



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 01:52 pm GMT

PDB ID : 1W2M  
Title : Ca-substituted form of E. coli aminopeptidase P  
Authors : Graham, S.C.; Bond, C.S.; Freeman, H.C.; Guss, J.M.  
Deposited on : 2004-07-07  
Resolution : 2.40 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

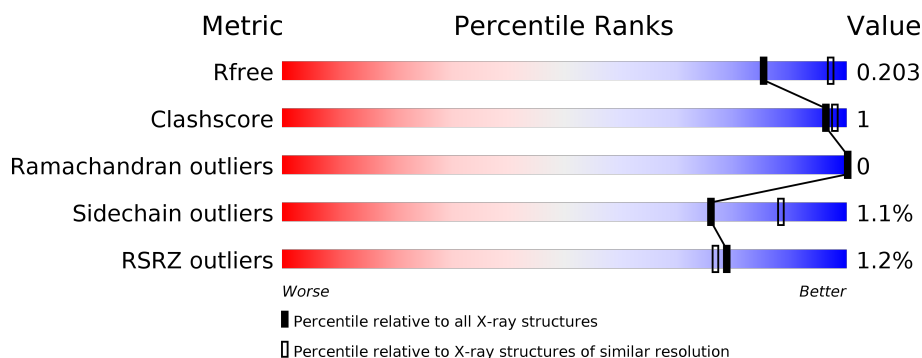
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	111664	3481 (2.40-2.40)
Clashscore	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)
RSRZ outliers	108989	3386 (2.40-2.40)

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	440	<div> <div>%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
1	B	440	<div> <div>2%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>
1	C	440	<div> <div>%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
1	D	440	<div> <div>%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
1	E	440	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> </div>
1	F	440	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>

## 2 Entry composition [i](#)

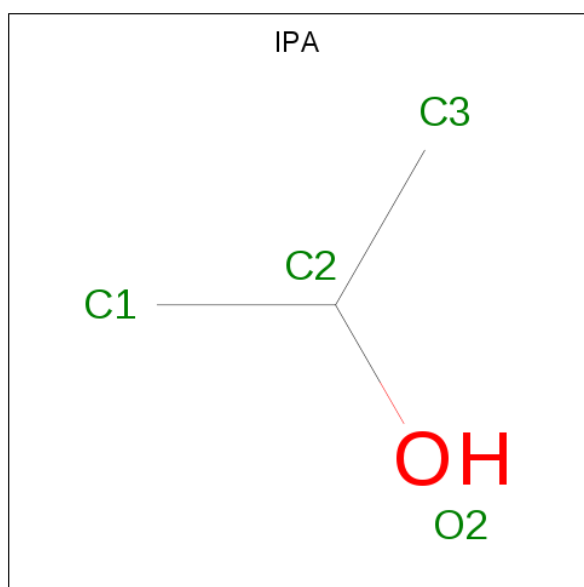
There are 5 unique types of molecules in this entry. The entry contains 22063 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 XAA-PRO AMINOPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3486	2194	615	662	15			
1	B	438	Total	C	N	O	S	0	0	1
			3471	2185	611	660	15			
1	C	439	Total	C	N	O	S	0	0	0
			3490	2197	616	662	15			
1	D	440	Total	C	N	O	S	0	0	0
			3494	2200	617	662	15			
1	E	439	Total	C	N	O	S	0	0	0
			3490	2197	616	662	15			
1	F	440	Total	C	N	O	S	0	0	0
			3500	2202	618	665	15			

- Molecule 2 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C<sub>3</sub>H<sub>8</sub>O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 3 1	0	0
2	A	1	Total C O 4 3 1	0	0
2	B	1	Total C O 4 3 1	0	0
2	B	1	Total C O 4 3 1	0	0
2	C	1	Total C O 4 3 1	0	0
2	D	1	Total C O 4 3 1	0	0
2	D	1	Total C O 4 3 1	0	0
2	D	1	Total C O 4 3 1	0	0
2	E	1	Total C O 4 3 1	0	0
2	E	1	Total C O 4 3 1	0	0
2	F	1	Total C O 4 3 1	0	0
2	F	1	Total C O 4 3 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total 1	Cl 1	0	0
4	E	1	Total 1	Cl 1	0	0
4	B	1	Total 1	Cl 1	0	0
4	C	1	Total 1	Cl 1	0	0
4	A	1	Total 1	Cl 1	0	0
4	F	1	Total 1	Cl 1	0	0

