



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:52 AM GMT

PDB ID : 2YN3  
Title : Structural insight into the giant calcium-binding adhesin SiiE: implications for the adhesion of Salmonella enterica to polarized epithelial cells  
Authors : Griessl, M.H.; Schmid, B.; Kassler, K.; Braunsmann, C.; Ritter, R.; Barlag, B.; Sturm, K.U.; Danzer, C.; Wagner, C.; Schaeffer, T.E.; Sticht, H.; Hensel, M.; Muller, Y.A.  
Deposited on : 2012-10-11  
Resolution : 2.12 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

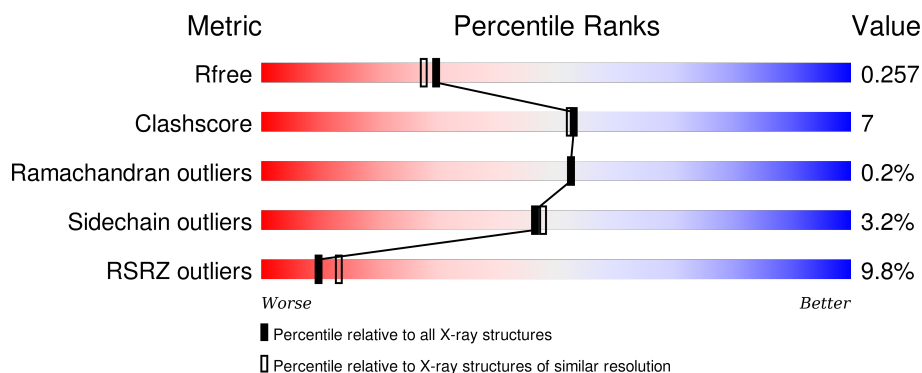
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.12 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	4587 (2.14-2.10)
Clashscore	102246	5132 (2.14-2.10)
Ramachandran outliers	100387	5080 (2.14-2.10)
Sidechain outliers	100360	5081 (2.14-2.10)
RSRZ outliers	91569	4597 (2.14-2.10)

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	288	<div> <div>11%</div> <div>84% 10% 5%</div> </div>
1	B	288	<div> <div>11%</div> <div>69% 15% 15%</div> </div>
1	C	288	<div> <div>2%</div> <div>93% 5%</div> </div>
1	D	288	<div> <div>9%</div> <div>55% 16% 28%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7988 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 PUTATIVE INNER MEMBRANE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	Se	0	0	0
			2028	1267	329	429	3			
1	B	246	Total	C	N	O	Se	0	0	0
			1832	1143	297	389	3			
1	C	284	Total	C	N	O	Se	0	0	0
			2108	1311	342	452	3			
1	D	208	Total	C	N	O	Se	0	0	0
			1538	959	246	330	3			

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	I	0	0
			2	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Ca	0	0
			3	3		
3	A	3	Total	Ca	0	0
			3	3		
3	D	3	Total	Ca	0	0
			3	3		
3	C	4	Total	Ca	0	0
			4	4		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	P	0	0
			5	4	1		

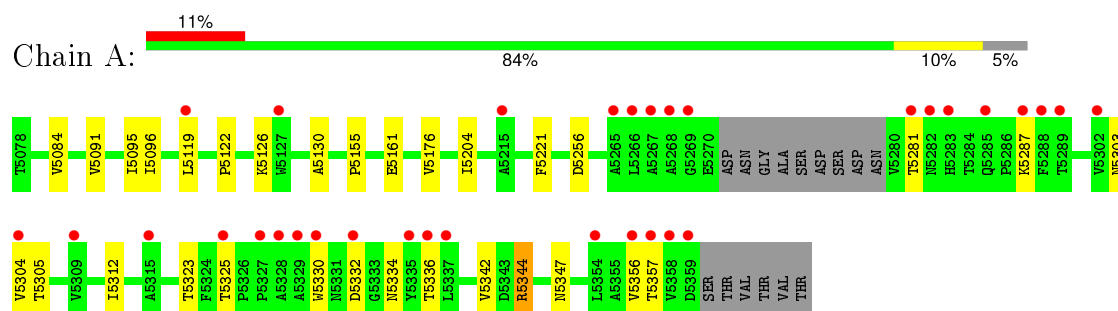
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	185	Total	O	0	0
			185	185		
5	B	53	Total	O	0	0
			53	53		
5	C	175	Total	O	0	0
			175	175		
5	D	49	Total	O	0	0
			49	49		

