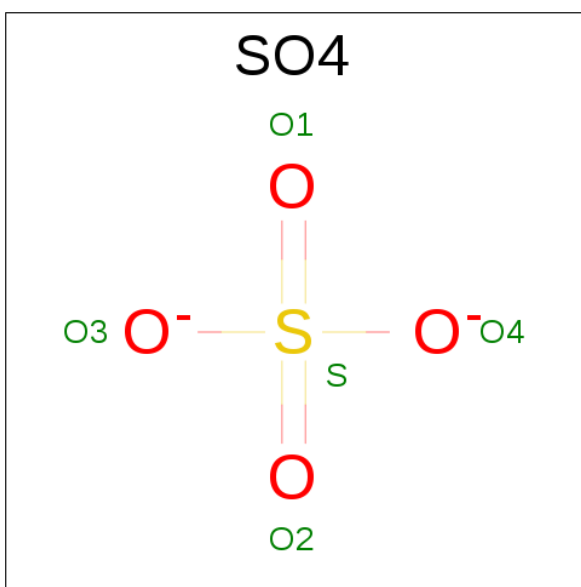
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	27	5	1		
2	B	1	Total	C	N	O	0	0
			33	27	5	1		
2	C	1	Total	C	N	O	0	0
			33	27	5	1		
2	D	1	Total	C	N	O	0	0
			33	27	5	1		
2	E	1	Total	C	N	O	0	0
			33	27	5	1		
2	F	1	Total	C	N	O	0	0
			33	27	5	1		
2	G	1	Total	C	N	O	0	0
			33	27	5	1		
2	H	1	Total	C	N	O	0	0
			33	27	5	1		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		

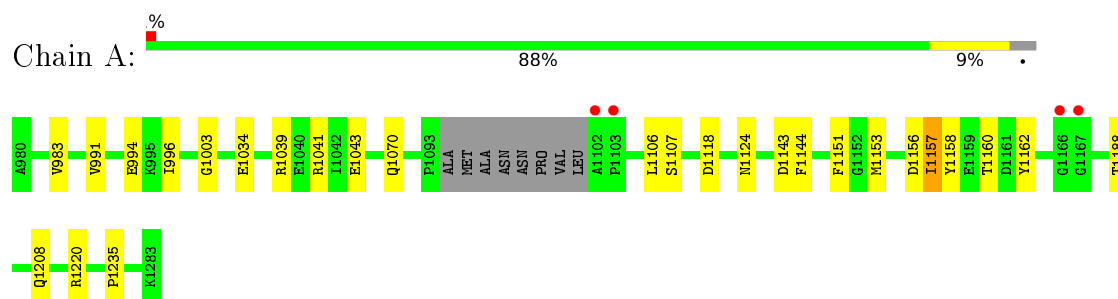
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	92	Total	O	0	0
			92	92		
5	B	42	Total	O	0	0
			42	42		
5	C	49	Total	O	0	0
			49	49		
5	D	92	Total	O	0	0
			92	92		
5	E	97	Total	O	0	0
			97	97		
5	F	43	Total	O	0	0
			43	43		
5	G	48	Total	O	0	0
			48	48		
5	H	88	Total	O	0	0
			88	88		

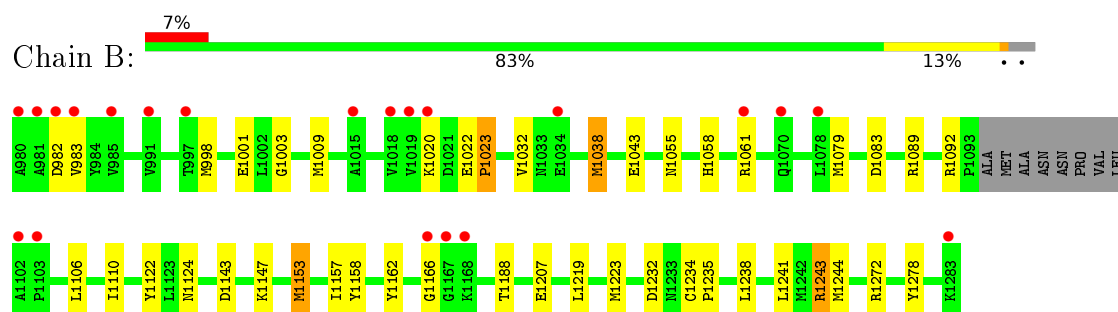
### 3 Residue-property plots [i](#)

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

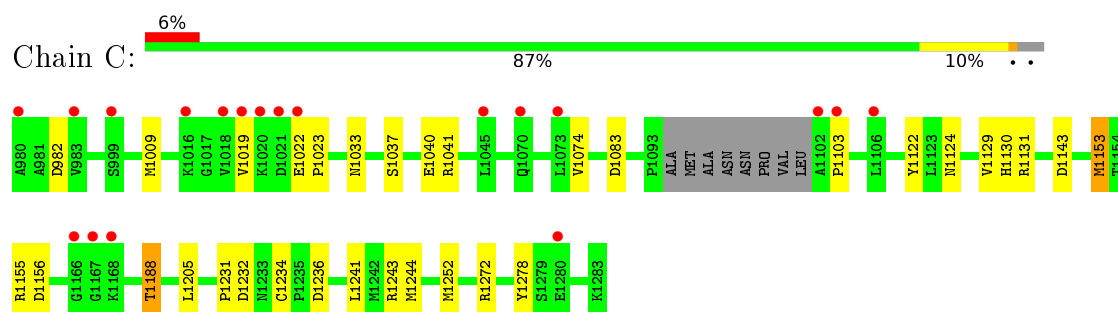
- Molecule 1: Insulin-like growth factor 1 receptor



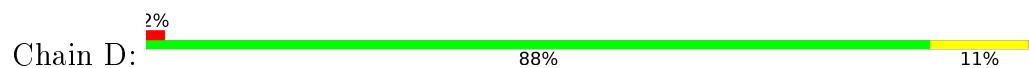
- Molecule 1: Insulin-like growth factor 1 receptor



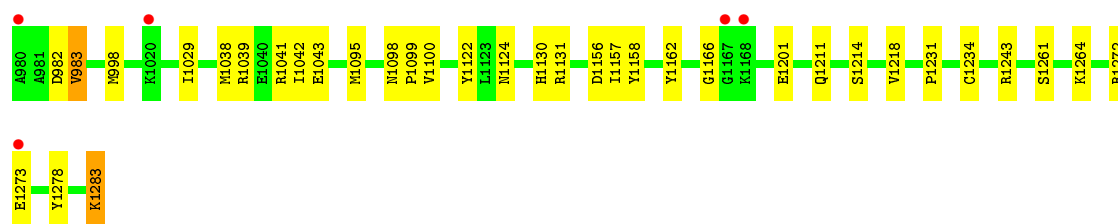
- Molecule 1: Insulin-like growth factor 1 receptor