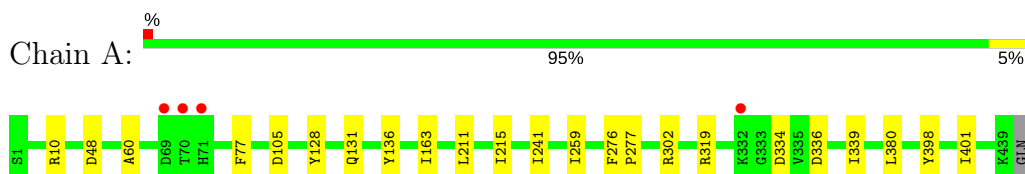
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	177	Total 177	O 177	0	0
5	B	145	Total 145	O 145	0	0
5	C	159	Total 159	O 159	0	0
5	D	179	Total 179	O 179	0	0
5	E	222	Total 222	O 222	0	0
5	F	190	Total 190	O 190	0	0

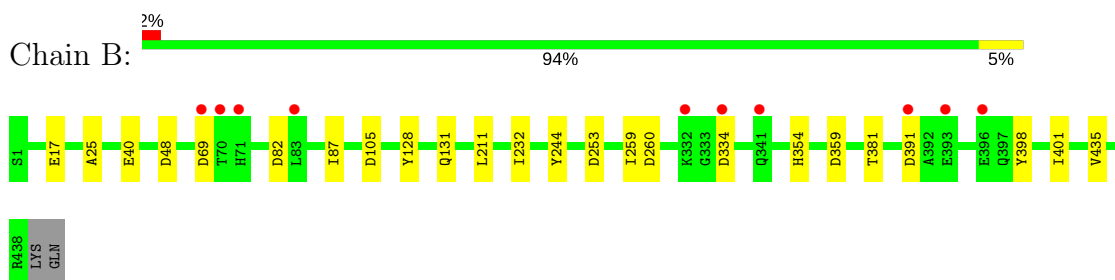
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

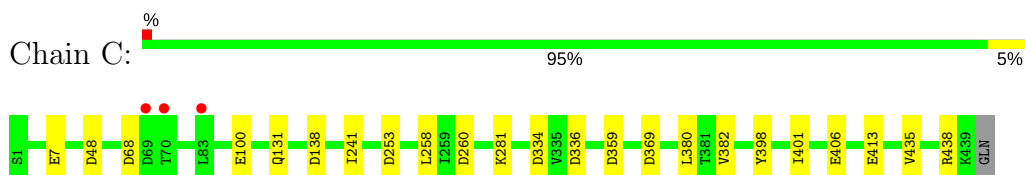
- Molecule 1: XAA-PRO AMINOPEPTIDASE



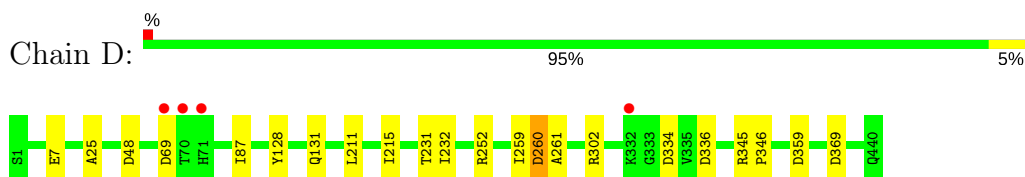
- Molecule 1: XAA-PRO AMINOPEPTIDASE



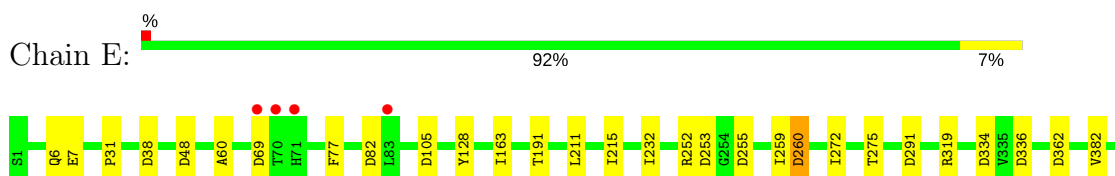
- Molecule 1: XAA-PRO AMINOPEPTIDASE



- Molecule 1: XAA-PRO AMINOPEPTIDASE



- Molecule 1: XAA-PRO AMINOPEPTIDASE





● Molecule 1: XAA-PRO AMINOPEPTIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.36Å 312.69Å 160.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	182.57 – 2.40 29.52 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.8 (182.57-2.40) 94.8 (29.52-2.40)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.57 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.175 , 0.200 0.181 , 0.203	Depositor DCC
$R_{free}$ test set	9688 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.0	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 33.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	22063	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.40% 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: CSO, IPA, CA, CL