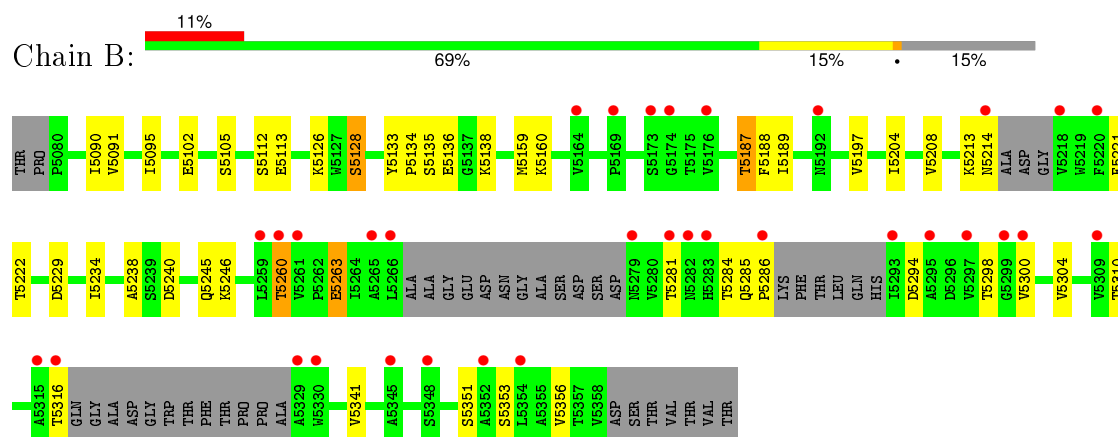
### 3 Residue-property plots [i](#)

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.

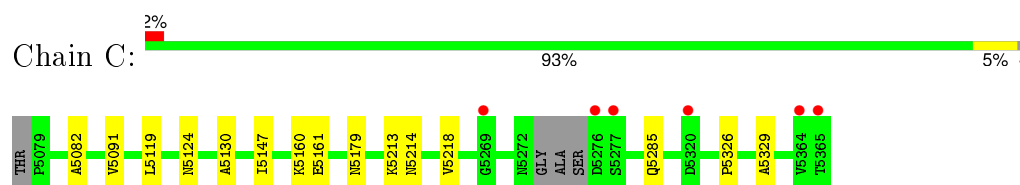
#### • Molecule 1: PUTATIVE INNER MEMBRANE PROTEIN



#### • Molecule 1: PUTATIVE INNER MEMBRANE PROTEIN



#### • Molecule 1: PUTATIVE INNER MEMBRANE PROTEIN



#### • Molecule 1: PUTATIVE INNER MEMBRANE PROTEIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.48Å 153.31Å 96.30Å 90.00° 103.88° 90.00°	Depositor
Resolution (Å)	34.32 – 2.12 34.32 – 2.12	Depositor EDS
% Data completeness (in resolution range)	98.0 (34.32-2.12) 98.1 (34.32-2.12)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.30 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.210 , 0.260 0.209 , 0.257	Depositor DCC
$R_{free}$ test set	3648 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.5	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 48.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 72954 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7988	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.25% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CA, IOD, PO4

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	0.69	0/2064	0.79	3/2835 (0.1%)
1	B	0.49	0/1857	0.67	0/2544
1	C	0.70	0/2144	0.78	0/2945
1	D	0.52	0/1559	0.71	0/2133
All	All	0.62	0/7624	0.74	3/10457 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5344	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	5344	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	A	5256	ASP	CB-CG-OD1	5.14	122.93	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	2028	0	1959	30	0
1	B	1832	0	1784	23	0
1	C	2108	0	2026	15	0
1	D	1538	0	1505	34	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	4	0	0	0	0
3	D	3	0	0	0	0
4	C	5	0	0	0	0
5	A	185	0	0	5	0
5	B	53	0	0	3	0
5	C	175	0	0	0	0
5	D	49	0	0	2	0
All	All	7988	0	7274	97	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 7.