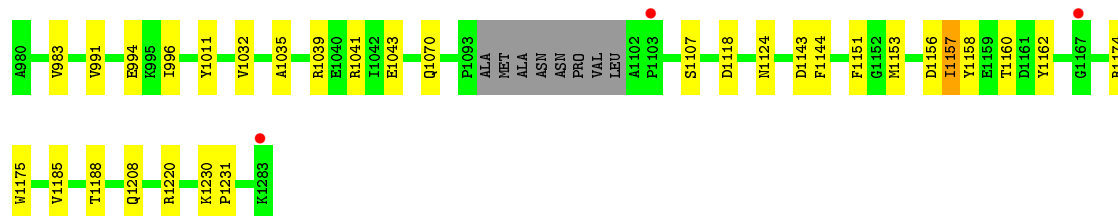
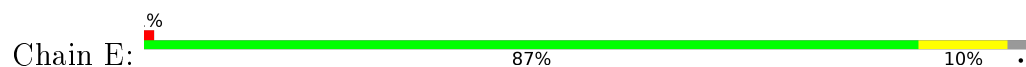
- Molecule 1: Insulin-like growth factor 1 receptor



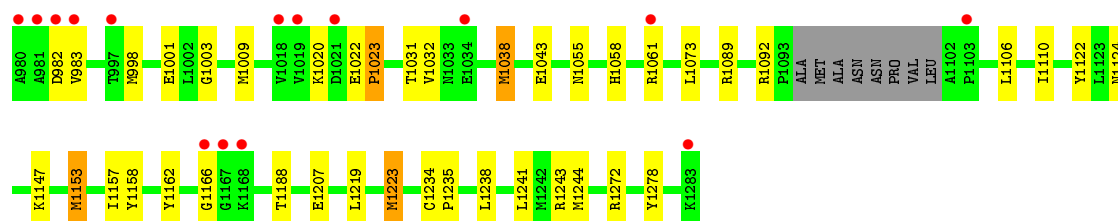
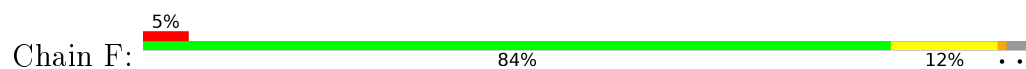




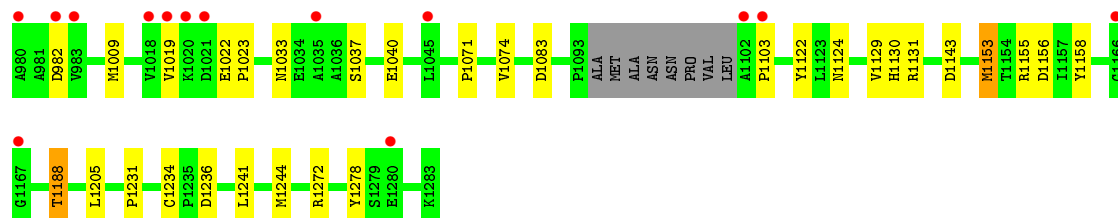
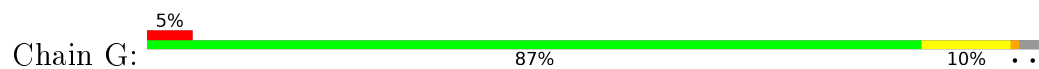
- Molecule 1: Insulin-like growth factor 1 receptor



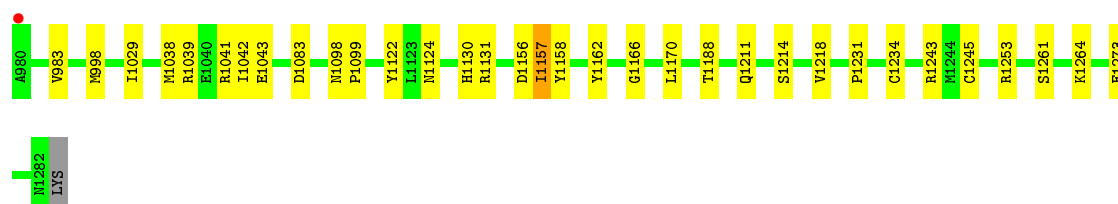
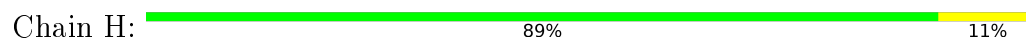
- Molecule 1: Insulin-like growth factor 1 receptor



- Molecule 1: Insulin-like growth factor 1 receptor



- Molecule 1: Insulin-like growth factor 1 receptor



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.44Å 190.04Å 155.49Å 90.00° 90.22° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 29.87 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.6 (30.00-2.20) 89.6 (29.87-2.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.194 , 0.218 0.221 , 0.242	Depositor DCC
$R_{free}$ test set	7400 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.0	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 25.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -1/2*h+1/2*k,3/2*h+1/2*k,-l 0.011 for -1/2*h-1/2*k,-3/2*h+1/2*k,-l 0.010 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.009 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.467 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	19906	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: SO4, MES, 66A

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	0.65	2/2409 (0.1%)	0.75	3/3250 (0.1%)
1	B	0.55	3/2409 (0.1%)	0.74	5/3250 (0.2%)
1	C	0.56	4/2409 (0.2%)	0.75	7/3250 (0.2%)
1	D	0.71	10/2467 (0.4%)	0.77	4/3332 (0.1%)
1	E	0.64	1/2409 (0.0%)	0.76	3/3250 (0.1%)
1	F	0.54	4/2409 (0.2%)	0.73	2/3250 (0.1%)
1	G	0.56	4/2409 (0.2%)	0.74	6/3250 (0.2%)
1	H	0.69	7/2458 (0.3%)	0.77	5/3321 (0.2%)
All	All	0.61	35/19379 (0.2%)	0.75	35/26153 (0.1%)