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	0.60	0/3550	0.77	5/4808 (0.1%)
1	B	0.60	0/3535	0.76	8/4789 (0.2%)
1	C	0.61	0/3554	0.76	9/4812 (0.2%)
1	D	0.59	0/3558	0.76	8/4818 (0.2%)
1	E	0.63	0/3554	0.79	11/4812 (0.2%)
1	F	0.61	0/3564	0.79	10/4824 (0.2%)
All	All	0.60	0/21315	0.77	51/28863 (0.2%)

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	105	ASP	CB-CG-OD2	7.69	125.22	118.30
1	F	105	ASP	CB-CG-OD2	7.39	124.95	118.30
1	E	291	ASP	CB-CG-OD2	7.24	124.81	118.30
1	F	253	ASP	CB-CG-OD2	7.18	124.77	118.30
1	D	336	ASP	CB-CG-OD2	6.81	124.43	118.30
1	D	260	ASP	CB-CG-OD1	6.81	124.43	118.30
1	C	336	ASP	CB-CG-OD2	6.68	124.31	118.30
1	C	253	ASP	CB-CG-OD2	6.63	124.27	118.30
1	B	69	ASP	CB-CG-OD2	6.62	124.26	118.30
1	A	336	ASP	CB-CG-OD2	6.52	124.17	118.30
1	B	253	ASP	CB-CG-OD2	6.37	124.03	118.30
1	B	105	ASP	CB-CG-OD2	6.36	124.03	118.30
1	D	48	ASP	CB-CG-OD2	6.32	123.99	118.30
1	E	255	ASP	CB-CG-OD2	6.30	123.97	118.30
1	E	82	ASP	CB-CG-OD2	6.30	123.97	118.30
1	F	336	ASP	CB-CG-OD2	6.15	123.83	118.30
1	B	82	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	48	ASP	CB-CG-OD2	5.97	123.67	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	125	ASP	CB-CG-OD2	5.95	123.65	118.30
1	F	334	ASP	CB-CG-OD2	5.88	123.60	118.30
1	F	138	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	10	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	F	82	ASP	CB-CG-OD2	5.82	123.54	118.30
1	D	69	ASP	CB-CG-OD2	5.76	123.48	118.30
1	F	69	ASP	CB-CG-OD2	5.68	123.42	118.30
1	C	138	ASP	CB-CG-OD2	5.64	123.37	118.30
1	A	334	ASP	CB-CG-OD2	5.63	123.36	118.30
1	C	48	ASP	CB-CG-OD2	5.57	123.31	118.30
1	D	359	ASP	CB-CG-OD2	5.55	123.30	118.30
1	D	302	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	E	48	ASP	CB-CG-OD2	5.52	123.27	118.30
1	F	359	ASP	CB-CG-OD2	5.51	123.26	118.30
1	E	253	ASP	CB-CG-OD2	5.49	123.24	118.30
1	E	362	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	105	ASP	CB-CG-OD2	5.48	123.24	118.30
1	C	68	ASP	CB-CG-OD2	5.47	123.23	118.30
1	B	391	ASP	CB-CG-OD2	5.45	123.20	118.30
1	C	260	ASP	CB-CG-OD1	5.44	123.20	118.30
1	C	334	ASP	CB-CG-OD2	5.39	123.15	118.30
1	D	334	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	334	ASP	CB-CG-OD2	5.32	123.09	118.30
1	E	260	ASP	CB-CG-OD1	5.24	123.02	118.30
1	F	38	ASP	CB-CG-OD2	5.17	122.95	118.30
1	E	38	ASP	CB-CG-OD2	5.11	122.90	118.30
1	D	369	ASP	CB-CG-OD2	5.08	122.88	118.30
1	C	369	ASP	CB-CG-OD2	5.06	122.86	118.30
1	E	334	ASP	CB-CG-OD2	5.05	122.84	118.30
1	E	69	ASP	CB-CG-OD2	5.04	122.84	118.30
1	C	359	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	359	ASP	CB-CG-OD2	5.02	122.82	118.30
1	B	48	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	3486	0	3409	9	0
1	B	3471	0	3394	9	0
1	C	3490	0	3420	7	0
1	D	3494	0	3422	10	0
1	E	3490	0	3420	10	0
1	F	3500	0	3428	6	0
2	A	8	0	16	0	0
2	B	8	0	16	0	0
2	C	4	0	8	0	0
2	D	12	0	24	0	0
2	E	8	0	16	0	0
2	F	8	0	16	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	177	0	0	0	0
5	B	145	0	0	1	0
5	C	159	0	0	0	0
5	D	179	0	0	0	0
5	E	222	0	0	1	0
5	F	190	0	0	0	0
All	All	22063	0	20589	45	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 1.