All (97) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5161:GLU:HG3	5:A:2088:HOH:O	1.33	1.29
1:A:5155:PRO:HD2	5:A:2080:HOH:O	1.41	1.20
1:A:5204:ILE:HD11	1:A:5221:PHE:CE2	2.09	0.87
1:A:5091:VAL:HG12	1:A:5096:ILE:HD11	1.57	0.86
1:A:5334:ASN:HB2	5:A:2180:HOH:O	1.74	0.86
1:A:5356:VAL:HG12	1:A:5357:THR:H	1.41	0.85
1:A:5091:VAL:CG1	1:A:5096:ILE:HD11	2.08	0.84
1:A:5305:THR:CG2	1:A:5336:THR:HB	2.11	0.81
1:D:5297:VAL:HG22	1:D:5341:VAL:HG13	1.66	0.77
1:D:5259:LEU:HD21	1:D:5341:VAL:HG12	1.74	0.69
1:D:5259:LEU:HD11	1:D:5341:VAL:HG11	1.75	0.69
1:D:5159:MSE:HG2	1:D:5244:ASN:CB	2.25	0.67
1:A:5287:LYS:HD2	1:A:5325:THR:OG1	1.95	0.66
1:A:5305:THR:HG23	1:A:5336:THR:HB	1.79	0.65
1:A:5356:VAL:HG12	1:A:5357:THR:N	2.13	0.63
1:B:5090:ILE:HD12	5:B:2037:HOH:O	1.99	0.63
1:C:5160:LYS:HE3	1:C:5161:GLU:OE2	1.99	0.63
1:C:5214:ASN:HD21	1:C:5218:VAL:CG1	2.11	0.62
1:A:5305:THR:HG22	1:A:5336:THR:HB	1.83	0.61
1:D:5216:ASP:OD1	1:D:5217:GLY:N	2.33	0.59
1:A:5344:ARG:NH1	5:A:2183:HOH:O	2.35	0.58
1:A:5204:ILE:HD11	1:A:5221:PHE:HE2	1.67	0.58
1:D:5294:ASP:O	1:D:5297:VAL:HG23	2.03	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5136:GLU:OE1	1:B:5138:LYS:NZ	2.32	0.58
1:D:5159:MSE:HG2	1:D:5244:ASN:HB3	1.85	0.57
1:D:5297:VAL:HG22	1:D:5341:VAL:CG1	2.34	0.56
1:C:5214:ASN:ND2	1:C:5218:VAL:HG13	2.20	0.56
1:B:5263:GLU:HA	1:B:5351:SER:HB2	1.88	0.56
1:D:5202:VAL:HG12	1:D:5204:ILE:HG13	1.88	0.56
1:D:5213:LYS:HE2	1:D:5217:GLY:HA2	1.87	0.56
1:A:5344:ARG:NH2	1:C:5124:ASN:O	2.39	0.55
1:D:5163:PRO:HG3	1:D:5193:LEU:HD21	1.87	0.55
1:A:5091:VAL:HG11	1:A:5096:ILE:HD11	1.86	0.55
1:B:5128:SER:HB2	1:C:5130:ALA:O	2.07	0.54
1:D:5133:TYR:CZ	1:D:5160:LYS:HB2	2.42	0.54
1:C:5214:ASN:HD21	1:C:5218:VAL:HG13	1.73	0.54
1:D:5136:GLU:OE2	1:D:5195:SER:OG	2.22	0.54
1:B:5189:ILE:HD11	5:B:2042:HOH:O	2.08	0.53
1:D:5144:VAL:HG22	1:D:5150:ARG:HB3	1.90	0.53
1:B:5304:VAL:O	1:B:5310:THR:HA	2.09	0.52
1:A:5204:ILE:CD1	1:A:5221:PHE:CE2	2.87	0.52
1:D:5297:VAL:CG2	1:D:5341:VAL:HG13	2.39	0.52
1:D:5160:LYS:HD3	1:D:5161:GLU:HG3	1.91	0.52
1:C:5285:GLN:HG3	1:C:5329:ALA:HA	1.92	0.51
1:B:5091:VAL:HG11	1:C:5091:VAL:HG21	1.93	0.51
1:A:5356:VAL:CG1	1:A:5357:THR:H	2.19	0.51
1:B:5188:PHE:CE2	1:B:5234:ILE:HD13	2.45	0.51
1:A:5091:VAL:HG12	1:A:5096:ILE:CD1	2.35	0.51
1:B:5285:GLN:N	1:B:5286:PRO:HD3	2.26	0.50
1:D:5159:MSE:CG	1:D:5244:ASN:HB3	2.41	0.50
1:B:5260:THR:N	1:B:5294:ASP:OD2	2.42	0.50
1:A:5084:VAL:HG11	1:C:5179:ASN:HB2	1.94	0.49