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1243	ARG	CZ-NH1	8.16	1.43	1.33
1	C	1122	TYR	CE1-CZ	-7.29	1.29	1.38
1	G	1122	TYR	CE2-CZ	-7.22	1.29	1.38
1	B	1122	TYR	CE1-CZ	-6.54	1.30	1.38
1	D	1162	TYR	CE1-CZ	-6.39	1.30	1.38
1	G	1122	TYR	CE1-CZ	-6.25	1.30	1.38
1	H	1122	TYR	CE1-CZ	-6.17	1.30	1.38
1	G	1122	TYR	CG-CD2	-6.02	1.31	1.39
1	F	1122	TYR	CE1-CZ	-6.02	1.30	1.38
1	C	1122	TYR	CG-CD1	-6.01	1.31	1.39
1	C	1122	TYR	CE2-CZ	-5.96	1.30	1.38
1	B	1122	TYR	CE2-CZ	-5.79	1.31	1.38
1	H	1162	TYR	CE2-CZ	-5.74	1.31	1.38
1	F	1223	MET	SD-CE	-5.68	1.46	1.77
1	D	1162	TYR	CG-CD2	-5.63	1.31	1.39
1	D	1201	GLU	CD-OE2	-5.63	1.19	1.25
1	H	1122	TYR	CE2-CZ	-5.60	1.31	1.38
1	F	1122	TYR	CE2-CZ	-5.55	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1122	TYR	CE1-CZ	-5.51	1.31	1.38
1	D	1122	TYR	CE2-CZ	-5.48	1.31	1.38
1	D	1162	TYR	CE2-CZ	-5.47	1.31	1.38
1	A	1151	PHE	CE1-CZ	-5.46	1.26	1.37
1	H	1162	TYR	CG-CD1	-5.40	1.32	1.39
1	H	1162	TYR	CE1-CZ	-5.33	1.31	1.38
1	B	1122	TYR	CG-CD2	-5.32	1.32	1.39
1	H	1162	TYR	CG-CD2	-5.31	1.32	1.39
1	D	1162	TYR	CG-CD1	-5.30	1.32	1.39
1	F	1122	TYR	CG-CD2	-5.19	1.32	1.39
1	D	1201	GLU	CD-OE1	-5.16	1.20	1.25
1	D	1039	ARG	CZ-NH1	-5.09	1.26	1.33
1	E	1151	PHE	CE1-CZ	-5.07	1.27	1.37
1	G	1122	TYR	CG-CD1	-5.04	1.32	1.39
1	H	1039	ARG	CZ-NH1	-5.04	1.26	1.33
1	C	1122	TYR	CG-CD2	-5.04	1.32	1.39
1	A	1151	PHE	CG-CD2	-5.01	1.31	1.38