All (45) 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:C:131:GLN:HE22	1:D:131:GLN:HE22	1.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:211:LEU:HD13	1:E:259:ILE:HD11	1.85	0.59
1:C:398:TYR:HA	1:C:401:ILE:HD12	1.88	0.55
1:E:435:VAL:HG23	5:E:2156:HOH:O	2.09	0.53
1:C:131:GLN:NE2	1:D:131:GLN:HE22	2.07	0.53
1:B:435:VAL:HG13	5:B:2119:HOH:O	2.09	0.53
1:F:232:ILE:HB	1:F:260:ASP:HB3	1.93	0.51
1:E:232:ILE:HB	1:E:260:ASP:HB3	1.94	0.49
1:B:398:TYR:HA	1:B:401:ILE:HD12	1.94	0.49
1:D:231:THR:HG23	1:D:261:ALA:HB2	1.95	0.49
1:D:215:ILE:HD11	1:D:259:ILE:HG21	1.95	0.49
1:D:232:ILE:HB	1:D:260:ASP:HB3	1.93	0.49
1:A:398:TYR:HA	1:A:401:ILE:HD12	1.95	0.48
1:C:131:GLN:HE22	1:D:131:GLN:NE2	2.11	0.47
1:B:232:ILE:HB	1:B:260:ASP:HB3	1.97	0.46
1:F:25:ALA:HA	1:F:128:TYR:HB2	1.97	0.46
1:F:211:LEU:HD13	1:F:259:ILE:HD11	1.96	0.46
1:A:215:ILE:HD11	1:A:259:ILE:HG21	1.98	0.45
1:B:87:ILE:O	1:C:241:ILE:HA	2.17	0.45
1:C:382:VAL:O	1:C:406:GLU:HA	2.17	0.45
1:B:354:HIS:CE1	1:B:381:THR:HG21	2.52	0.45
1:A:241:ILE:HA	1:D:87:ILE:O	2.18	0.44
1:D:25:ALA:HA	1:D:128:TYR:HB2	2.00	0.44
1:B:232:ILE:HG23	1:B:244:TYR:O	2.17	0.44
1:A:131:GLN:HE22	1:B:131:GLN:HE22	1.65	0.44
1:A:319:ARG:HA	1:A:339:ILE:HD11	2.00	0.44
1:D:211:LEU:HD13	1:D:259:ILE:HD11	1.99	0.44
1:B:25:ALA:HA	1:B:128:TYR:HB2	2.01	0.43
1:B:211:LEU:HD13	1:B:259:ILE:HD11	2.00	0.43
1:E:191:THR:HG22	1:E:272:ILE:HD12	1.99	0.43
1:E:60:ALA:HA	1:E:77:PHE:O	2.18	0.43
1:A:60:ALA:HA	1:A:77:PHE:O	2.19	0.43
1:E:128:TYR:HA	1:E:163:ILE:O	2.19	0.43
1:A:211:LEU:HD13	1:A:259:ILE:HD11	2.02	0.42
1:F:398:TYR:HA	1:F:401:ILE:HD12	2.01	0.42
1:E:382:VAL:O	1:E:406:GLU:HA	2.21	0.41
1:F:345:ARG:N	1:F:346:PRO:CD	2.84	0.41
1:D:345:ARG:N	1:D:346:PRO:CD	2.84	0.41
1:C:258:LEU:HD23	1:C:258:LEU:C	2.41	0.41
1:E:215:ILE:HD11	1:E:259:ILE:HG21	2.03	0.41
1:E:275:THR:HG21	1:E:403:ILE:HG12	2.03	0.40
1:E:319:ARG:NH2	1:E:336:ASP:OD1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:TYR:HA	1:A:163:ILE:O	2.21	0.40
1:A:276:PHE:HB2	1:A:277:PRO:HD2	2.04	0.40
1:F:35:ARG:HA	1:F:41:TYR:CE2	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/440 (99%)	426 (98%)	10 (2%)	0	100	100
1	B	435/440 (99%)	424 (98%)	11 (2%)	0	100	100
1	C	436/440 (99%)	424 (97%)	12 (3%)	0	100	100
1	D	437/440 (99%)	425 (97%)	12 (3%)	0	100	100
1	E	436/440 (99%)	425 (98%)	11 (2%)	0	100	100
1	F	437/440 (99%)	425 (97%)	12 (3%)	0	100	100
All	All	2617/2640 (99%)	2549 (97%)	68 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	368/370 (100%)	365 (99%)	3 (1%)	83	92
1	B	367/370 (99%)	365 (100%)	2 (0%)	90	96
1	C	369/370 (100%)	362 (98%)	7 (2%)	60	78
1	D	369/370 (100%)	367 (100%)	2 (0%)	90	96
1	E	369/370 (100%)	364 (99%)	5 (1%)	69	84
1	F	370/370 (100%)	365 (99%)	5 (1%)	69	84
All	All	2212/2220 (100%)	2188 (99%)	24 (1%)	76	88