1:D:5261:VAL:HG22	1:D:5349:GLN:OE1	2.13	0.49
1:B:5187:THR:HB	1:B:5222:THR:OG1	2.13	0.49
1:D:5168:SER:O	1:D:5171:SER:N	2.41	0.49
5:A:2158:HOH:O	1:C:5082:ALA:HB3	2.12	0.48
1:B:5090:ILE:HG21	1:B:5160:LYS:HG3	1.95	0.48
1:D:5136:GLU:OE1	1:D:5138:LYS:NZ	2.44	0.48
1:D:5259:LEU:HD11	1:D:5341:VAL:CG1	2.43	0.48
1:D:5202:VAL:CG1	1:D:5204:ILE:HG13	2.44	0.48
1:D:5084:VAL:O	1:D:5099:GLY:HA3	2.14	0.47
1:A:5095:ILE:O	1:A:5130:ALA:HA	2.14	0.47
1:B:5246:LYS:NZ	5:B:2037:HOH:O	2.48	0.47
1:D:5215:ALA:O	1:D:5216:ASP:HB2	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5204:ILE:HD11	1:B:5221:PHE:CE2	2.50	0.46
1:D:5080:PRO:HG2	5:D:2016:HOH:O	2.15	0.46
1:B:5213:LYS:HG2	1:B:5214:ASN:N	2.31	0.46
1:C:5147:ILE:O	1:C:5147:ILE:HG22	2.15	0.46
1:C:5213:LYS:HE2	1:C:5213:LYS:HB3	1.77	0.46
1:D:5147:ILE:CG2	1:D:5147:ILE:O	2.63	0.46
1:B:5197:VAL:HA	1:B:5240:ASP:HA	1.97	0.46
1:C:5214:ASN:ND2	1:C:5218:VAL:CG1	2.77	0.45
1:D:5093:ASP:HB3	5:D:2012:HOH:O	2.15	0.45
1:A:5305:THR:HG22	1:A:5336:THR:O	2.17	0.45
1:D:5185:GLN:HG3	1:D:5226:PRO:HA	1.98	0.44
1:A:5303:ASN:HD22	1:A:5312:ILE:HG12	1.83	0.43
1:A:5204:ILE:CD1	1:A:5221:PHE:HE2	2.28	0.43
1:A:5091:VAL:HG11	1:D:5091:VAL:HG21	2.00	0.43
1:D:5095:ILE:HD11	1:D:5134:PRO:HD2	2.00	0.43
1:A:5342:VAL:HA	1:A:5347:ASN:O	2.18	0.43
1:B:5095:ILE:HD11	1:B:5134:PRO:HD2	1.99	0.43
1:C:5119:LEU:C	1:C:5119:LEU:HD12	2.40	0.43
1:A:5287:LYS:HD2	1:A:5325:THR:HG1	1.84	0.42
1:B:5284:THR:O	1:B:5285:GLN:HG3	2.19	0.42
1:A:5119:LEU:C	1:A:5119:LEU:HD12	2.40	0.42
1:B:5238:ALA:O	1:B:5245:GLN:HG3	2.18	0.42
1:D:5180:ILE:HG12	1:D:5254:THR:HB	2.02	0.42
1:C:5285:GLN:HA	1:C:5326:PRO:HG2	2.03	0.41
1:D:5262:PRO:HG2	1:D:5351:SER:HB3	2.00	0.41
1:A:5122:PRO:HD2	1:A:5126:LYS:O	2.21	0.41
1:B:5263:GLU:HA	1:B:5351:SER:CB	2.51	0.41
1:A:5304:VAL:HG21	1:A:5330:TRP:HH2	1.86	0.41
1:B:5133:TYR:CZ	1:B:5160:LYS:HB2	2.56	0.41
1:B:5102:GLU:O	1:B:5105:SER:OG	2.26	0.40
1:B:5300:VAL:HG22	1:B:5341:VAL:HG12	2.03	0.40
1:D:5293:ILE:HG23	1:D:5297:VAL:HG21	2.03	0.40
1:D:5083:PRO:HD3	1:D:5143:SER:HB3	2.04	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	269/288 (93%)	264 (98%)	5 (2%)	0	100	100
1	B	236/288 (82%)	225 (95%)	11 (5%)	0	100	100
1	C	280/288 (97%)	276 (99%)	4 (1%)	0	100	100
1	D	202/288 (70%)	188 (93%)	12 (6%)	2 (1%)	19	12
All	All	987/1152 (86%)	953 (97%)	32 (3%)	2 (0%)	52	52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	5216	ASP
1	D	5214	ASN