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1083	ASP	CB-CG-OD2	10.48	127.73	118.30
1	C	1083	ASP	CB-CG-OD2	9.90	127.21	118.30
1	B	1243	ARG	NE-CZ-NH2	9.44	125.02	120.30
1	F	1243	ARG	NE-CZ-NH2	8.83	124.72	120.30
1	D	1039	ARG	NE-CZ-NH2	8.64	124.62	120.30
1	G	1083	ASP	OD1-CG-OD2	-6.88	110.24	123.30
1	C	1083	ASP	OD1-CG-OD2	-6.67	110.62	123.30
1	H	1243	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	H	1039	ARG	NE-CZ-NH2	6.41	123.50	120.30
1	H	1243	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	H	1156	ASP	CB-CG-OD2	5.80	123.52	118.30
1	D	1156	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	1156	ASP	CB-CG-OD2	5.60	123.34	118.30
1	D	982	ASP	CB-CG-OD2	5.52	123.27	118.30
1	G	1156	ASP	CB-CG-OD2	5.49	123.24	118.30
1	E	1156	ASP	CB-CG-OD2	5.49	123.24	118.30
1	D	1201	GLU	OE1-CD-OE2	-5.48	116.72	123.30
1	E	1118	ASP	CB-CG-OD2	5.47	123.23	118.30
1	G	1236	ASP	CB-CG-OD2	5.42	123.18	118.30
1	C	1143	ASP	CB-CG-OD2	5.38	123.14	118.30
1	C	982	ASP	CB-CG-OD2	5.33	123.10	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1236	ASP	CB-CG-OD2	5.28	123.05	118.30
1	C	1232	ASP	CB-CG-OD2	5.24	123.02	118.30
1	F	982	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	1143	ASP	CB-CG-OD2	5.22	123.00	118.30
1	C	1156	ASP	CB-CG-OD2	5.22	123.00	118.30
1	G	982	ASP	CB-CG-OD2	5.18	122.97	118.30
1	G	1143	ASP	CB-CG-OD2	5.18	122.96	118.30
1	E	1220	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	H	1083	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	1220	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	1118	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	982	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	1232	ASP	CB-CG-OD2	5.02	122.82	118.30
1	B	1083	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2359	0	2318	15	0
1	B	2359	0	2318	31	0
1	C	2359	0	2318	17	0
1	D	2415	0	2377	19	0
1	E	2359	0	2318	17	0
1	F	2359	0	2318	32	0
1	G	2359	0	2318	15	0
1	H	2406	0	2364	17	0
2	A	33	0	0	0	0
2	B	33	0	0	0	0
2	C	33	0	0	0	0
2	D	33	0	0	0	0
2	E	33	0	0	0	0
2	F	33	0	0	0	0
2	G	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	33	0	0	0	0
3	A	12	0	12	0	0
3	B	12	0	12	0	0
3	C	12	0	12	1	0
3	D	12	0	12	0	0
3	E	12	0	12	0	0
3	F	12	0	12	0	0
3	G	12	0	12	1	0
3	H	12	0	12	0	0
4	A	5	0	0	0	0
4	C	5	0	0	0	0
4	E	5	0	0	0	0
4	G	5	0	0	0	0
5	A	92	0	0	1	0
5	B	42	0	0	0	0
5	C	49	0	0	3	0
5	D	92	0	0	1	0
5	E	97	0	0	1	0
5	F	43	0	0	1	0
5	G	48	0	0	2	0
5	H	88	0	0	1	0
All	All	19906	0	18745	153	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 (153) 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:G:1124:ASN:OD1	1:G:1188:THR:HB	1.60	1.01
1:C:1124:ASN:OD1	1:C:1188:THR:HB	1.71	0.91
1:B:1003:GLY:H	1:B:1009:MET:HE3	1.41	0.85
1:F:1003:GLY:H	1:F:1009:MET:HE3	1.43	0.84
1:F:1219:LEU:HD21	1:F:1223:MET:HE1	1.64	0.80
1:F:1124:ASN:OD1	1:F:1188:THR:OG1	2.04	0.76
1:B:1272:ARG:HH11	1:B:1272:ARG:HG2	1.54	0.72
1:B:1219:LEU:HD21	1:B:1223:MET:HE3	1.72	0.72
1:B:1124:ASN:OD1	1:B:1188:THR:OG1	2.11	0.69
1:F:1272:ARG:HG2	1:F:1272:ARG:HH11	1.57	0.69
1:F:1219:LEU:CD2	1:F:1223:MET:HE1	2.23	0.68
1:B:1003:GLY:H	1:B:1009:MET:CE	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1001:GLU:HB3	1:F:1009:MET:HE2	1.76	0.67
1:B:1001:GLU:HB3	1:B:1009:MET:HE2	1.76	0.67
1:C:1037:SER:OG	1:C:1040:GLU:HG3	1.95	0.67
1:F:1003:GLY:H	1:F:1009:MET:CE	2.09	0.65
1:G:1037:SER:OG	1:G:1040:GLU:HG3	1.97	0.65
1:B:1038:MET:SD	1:C:1009:MET:HB2	2.41	0.61
1:H:1124:ASN:HB3	5:H:1477:HOH:O	1.99	0.60
1:F:1055:ASN:OD1	1:F:1061:ARG:NH1	2.34	0.60
1:E:1124:ASN:OD1	1:E:1188:THR:HB	2.01	0.60
1:B:1219:LEU:CD2	1:B:1223:MET:CE	2.79	0.60
1:F:1038:MET:HG3	5:F:1440:HOH:O	2.03	0.59
1:C:1103:PRO:HB3	1:C:1205:LEU:HD11	1.84	0.59
1:A:1124:ASN:OD1	1:A:1188:THR:HB	2.03	0.59
1:F:1153:MET:HA	1:F:1153:MET:HE3	1.84	0.59
1:G:1188:THR:HG23	5:G:1441:HOH:O	2.01	0.58
1:B:1219:LEU:HD21	1:B:1223:MET:CE	2.33	0.58
1:F:1219:LEU:CD2	1:F:1223:MET:CE	2.81	0.58
1:B:1055:ASN:OD1	1:B:1061:ARG:NH1	2.37	0.57
1:E:1043:GLU:OE1	1:E:1157:ILE:HG22	2.04	0.57
1:A:1043:GLU:OE1	1:A:1157:ILE:HG22	2.04	0.57
1:D:1100:VAL:HA	1:E:1035:ALA:HB2	1.85	0.57
1:G:1103:PRO:HB3	1:G:1205:LEU:HD11	1.88	0.56
1:H:1043:GLU:CD	1:H:1157:ILE:HG22	2.26	0.56
1:D:1043:GLU:CD	1:D:1157:ILE:HG22	2.26	0.55
1:H:998:MET:HG2	1:H:1029:ILE:HD13	1.88	0.55
1:A:994:GLU:H	1:A:994:GLU:CD	2.08	0.55
1:F:1038:MET:SD	1:G:1009:MET:HB2	2.47	0.55
1:F:1241:LEU:HD12	1:F:1244:MET:HE3	1.89	0.55
1:E:994:GLU:H	1:E:994:GLU:CD	2.08	0.55
1:F:1043:GLU:HG2	1:F:1157:ILE:HG22	1.88	0.55
1:F:1092:ARG:HH22	1:F:1207:GLU:CD	2.10	0.54
1:C:1188:THR:HG23	5:C:1442:HOH:O	2.07	0.54
1:B:1241:LEU:HD12	1:B:1244:MET:HE3	1.89	0.54
1:B:1092:ARG:HH22	1:B:1207:GLU:CD	2.11	0.54
1:D:998:MET:HG2	1:D:1029:ILE:HD13	1.89	0.54
1:B:1219:LEU:CD2	1:B:1223:MET:HE3	2.37	0.53
1:F:1219:LEU:HD21	1:F:1223:MET:CE	2.36	0.53
1:E:991:VAL:HG11	1:E:996:ILE:HD11	1.91	0.53
1:F:1235:PRO:HG2	1:F:1238:LEU:HD12	1.91	0.52
1:B:1272:ARG:NH1	1:B:1278:TYR:CE1	2.77	0.52
1:B:1043:GLU:HG2	1:B:1157:ILE:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1003:GLY:N	1:B:1009:MET:CE	2.72	0.52