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

Mol	Chain	Res	Type
1	A	136	TYR
1	A	302	ARG
1	A	380	LEU
1	B	17	GLU
1	B	40	GLU
1	C	7	GLU
1	C	100	GLU
1	C	281	LYS
1	C	380	LEU
1	C	413	GLU
1	C	435	VAL
1	C	438	ARG
1	D	7	GLU
1	D	252	ARG
1	E	6	GLN
1	E	7	GLU
1	E	31	PRO
1	E	252	ARG
1	E	396	GLU
1	F	69	ASP
1	F	281	LYS
1	F	435	VAL
1	F	438	ARG
1	F	439	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	131	GLN

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Mol	Chain	Res	Type
1	C	131	GLN
1	E	131	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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	CSO	A	249	1	4,6,7	0.49	0	1,6,8	0.70	0
1	CSO	B	249	1	4,6,7	0.64	0	1,6,8	1.17	0
1	CSO	C	249	1	4,6,7	0.42	0	1,6,8	0.61	0
1	CSO	D	249	1	4,6,7	1.31	1 (25%)	1,6,8	0.75	0
1	CSO	E	249	1	4,6,7	0.48	0	1,6,8	1.14	0
1	CSO	F	249	1	4,6,7	0.72	0	1,6,8	1.11	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
1	CSO	A	249	1	-	0/1/5/7	0/0/0/0
1	CSO	B	249	1	-	0/1/5/7	0/0/0/0
1	CSO	C	249	1	-	0/1/5/7	0/0/0/0
1	CSO	D	249	1	-	0/1/5/7	0/0/0/0
1	CSO	E	249	1	-	0/1/5/7	0/0/0/0
1	CSO	F	249	1	-	0/1/5/7	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	249	CSO	CA-C	2.14	1.53	1.50