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	231/241 (96%)	227 (98%)	4 (2%)	68	73
1	B	213/241 (88%)	197 (92%)	16 (8%)	17	12
1	C	242/241 (100%)	242 (100%)	0	100	100
1	D	180/241 (75%)	172 (96%)	8 (4%)	35	32
All	All	866/964 (90%)	838 (97%)	28 (3%)	46	48

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5176	VAL
1	A	5281	THR
1	A	5323	THR
1	A	5332	ASP
1	B	5112	SER
1	B	5113	GLU
1	B	5126	LYS
1	B	5128	SER
1	B	5135	SER
1	B	5159	MSE
1	B	5187	THR
1	B	5208	VAL
1	B	5229	ASP
1	B	5260	THR
1	B	5263	GLU
1	B	5281	THR
1	B	5298	THR
1	B	5316	THR
1	B	5353	SER
1	B	5356	VAL
1	D	5135	SER
1	D	5143	SER
1	D	5159	MSE
1	D	5167	LEU
1	D	5212	GLU
1	D	5245	GLN
1	D	5249	LEU
1	D	5252	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5303	ASN
1	A	5350	GLN
1	C	5081	ASN
1	C	5106	GLN

### 5.3.3 RNA ⓘ

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](#)

Of 16 ligands modelled in this entry, 15 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	PO4	C	6366	-	4,4,4	1.15	0	6,6,6	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PO4	C	6366	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	270/288 (93%)	0.65	33 (12%) 5 7	15, 28, 80, 100	0
1	B	243/288 (84%)	0.67	33 (13%) 4 6	24, 54, 75, 95	0
1	C	281/288 (97%)	0.09	6 (2%) 67 72	15, 26, 51, 96	0
1	D	205/288 (71%)	0.67	26 (12%) 5 6	23, 52, 81, 93	0
All	All	999/1152 (86%)	0.50	98 (9%) 10 13	15, 39, 77, 100	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5268	ALA	9.3
1	D	5336	THR	5.9
1	D	5164	VAL	5.6
1	B	5352	ALA	5.5
1	A	5358	VAL	5.4
1	D	5192	ASN	5.1
1	B	5286	PRO	5.0
1	A	5356	VAL	5.0
1	A	5337	LEU	4.9
1	D	5293	ILE	4.8
1	A	5304	VAL	4.8
1	D	5341	VAL	4.8
1	D	5339	VAL	4.7
1	A	5328	ALA	4.6
1	A	5329	ALA	4.5
1	D	5352	ALA	4.4
1	C	5365	THR	4.2
1	A	5267	ALA	4.2
1	A	5282	ASN	4.2
1	D	5337	LEU	4.1
1	D	5353	SER	4.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	5260	THR	4.0
1	A	5269	GLY	4.0
1	B	5261	VAL	3.9
1	A	5357	THR	3.9
1	B	5315	ALA	3.8
1	A	5325	THR	3.8
1	A	5327	PRO	3.8
1	B	5297	VAL	3.8
1	A	5330	TRP	3.6
1	C	5276	ASP	3.4
1	B	5265	ALA	3.4
1	B	5266	LEU	3.3
1	B	5174	GLY	3.3