1:B:1235:PRO:HG2	1:B:1238:LEU:HD12	1.92	0.51
1:A:1153:MET:HE1	1:D:1158:TYR:CE1	2.45	0.51
1:E:1158:TYR:HB3	1:E:1162:TYR:HB2	1.93	0.51
1:F:1272:ARG:NH1	1:F:1278:TYR:CE1	2.78	0.51
1:F:1003:GLY:N	1:F:1009:MET:CE	2.73	0.51
1:H:1130:HIS:O	1:H:1131:ARG:HB2	2.11	0.51
1:E:991:VAL:CG1	1:E:996:ILE:HD11	2.42	0.50
1:C:1153:MET:CE	3:C:1302:MES:H52	2.40	0.49
1:B:1003:GLY:N	1:B:1009:MET:HE3	2.19	0.49
1:B:1272:ARG:NH1	1:B:1272:ARG:HG2	2.26	0.49
1:E:1043:GLU:CD	1:E:1157:ILE:HG22	2.33	0.49
1:F:1106:LEU:HG	1:F:1110:ILE:HD11	1.93	0.49
1:A:983:VAL:HG11	1:B:1001:GLU:HB3	1.94	0.49
1:C:1252:MET:HG3	5:C:1438:HOH:O	2.13	0.49
1:C:1272:ARG:HA	1:C:1278:TYR:CD2	2.48	0.49
1:A:991:VAL:HG11	1:A:996:ILE:HD11	1.95	0.49
1:F:1003:GLY:N	1:F:1009:MET:HE3	2.21	0.49
1:H:1231:PRO:HB2	1:H:1234:CYS:HB2	1.95	0.48
1:H:1038:MET:HE2	1:H:1042:ILE:HD11	1.94	0.48
1:D:1130:HIS:O	1:D:1131:ARG:HB2	2.13	0.48
1:D:1038:MET:HE2	1:D:1042:ILE:HD11	1.94	0.48
1:B:1106:LEU:HG	1:B:1110:ILE:HD11	1.94	0.48
1:F:1158:TYR:HB3	1:F:1162:TYR:HB2	1.95	0.48
1:B:1153:MET:HE3	1:B:1153:MET:HA	1.96	0.47
1:F:1272:ARG:HG2	1:F:1272:ARG:NH1	2.29	0.47
1:H:1038:MET:HE1	1:H:1041:ARG:NH1	2.28	0.47
1:D:1214:SER:O	1:D:1218:VAL:HG23	2.15	0.47
1:B:1158:TYR:HB3	1:B:1162:TYR:HB2	1.96	0.47
1:G:1019:VAL:HB	1:G:1022:GLU:HB3	1.95	0.47
1:G:1272:ARG:HA	1:G:1278:TYR:CD2	2.50	0.47
1:A:1158:TYR:HB3	1:A:1162:TYR:HB2	1.97	0.47
1:H:1214:SER:O	1:H:1218:VAL:HG23	2.15	0.47
1:C:1019:VAL:HB	1:C:1022:GLU:HB3	1.96	0.46
1:F:1058:HIS:HA	1:F:1147:LYS:HG2	1.97	0.46
1:E:1041:ARG:HE	1:E:1070:GLN:HE22	1.64	0.46
1:A:1043:GLU:CD	1:A:1157:ILE:HG22	2.36	0.46
1:F:1272:ARG:HA	1:F:1278:TYR:CD2	2.51	0.46
1:G:1153:MET:CE	3:G:1302:MES:H52	2.45	0.46
1:H:1273:GLU:OE1	1:H:1273:GLU:HA	2.16	0.46
1:A:991:VAL:CG1	1:A:996:ILE:HD11	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:983:VAL:HG11	1:F:1001:GLU:HB3	1.97	0.45
1:H:1038:MET:CE	1:H:1041:ARG:HH11	2.29	0.45
1:G:1188:THR:CG2	5:G:1441:HOH:O	2.63	0.45
1:A:1034:GLU:HG3	5:A:1429:HOH:O	2.17	0.45
1:G:1130:HIS:O	1:G:1131:ARG:HB2	2.17	0.45
1:A:1041:ARG:HE	1:A:1070:GLN:HE22	1.65	0.45
1:B:1272:ARG:HA	1:B:1278:TYR:CD2	2.52	0.45
1:C:1033:ASN:HD22	1:C:1033:ASN:H	1.64	0.45
1:B:1001:GLU:CB	1:B:1009:MET:HE2	2.43	0.45
1:D:1273:GLU:HA	1:D:1273:GLU:OE1	2.17	0.45
1:E:1143:ASP:O	1:E:1144:PHE:HB2	2.17	0.45
1:F:1001:GLU:CB	1:F:1009:MET:HE2	2.44	0.45
1:D:1231:PRO:HB2	1:D:1234:CYS:HB2	2.00	0.44
1:C:1241:LEU:HD23	1:C:1244:MET:CE	2.46	0.44
1:D:1124:ASN:HB3	5:D:1482:HOH:O	2.17	0.44
1:C:1129:VAL:O	1:C:1155:ARG:NH2	2.49	0.44
1:D:1038:MET:HE3	1:D:1041:ARG:HH11	1.83	0.44
1:B:1241:LEU:HD12	1:B:1244:MET:CE	2.47	0.44
1:E:1039:ARG:HD3	1:E:1157:ILE:HD11	1.99	0.44
1:G:1241:LEU:HD23	1:G:1244:MET:CE	2.47	0.44
1:D:1038:MET:CE	1:D:1041:ARG:HH11	2.32	0.43
1:E:1153:MET:HE1	1:H:1158:TYR:CE1	2.52	0.43
1:B:1058:HIS:HA	1:B:1147:LYS:HG2	2.00	0.43
1:G:1033:ASN:H	1:G:1033:ASN:HD22	1.66	0.43
1:A:1003:GLY:HA2	1:D:983:VAL:HG13	1.99	0.43
1:A:1039:ARG:HD3	1:A:1157:ILE:HD11	1.99	0.43
1:C:1041:ARG:NH1	5:C:1401:HOH:O	2.35	0.43
1:H:1098:ASN:HA	1:H:1099:PRO:HD3	1.86	0.43
1:H:1157:ILE:HG13	1:H:1158:TYR:CD2	2.53	0.43
1:D:1157:ILE:HG13	1:D:1158:TYR:CD2	2.54	0.42
1:E:1174:ARG:HB2	1:E:1175:TRP:CZ3	2.55	0.42
1:C:1244:MET:HE2	1:C:1244:MET:HB2	1.88	0.42
1:F:1241:LEU:HD12	1:F:1244:MET:CE	2.48	0.42
1:B:1106:LEU:HG	1:B:1110:ILE:CD1	2.49	0.42
1:F:1022:GLU:HA	1:F:1023:PRO:HD3	1.87	0.42
1:G:1231:PRO:HB2	1:G:1234:CYS:HB2	2.02	0.42
1:C:1130:HIS:O	1:C:1131:ARG:HB2	2.20	0.42
1:C:1231:PRO:HB2	1:C:1234:CYS:HB2	2.02	0.42
1:B:1234:CYS:HA	1:B:1235:PRO:HD2	1.82	0.42
1:C:1124:ASN:CG	1:C:1188:THR:HB	2.39	0.42
1:E:1032:VAL:HG21	5:E:1426:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1230:LYS:HA	1:E:1231:PRO:HD3	1.96	0.41
1:F:1106:LEU:HG	1:F:1110:ILE:CD1	2.49	0.41
1:D:1095:MET:HG3	1:E:1011:TYR:CE1	2.54	0.41
1:B:1022:GLU:HA	1:B:1023:PRO:HD3	1.87	0.41
1:A:1143:ASP:O	1:A:1144:PHE:HB2	2.20	0.41
1:D:1098:ASN:HA	1:D:1099:PRO:HD3	1.88	0.41
1:D:1283:LYS:HB3	1:D:1283:LYS:HE3	1.83	0.41
1:B:1079:MET:CE	1:B:1147:LYS:HD2	2.50	0.41
1:D:1272:ARG:HA	1:D:1278:TYR:CD2	2.56	0.41
1:G:1158:TYR:CD2	1:H:1170:LEU:HD21	2.56	0.41
1:D:1261:SER:HA	1:D:1264:LYS:HD3	2.02	0.41
1:H:1245:CYS:O	1:H:1253:ARG:HD3	2.21	0.41
1:H:1261:SER:HA	1:H:1264:LYS:HD3	2.02	0.41
1:G:1129:VAL:O	1:G:1155:ARG:NH2	2.53	0.41
1:H:1124:ASN:OD1	1:H:1188:THR:HB	2.20	0.41
1:A:1106:LEU:HD13	1:A:1235:PRO:HG2	2.02	0.40
1:F:1031:THR:HG22	1:F:1073:LEU:CD2	2.51	0.40
1:F:1234:CYS:HA	1:F:1235:PRO:HD2	1.81	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	292/304 (96%)	281 (96%)	11 (4%)	0	100	100
1	B	292/304 (96%)	280 (96%)	10 (3%)	2 (1%)	26	25
1	C	292/304 (96%)	277 (95%)	14 (5%)	1 (0%)	46	50
1	D	302/304 (99%)	294 (97%)	7 (2%)	1 (0%)	46	50
1	E	292/304 (96%)	282 (97%)	10 (3%)	0	100	100
1	F	292/304 (96%)	279 (96%)	11 (4%)	2 (1%)	26	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	292/304 (96%)	276 (94%)	15 (5%)	1 (0%)	46	50
1	H	301/304 (99%)	293 (97%)	7 (2%)	1 (0%)	46	50
All	All	2355/2432 (97%)	2262 (96%)	85 (4%)	8 (0%)	46	50

