



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 07:36 AM BST

PDB ID : 6STU  
Title : Adenovirus 30 Fiber Knob protein  
Authors : Baker, A.T.; Mundy, R.M.; Rizkallah, P.J.; Parker, A.L.  
Deposited on : 2019-09-11  
Resolution : 2.39 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.4.dev1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

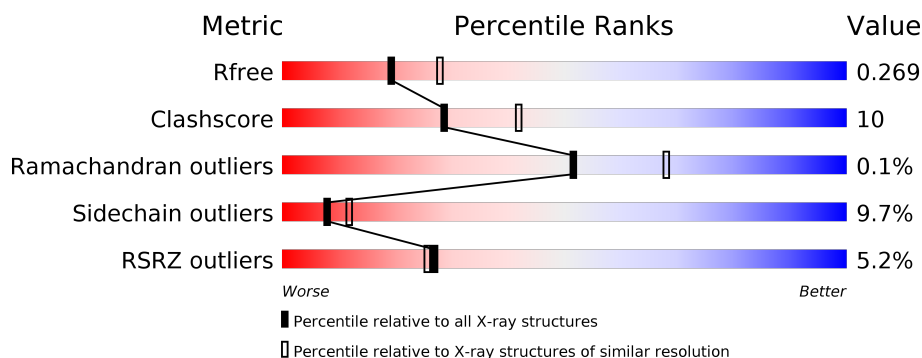
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 respectively. 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	208	<div> <div>0%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>• • •</div> </div> </div>
1	B	208	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>• •</div> </div> </div>
1	C	208	<div> <div>7%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>• •</div> </div> </div>
1	D	208	<div> <div>9%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>• •</div> </div> </div>
1	E	208	<div> <div>7%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>• •</div> </div> </div>
1	F	208	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>25%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9637 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 Fiber.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	204	Total	C	N	O	S	0	0	0
			1577	999	255	319	4			
1	B	203	Total	C	N	O	S	0	0	0
			1570	994	252	320	4			
1	C	206	Total	C	N	O	S	0	0	0
			1588	1006	257	321	4			
1	D	201	Total	C	N	O	S	0	0	0
			1552	985	249	314	4			
1	E	201	Total	C	N	O	S	0	0	0
			1552	985	249	314	4			
1	F	205	Total	C	N	O	S	0	0	0
			1587	1004	256	323	4			

There are 30 discrepancies between the modelled and reference sequences:

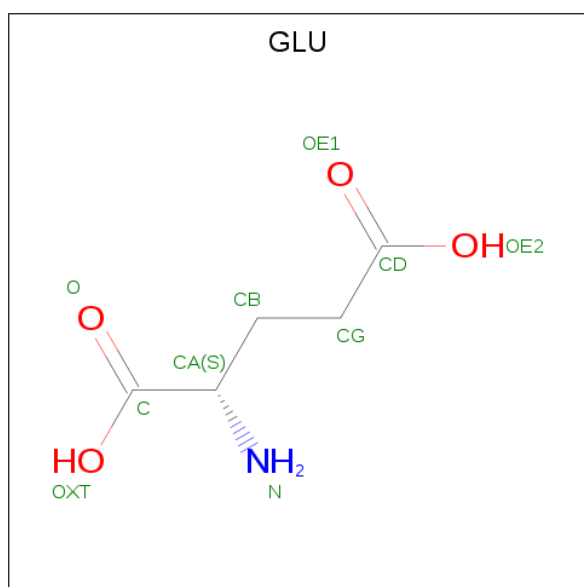
Chain	Residue	Modelled	Actual	Comment	Reference
A	178	VAL	ALA	conflict	UNP M0QTV3
A	179	GLY	TRP	conflict	UNP M0QTV3
A	182	ASN	GLU	conflict	UNP M0QTV3
A	185	LYS	ARG	conflict	UNP M0QTV3
A	186	LEU	ARG	conflict	UNP M0QTV3
B	178	VAL	ALA	conflict	UNP M0QTV3
B	179	GLY	TRP	conflict	UNP M0QTV3
B	182	ASN	GLU	conflict	UNP M0QTV3
B	185	LYS	ARG	conflict	UNP M0QTV3
B	186	LEU	ARG	conflict	UNP M0QTV3
C	178	VAL	ALA	conflict	UNP M0QTV3
C	179	GLY	TRP	conflict	UNP M0QTV3
C	182	ASN	GLU	conflict	UNP M0QTV3
C	185	LYS	ARG	conflict	UNP M0QTV3
C	186	LEU	ARG	conflict	UNP M0QTV3
D	178	VAL	ALA	conflict	UNP M0QTV3
D	179	GLY	TRP	conflict	UNP M0QTV3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	182	ASN	GLU	conflict	UNP M0QTV3
D	185	LYS	ARG	conflict	UNP M0QTV3
D	186	LEU	ARG	conflict	UNP M0QTV3
E	178	VAL	ALA	conflict	UNP M0QTV3
E	179	GLY	TRP	conflict	UNP M0QTV3
E	182	ASN	GLU	conflict	UNP M0QTV3
E	185	LYS	ARG	conflict	UNP M0QTV3
E	186	LEU	ARG	conflict	UNP M0QTV3
F	178	VAL	ALA	conflict	UNP M0QTV3
F	179	GLY	TRP	conflict	UNP M0QTV3
F	182	ASN	GLU	conflict	UNP M0QTV3
F	185	LYS	ARG	conflict	UNP M0QTV3
F	186	LEU	ARG	conflict	UNP M0QTV3

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula:  $C_5H_9NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