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.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	IPA	A	1440	-	3,3,3	0.55	0	3,3,3	0.26	0
2	IPA	A	1441	-	3,3,3	0.45	0	3,3,3	0.53	0
2	IPA	B	1439	-	3,3,3	0.56	0	3,3,3	0.22	0
2	IPA	B	1440	-	3,3,3	0.35	0	3,3,3	0.37	0
2	IPA	C	1440	-	3,3,3	0.56	0	3,3,3	0.20	0
2	IPA	D	1441	-	3,3,3	0.47	0	3,3,3	0.25	0
2	IPA	D	1442	-	3,3,3	0.55	0	3,3,3	0.13	0
2	IPA	D	1443	-	3,3,3	0.43	0	3,3,3	0.37	0
2	IPA	E	1440	-	3,3,3	0.43	0	3,3,3	0.29	0
2	IPA	E	1441	-	3,3,3	0.47	0	3,3,3	0.27	0
2	IPA	F	1441	-	3,3,3	0.61	0	3,3,3	0.44	0
2	IPA	F	1442	-	3,3,3	0.42	0	3,3,3	0.40	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	IPA	A	1440	-	-	0/0/0/0	0/0/0/0
2	IPA	A	1441	-	-	0/0/0/0	0/0/0/0
2	IPA	B	1439	-	-	0/0/0/0	0/0/0/0
2	IPA	B	1440	-	-	0/0/0/0	0/0/0/0
2	IPA	C	1440	-	-	0/0/0/0	0/0/0/0
2	IPA	D	1441	-	-	0/0/0/0	0/0/0/0
2	IPA	D	1442	-	-	0/0/0/0	0/0/0/0
2	IPA	D	1443	-	-	0/0/0/0	0/0/0/0
2	IPA	E	1440	-	-	0/0/0/0	0/0/0/0
2	IPA	E	1441	-	-	0/0/0/0	0/0/0/0
2	IPA	F	1441	-	-	0/0/0/0	0/0/0/0
2	IPA	F	1442	-	-	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	438/440 (99%)	-0.48	4 (0%) 84 82	16, 23, 40, 47	0
1	B	437/440 (99%)	-0.42	10 (2%) 60 57	16, 23, 40, 46	0
1	C	438/440 (99%)	-0.46	3 (0%) 87 86	16, 23, 41, 52	0
1	D	439/440 (99%)	-0.45	4 (0%) 84 82	16, 23, 40, 47	0
1	E	438/440 (99%)	-0.49	5 (1%) 80 78	16, 23, 40, 50	0
1	F	439/440 (99%)	-0.47	5 (1%) 80 78	16, 23, 41, 63	0
All	All	2629/2640 (99%)	-0.46	31 (1%) 79 77	16, 23, 40, 63	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	440	GLN	5.5
1	A	70	THR	3.7
1	D	70	THR	3.6
1	B	332	LYS	3.5
1	C	70	THR	3.2
1	D	69	ASP	3.1
1	B	70	THR	2.9
1	B	393	GLU	2.8
1	B	71	HIS	2.8
1	B	83	LEU	2.8
1	F	71	HIS	2.7
1	E	69	ASP	2.6
1	F	70	THR	2.5
1	F	83	LEU	2.5
1	C	69	ASP	2.5
1	B	341	GLN	2.4
1	F	69	ASP	2.4
1	E	83	LEU	2.4
1	D	71	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	396	GLU	2.2
1	A	69	ASP	2.2
1	E	70	THR	2.2
1	B	391	ASP	2.1
1	E	439	LYS	2.1
1	A	332	LYS	2.1
1	B	334	ASP	2.1
1	C	83	LEU	2.1
1	B	69	ASP	2.1
1	A	71	HIS	2.0
1	E	71	HIS	2.0
1	D	332	LYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	CSO	B	249	7/8	0.93	0.10	29,31,34,35	0
1	CSO	A	249	7/8	0.95	0.10	29,31,35,36	0
1	CSO	D	249	7/8	0.95	0.12	29,31,35,35	0
1	CSO	E	249	7/8	0.96	0.08	29,31,33,36	0
1	CSO	C	249	7/8	0.98	0.08	29,31,34,36	0
1	CSO	F	249	7/8	0.98	0.07	29,31,33,35	0

## 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	IPA	F	1442	4/4	0.88	0.30	38,39,39,42	0
2	IPA	E	1441	4/4	0.90	0.28	33,34,36,37	0
2	IPA	D	1443	4/4	0.90	0.27	38,39,40,40	0
2	IPA	D	1441	4/4	0.93	0.24	40,40,40,42	0
2	IPA	B	1440	4/4	0.94	0.24	36,36,37,40	0
2	IPA	A	1441	4/4	0.94	0.23	35,36,37,38	0
3	CA	D	1444	1/1	0.95	0.15	35,35,35,35	0
3	CA	A	1442	1/1	0.97	0.16	32,32,32,32	0
3	CA	B	1441	1/1	0.97	0.12	34,34,34,34	0
2	IPA	B	1439	4/4	0.98	0.10	27,29,30,31	0
4	CL	F	1444	1/1	0.98	0.04	40,40,40,40	0
3	CA	E	1442	1/1	0.98	0.15	26,26,26,26	0
2	IPA	F	1441	4/4	0.98	0.19	29,30,31,32	0
3	CA	F	1443	1/1	0.98	0.15	30,30,30,30	0
2	IPA	D	1442	4/4	0.98	0.17	26,28,28,28	0
2	IPA	C	1440	4/4	0.98	0.11	31,31,32,32	0
2	IPA	A	1440	4/4	0.98	0.16	32,35,36,36	0
4	CL	E	1443	1/1	0.99	0.08	35,35,35,35	0
4	CL	A	1443	1/1	0.99	0.12	45,45,45,45	0
3	CA	C	1441	1/1	0.99	0.12	29,29,29,29	0
4	CL	C	1442	1/1	0.99	0.09	45,45,45,45	0
4	CL	D	1445	1/1	0.99	0.12	42,42,42,42	0
2	IPA	E	1440	4/4	0.99	0.16	27,29,30,30	0
4	CL	B	1442	1/1	0.99	0.09	44,44,44,44	0

## 6.5 Other polymers

There are no such residues in this entry.