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1023	PRO
1	F	1023	PRO
1	C	1023	PRO
1	G	1023	PRO
1	D	1166	GLY
1	H	1166	GLY
1	B	1166	GLY
1	F	1166	GLY

### 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	256/263 (97%)	252 (98%)	4 (2%)	70	82
1	B	256/263 (97%)	248 (97%)	8 (3%)	47	59
1	C	256/263 (97%)	252 (98%)	4 (2%)	70	82
1	D	262/263 (100%)	259 (99%)	3 (1%)	80	89
1	E	256/263 (97%)	251 (98%)	5 (2%)	63	76
1	F	256/263 (97%)	249 (97%)	7 (3%)	52	64
1	G	256/263 (97%)	252 (98%)	4 (2%)	70	82
1	H	261/263 (99%)	258 (99%)	3 (1%)	80	89
All	All	2059/2104 (98%)	2021 (98%)	38 (2%)	66	79

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1107	SER
1	A	1157	ILE
1	A	1160	THR
1	A	1208	GLN
1	B	983	VAL
1	B	998	MET
1	B	1020	LYS
1	B	1032	VAL
1	B	1038	MET
1	B	1089	ARG
1	B	1153	MET
1	B	1243	ARG
1	C	1074	VAL
1	C	1153	MET
1	C	1188	THR
1	C	1243	ARG
1	D	983	VAL
1	D	1211	GLN
1	D	1283	LYS
1	E	1107	SER
1	E	1157	ILE
1	E	1160	THR
1	E	1185	VAL
1	E	1208	GLN
1	F	983	VAL
1	F	998	MET
1	F	1020	LYS
1	F	1032	VAL
1	F	1038	MET
1	F	1089	ARG
1	F	1153	MET
1	G	1071	PRO
1	G	1074	VAL
1	G	1153	MET
1	G	1188	THR
1	H	983	VAL
1	H	1157	ILE
1	H	1211	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1046	ASN

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Mol	Chain	Res	Type
1	B	1046	ASN
1	C	1033	ASN
1	C	1046	ASN
1	E	1046	ASN
1	F	1046	ASN
1	G	1033	ASN
1	G	1046	ASN
1	H	1068	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

20 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	66A	A	1301	-	32,38,38	1.67	3 (9%)	35,54,54	2.46	8 (22%)
3	MES	A	1302	-	12,12,12	1.76	1 (8%)	15,16,16	2.47	5 (33%)
4	SO4	A	1303	-	4,4,4	0.19	0	6,6,6	0.14	0
2	66A	B	1301	-	32,38,38	1.71	3 (9%)	35,54,54	2.13	4 (11%)
3	MES	B	1302	-	12,12,12	1.96	1 (8%)	15,16,16	2.50	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	66A	C	1301	-	32,38,38	1.79	3 (9%)	35,54,54	2.33	4 (11%)
3	MES	C	1302	-	12,12,12	1.86	1 (8%)	15,16,16	2.78	5 (33%)
4	SO4	C	1303	-	4,4,4	0.13	0	6,6,6	0.27	0
2	66A	D	1301	-	32,38,38	1.80	3 (9%)	35,54,54	2.23	7 (20%)
3	MES	D	1302	-	12,12,12	1.65	1 (8%)	15,16,16	2.46	4 (26%)
2	66A	E	1301	-	32,38,38	1.62	3 (9%)	35,54,54	2.39	9 (25%)
3	MES	E	1302	-	12,12,12	1.74	1 (8%)	15,16,16	2.95	6 (40%)
4	SO4	E	1303	-	4,4,4	0.20	0	6,6,6	0.15	0
2	66A	F	1301	-	32,38,38	1.71	4 (12%)	35,54,54	2.04	4 (11%)
3	MES	F	1302	-	12,12,12	1.91	1 (8%)	15,16,16	2.82	5 (33%)
2	66A	G	1301	-	32,38,38	1.80	3 (9%)	35,54,54	2.36	5 (14%)
3	MES	G	1302	-	12,12,12	1.89	1 (8%)	15,16,16	2.82	5 (33%)
4	SO4	G	1303	-	4,4,4	0.13	0	6,6,6	0.31	0
2	66A	H	1301	-	32,38,38	1.82	3 (9%)	35,54,54	2.15	4 (11%)
3	MES	H	1302	-	12,12,12	1.76	1 (8%)	15,16,16	3.04	5 (33%)

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	66A	A	1301	-	-	0/11/31/31	0/6/6/6
3	MES	A	1302	-	-	0/6/14/14	0/1/1/1
4	SO4	A	1303	-	-	0/0/0/0	0/0/0/0
2	66A	B	1301	-	-	0/11/31/31	0/6/6/6
3	MES	B	1302	-	-	0/6/14/14	0/1/1/1
2	66A	C	1301	-	-	0/11/31/31	0/6/6/6
3	MES	C	1302	-	-	0/6/14/14	0/1/1/1
4	SO4	C	1303	-	-	0/0/0/0	0/0/0/0
2	66A	D	1301	-	-	0/11/31/31	0/6/6/6
3	MES	D	1302	-	-	0/6/14/14	0/1/1/1
2	66A	E	1301	-	-	0/11/31/31	0/6/6/6
3	MES	E	1302	-	-	0/6/14/14	0/1/1/1
4	SO4	E	1303	-	-	0/0/0/0	0/0/0/0
2	66A	F	1301	-	-	0/11/31/31	0/6/6/6
3	MES	F	1302	-	-	0/6/14/14	0/1/1/1
2	66A	G	1301	-	-	0/11/31/31	0/6/6/6
3	MES	G	1302	-	-	0/6/14/14	0/1/1/1
4	SO4	G	1303	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	66A	H	1301	-	-	0/11/31/31	0/6/6/6
3	MES	H	1302	-	-	0/6/14/14	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1302	MES	C8-S	-6.46	1.67	1.77
3	F	1302	MES	C8-S	-6.22	1.68	1.77
3	G	1302	MES	C8-S	-6.13	1.68	1.77
3	C	1302	MES	C8-S	-6.02	1.68	1.77
3	A	1302	MES	C8-S	-5.52	1.69	1.77
3	E	1302	MES	C8-S	-5.50	1.69	1.77
3	H	1302	MES	C8-S	-5.47	1.69	1.77
3	D	1302	MES	C8-S	-5.11	1.69	1.77
2	B	1301	66A	C07-C02	-4.82	1.30	1.43
2	F	1301	66A	C07-C02	-4.80	1.30	1.43
2	G	1301	66A	C07-C02	-4.63	1.30	1.43
2	D	1301	66A	C07-C02	-4.62	1.30	1.43
2	H	1301	66A	C07-C02	-4.60	1.30	1.43
2	E	1301	66A	C07-C02	-4.56	1.30	1.43
2	A	1301	66A	C07-C02	-4.55	1.30	1.43
2	C	1301	66A	C07-C02	-4.53	1.31	1.43
2	F	1301	66A	C04-N03	2.08	1.35	1.32
2	H	1301	66A	C08-C07	3.60	1.47	1.41
2	D	1301	66A	C08-C07	3.72	1.47	1.41
2	B	1301	66A	C08-C07	4.09	1.48	1.41
2	F	1301	66A	C08-C07	4.09	1.48	1.41
2	C	1301	66A	C08-C07	4.62	1.48	1.41
2	G	1301	66A	C08-C07	4.64	1.48	1.41
2	E	1301	66A	C08-C07	4.67	1.49	1.41
2	A	1301	66A	C08-C07	5.08	1.49	1.41
2	E	1301	66A	C02-N03	5.64	1.43	1.35
2	A	1301	66A	C02-N03	5.81	1.44	1.35
2	F	1301	66A	C02-N03	6.42	1.45	1.35
2	B	1301	66A	C02-N03	6.49	1.45	1.35
2	C	1301	66A	C02-N03	6.93	1.45	1.35
2	G	1301	66A	C02-N03	6.98	1.45	1.35
2	D	1301	66A	C02-N03	7.43	1.46	1.35
2	H	1301	66A	C02-N03	7.51	1.46	1.35