1	B	5309	VAL	3.3
1	D	5079	PRO	3.2
1	B	5295	ALA	3.2
1	D	5242	ALA	3.2
1	B	5354	LEU	3.2
1	B	5316	THR	3.1
1	B	5164	VAL	3.1
1	A	5335	TYR	3.1
1	A	5336	THR	3.1
1	A	5302	VAL	3.0
1	D	5338	SER	3.0
1	B	5330	TRP	3.0
1	A	5289	THR	3.0
1	A	5287	LYS	3.0
1	D	5262	PRO	2.9
1	B	5220	PHE	2.9
1	A	5281	THR	2.9
1	A	5359	ASP	2.8
1	D	5295	ALA	2.8
1	A	5354	LEU	2.8
1	A	5285	GLN	2.8
1	A	5265	ALA	2.7
1	C	5320	ASP	2.7
1	B	5300	VAL	2.7
1	D	5261	VAL	2.7
1	B	5281	THR	2.7
1	A	5266	LEU	2.6
1	B	5218	VAL	2.6
1	B	5259	LEU	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	5277	SER	2.6
1	D	5218	VAL	2.6
1	B	5173	SER	2.5
1	B	5279	ASN	2.5
1	D	5175	THR	2.5
1	B	5282	ASN	2.4
1	A	5315	ALA	2.4
1	D	5174	GLY	2.4
1	D	5191	GLY	2.4
1	D	5217	GLY	2.3
1	A	5332	ASP	2.3
1	B	5169	PRO	2.3
1	B	5214	ASN	2.3
1	D	5340	THR	2.3
1	B	5283	HIS	2.3
1	D	5161	GLU	2.3
1	A	5119	LEU	2.3
1	A	5283	HIS	2.3
1	B	5192	ASN	2.2
1	C	5269	GLY	2.2
1	A	5127	TRP	2.2
1	B	5329	ALA	2.2
1	D	5245	GLN	2.2
1	C	5364	VAL	2.2
1	B	5299	GLY	2.1
1	B	5348	SER	2.1
1	A	5288	PHE	2.1
1	A	5309	VAL	2.1
1	B	5176	VAL	2.1
1	B	5293	ILE	2.1
1	D	5214	ASN	2.1
1	D	5243	GLY	2.0
1	B	5345	ALA	2.0
1	A	5215	ALA	2.0
1	D	5176	VAL	2.0

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

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
3	CA	A	6363	1/1	0.99	0.16	1.31	20,20,20,20	0
3	CA	A	6362	1/1	0.99	0.13	1.25	19,19,19,19	0
3	CA	C	6369	1/1	1.00	0.12	0.66	24,24,24,24	0
3	CA	C	6368	1/1	1.00	0.12	0.14	22,22,22,22	0
2	IOD	A	6361	1/1	0.99	0.13	-0.03	32,32,32,32	1
3	CA	D	6356	1/1	0.90	0.12	-0.44	58,58,58,58	0
3	CA	C	6367	1/1	1.00	0.10	-0.49	20,20,20,20	0
4	PO4	C	6366	5/5	1.00	0.12	-0.78	21,22,24,25	0
3	CA	C	6370	1/1	0.89	0.12	-1.03	60,60,60,60	0
2	IOD	A	6360	1/1	0.97	0.12	-1.38	47,47,47,47	1
3	CA	B	6361	1/1	0.95	0.04	-1.78	57,57,57,57	0
3	CA	A	6364	1/1	0.98	0.09	-2.26	29,29,29,29	0
3	CA	D	6355	1/1	0.97	0.06	-2.34	75,75,75,75	0
3	CA	D	6354	1/1	0.99	0.04	-2.55	40,40,40,40	0
3	CA	B	6360	1/1	0.98	0.03	-2.62	61,61,61,61	0
3	CA	B	6359	1/1	0.99	0.06	-2.66	39,39,39,39	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.