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1301	66A	N03-C04-N05	-9.59	121.33	128.87
2	G	1301	66A	N03-C04-N05	-9.34	121.54	128.87
2	H	1301	66A	N03-C04-N05	-9.20	121.65	128.87
2	A	1301	66A	N03-C04-N05	-9.05	121.76	128.87
2	C	1301	66A	N03-C04-N05	-8.98	121.82	128.87
2	E	1301	66A	N03-C04-N05	-8.93	121.86	128.87
2	B	1301	66A	N03-C04-N05	-8.63	122.09	128.87
2	F	1301	66A	N03-C04-N05	-8.23	122.41	128.87
2	C	1301	66A	C27-C29-N30	-7.28	104.69	115.09
2	G	1301	66A	C27-C29-N30	-6.45	105.88	115.09
2	A	1301	66A	C27-C29-N30	-6.03	106.48	115.09
2	F	1301	66A	C27-C29-N30	-5.75	106.87	115.09
2	E	1301	66A	C27-C29-N30	-5.39	107.39	115.09
2	H	1301	66A	C27-C29-N30	-5.39	107.40	115.09
2	D	1301	66A	C27-C29-N30	-5.09	107.82	115.09
2	B	1301	66A	C27-C29-N30	-4.73	108.33	115.09
2	A	1301	66A	C09-C08-C10	-3.20	119.29	125.37
2	A	1301	66A	C15-C10-C08	-2.88	115.69	120.86
2	A	1301	66A	C07-C06-N05	-2.76	115.29	122.73
2	E	1301	66A	C07-C06-N05	-2.76	115.29	122.73
2	E	1301	66A	C09-C08-C10	-2.66	120.31	125.37
2	D	1301	66A	C07-C06-N05	-2.62	115.66	122.73
2	B	1301	66A	C07-C06-N05	-2.52	115.93	122.73
2	G	1301	66A	C07-C06-N05	-2.44	116.14	122.73
2	H	1301	66A	C07-C06-N05	-2.44	116.14	122.73
2	C	1301	66A	C07-C06-N05	-2.34	116.40	122.73
2	F	1301	66A	C07-C06-N05	-2.33	116.44	122.73
2	D	1301	66A	C09-C08-C10	-2.29	121.02	125.37
3	E	1302	MES	O2S-S-O1S	-2.19	107.78	113.96
2	E	1301	66A	C15-C10-C08	-2.18	116.95	120.86
2	D	1301	66A	O16-C17-C18	2.02	114.94	109.17
2	E	1301	66A	C15-C10-C11	2.03	120.74	118.17
2	D	1301	66A	C04-N05-C06	2.06	122.44	118.77
2	G	1301	66A	C04-N05-C06	2.10	122.51	118.77
3	D	1302	MES	C7-N4-C5	2.21	116.06	111.25
3	H	1302	MES	C7-N4-C5	2.26	116.17	111.25
3	B	1302	MES	O2S-S-C8	2.37	108.54	106.87
2	E	1301	66A	C04-N05-C06	2.38	123.01	118.77
3	A	1302	MES	C7-N4-C5	2.42	116.53	111.25
2	A	1301	66A	C04-N05-C06	2.47	123.18	118.77
3	H	1302	MES	O2S-S-C8	2.74	108.81	106.87
2	A	1301	66A	C07-C06-N24	2.77	128.18	122.73
3	G	1302	MES	O3S-S-C8	2.77	110.75	104.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1301	66A	C07-C06-N24	2.79	128.23	122.73
3	B	1302	MES	O3S-S-C8	2.87	110.94	104.99
3	E	1302	MES	C7-N4-C5	2.90	117.56	111.25
3	E	1302	MES	O2S-S-C8	2.90	108.92	106.87
2	H	1301	66A	C09-N01-C25	3.07	127.84	125.45
3	A	1302	MES	O1S-S-C8	3.08	109.05	106.87
3	C	1302	MES	O3S-S-C8	3.20	111.65	104.99
2	D	1301	66A	C09-N01-C25	3.27	128.00	125.45
3	F	1302	MES	O1S-S-C8	3.32	109.21	106.87
3	B	1302	MES	C7-N4-C5	3.35	118.53	111.25
3	A	1302	MES	O3S-S-C8	3.35	111.95	104.99
3	G	1302	MES	C7-N4-C5	3.45	118.76	111.25
3	F	1302	MES	C7-N4-C5	3.49	118.85	111.25
3	B	1302	MES	O1S-S-C8	3.59	109.40	106.87
3	C	1302	MES	C7-N4-C5	3.62	119.12	111.25
2	F	1301	66A	C09-N01-C25	3.70	128.34	125.45
3	G	1302	MES	C7-N4-C3	3.71	119.33	111.25
3	C	1302	MES	C7-N4-C3	3.76	119.42	111.25
3	F	1302	MES	C7-N4-C3	4.09	120.15	111.25
3	B	1302	MES	C7-N4-C3	4.12	120.21	111.25
3	D	1302	MES	O3S-S-C8	4.25	113.83	104.99
3	E	1302	MES	C7-N4-C3	4.61	121.29	111.25
2	A	1301	66A	C09-N01-C25	4.72	129.13	125.45
2	C	1301	66A	C09-N01-C25	4.84	129.23	125.45
3	A	1302	MES	C7-N4-C3	5.07	122.29	111.25
2	B	1301	66A	C09-N01-C25	5.11	129.44	125.45
3	H	1302	MES	C7-N4-C3	5.12	122.39	111.25
2	G	1301	66A	C09-N01-C25	5.24	129.53	125.45
3	D	1302	MES	C5-N4-C3	5.25	120.61	108.87
3	F	1302	MES	C5-N4-C3	5.42	121.00	108.87
3	E	1302	MES	C5-N4-C3	5.47	121.11	108.87
3	A	1302	MES	C5-N4-C3	5.49	121.17	108.87
3	B	1302	MES	C5-N4-C3	5.53	121.26	108.87
3	D	1302	MES	C7-N4-C3	5.54	123.31	111.25
2	E	1301	66A	C09-N01-C25	5.55	129.78	125.45
3	H	1302	MES	C5-N4-C3	5.61	121.43	108.87
3	C	1302	MES	C5-N4-C3	5.62	121.45	108.87
3	G	1302	MES	C5-N4-C3	5.82	121.91	108.87
3	C	1302	MES	O1S-S-C8	6.23	111.27	106.87
3	F	1302	MES	O2S-S-C8	6.24	111.28	106.87
3	G	1302	MES	O1S-S-C8	6.61	111.54	106.87
3	E	1302	MES	O1S-S-C8	7.20	111.96	106.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1302	MES	O1S-S-C8	7.85	112.42	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1302	MES	1	0
3	G	1302	MES	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	296/304 (97%)	0.01	4 (1%) 78 77	28, 44, 62, 72	0
1	B	296/304 (97%)	0.26	21 (7%) 19 18	30, 46, 64, 74	0
1	C	296/304 (97%)	0.14	19 (6%) 23 22	29, 46, 65, 74	0
1	D	304/304 (100%)	-0.02	5 (1%) 74 73	27, 44, 63, 73	0
1	E	296/304 (97%)	0.08	3 (1%) 84 83	28, 44, 62, 73	0
1	F	296/304 (97%)	0.20	15 (5%) 32 31	30, 46, 64, 73	0
1	G	296/304 (97%)	0.07	14 (4%) 35 34	29, 45, 65, 74	0
1	H	303/304 (99%)	0.01	1 (0%) 94 94	27, 44, 62, 74	0
All	All	2383/2432 (97%)	0.09	82 (3%) 49 47	27, 45, 64, 74	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1102	ALA	6.5
1	G	1102	ALA	5.5
1	B	1019	VAL	5.2
1	B	980	ALA	5.1
1	B	981	ALA	5.0
1	D	980	ALA	4.5
1	F	1019	VAL	4.5
1	F	981	ALA	4.3
1	F	1167	GLY	4.3
1	G	1021	ASP	4.2
1	C	1020	LYS	4.2
1	D	1167	GLY	4.0
1	C	1019	VAL	3.9
1	F	982	ASP	3.9
1	F	983	VAL	3.8
1	F	1166	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	1283	LYS	3.7
1	F	980	ALA	3.6
1	B	983	VAL	3.6
1	B	1283	LYS	3.6
1	C	1021	ASP	3.5
1	D	1020	LYS	3.5
1	G	983	VAL	3.4
1	G	1020	LYS	3.4
1	F	1103	PRO	3.3
1	F	1021	ASP	3.3
1	B	1166	GLY	3.3
1	F	1018	VAL	3.2
1	G	1019	VAL	3.2
1	E	1103	PRO	3.1
1	B	1102	ALA	3.1
1	B	1167	GLY	3.1
1	B	991	VAL	3.0
1	B	1070	GLN	3.0
1	G	1167	GLY	3.0
1	F	1034	GLU	3.0
1	G	1280	GLU	2.9
1	E	1167	GLY	2.9
1	B	1018	VAL	2.9
1	B	982	ASP	2.9
1	C	1166	GLY	2.9
1	G	1018	VAL	2.8
1	D	1168	LYS	2.8
1	G	982	ASP	2.7
1	C	983	VAL	2.7
1	C	1045	LEU	2.7
1	B	997	THR	2.7
1	C	1106	LEU	2.7
1	G	1103	PRO	2.6
1	G	1035	ALA	2.6
1	C	1070	GLN	2.6
1	A	1102	ALA	2.5
1	F	1168	LYS	2.5
1	B	1168	LYS	2.5
1	G	1166	GLY	2.4
1	B	1015	ALA	2.4
1	C	1167	GLY	2.3
1	H	980	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	1273	GLU	2.3
1	B	985	VAL	2.3
1	F	1061	ARG	2.3
1	C	1103	PRO	2.3
1	A	1103	PRO	2.2
1	B	1103	PRO	2.2
1	C	1280	GLU	2.2
1	C	1018	VAL	2.2
1	C	1168	LYS	2.2
1	C	999	SER	2.2
1	A	1166	GLY	2.2
1	C	1073	LEU	2.1
1	G	980	ALA	2.1
1	C	1022	GLU	2.1
1	B	1034	GLU	2.0
1	G	1045	LEU	2.0
1	F	997	THR	2.0
1	C	980	ALA	2.0
1	B	1020	LYS	2.0
1	C	1016	LYS	2.0
1	B	1078	LEU	2.0
1	A	1167	GLY	2.0
1	B	1061	ARG	2.0
1	E	1283	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 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( $\text{\AA}^2$ )	Q<0.9
4	SO4	E	1303	5/5	0.87	0.14	1.05	87,87,89,90	0
2	66A	F	1301	33/33	0.92	0.15	0.69	39,43,51,52	0
4	SO4	A	1303	5/5	0.88	0.13	0.52	86,87,88,89	0
2	66A	B	1301	33/33	0.93	0.15	0.43	35,43,50,51	0
2	66A	D	1301	33/33	0.93	0.14	0.37	37,40,48,49	0
2	66A	H	1301	33/33	0.94	0.15	0.25	37,40,50,50	0
3	MES	F	1302	12/12	0.81	0.17	0.21	74,78,84,84	0
3	MES	B	1302	12/12	0.89	0.17	0.17	85,87,91,91	0
2	66A	G	1301	33/33	0.92	0.13	0.01	42,45,51,51	0
3	MES	C	1302	12/12	0.96	0.14	-0.01	52,59,69,69	0
2	66A	A	1301	33/33	0.94	0.13	-0.13	31,36,48,49	0
3	MES	G	1302	12/12	0.94	0.14	-0.15	53,59,71,71	0
2	66A	C	1301	33/33	0.89	0.13	-0.19	43,45,53,53	0
3	MES	D	1302	12/12	0.91	0.12	-0.30	52,57,67,68	0
2	66A	E	1301	33/33	0.95	0.14	-0.32	30,35,48,49	0
3	MES	E	1302	12/12	0.94	0.13	-0.52	49,55,60,61	0
3	MES	H	1302	12/12	0.93	0.12	-0.55	52,56,69,69	0
4	SO4	C	1303	5/5	0.97	0.11	-0.57	64,65,67,67	0
3	MES	A	1302	12/12	0.94	0.13	-0.59	45,50,59,60	0
4	SO4	G	1303	5/5	0.98	0.08	-1.83	61,61,61,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.