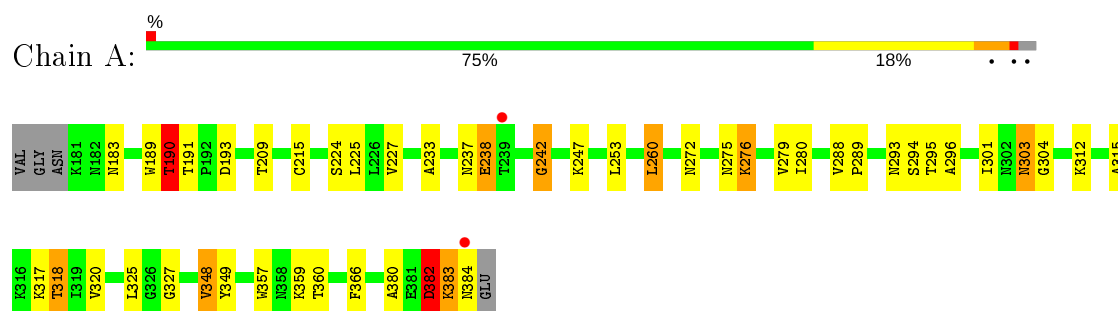
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	37	Total	O	0	0
			37	37		
4	B	53	Total	O	0	0
			53	53		
4	C	36	Total	O	0	0
			36	36		
4	D	19	Total	O	0	0
			19	19		
4	E	16	Total	O	0	0
			16	16		
4	F	32	Total	O	0	0
			32	32		

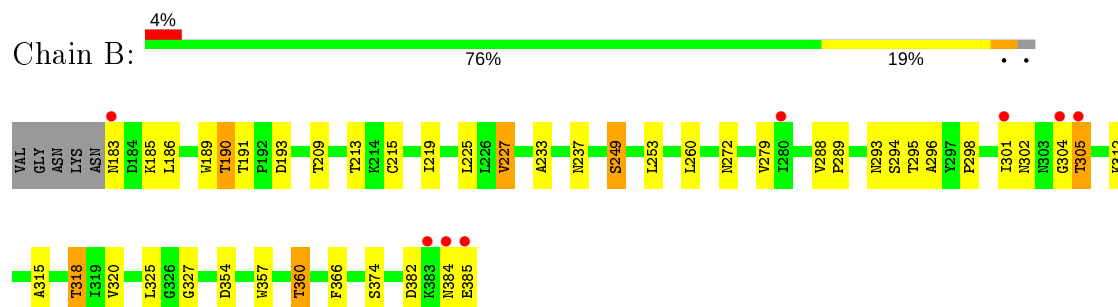
### 3 Residue-property plots

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

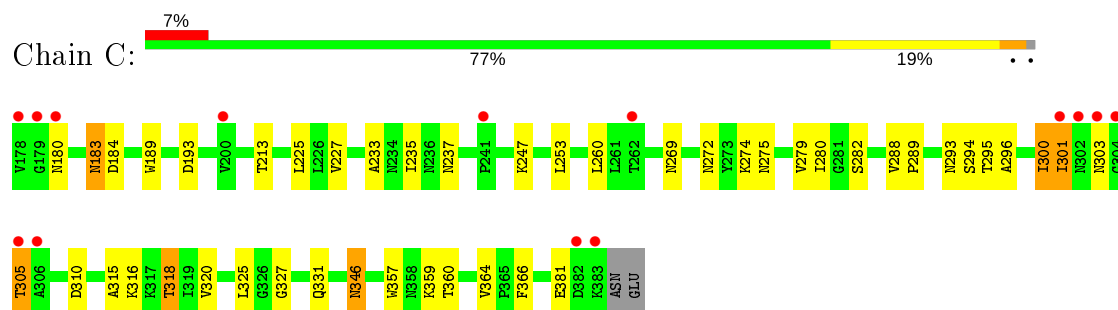
#### • Molecule 1: Fiber



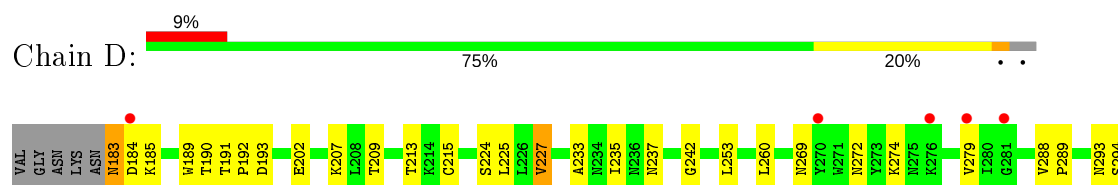
#### • Molecule 1: Fiber



#### • Molecule 1: Fiber

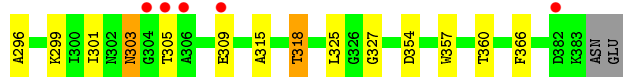
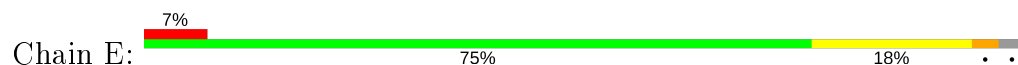


#### • Molecule 1: Fiber

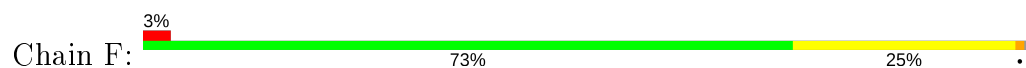




• Molecule 1: Fiber



• Molecule 1: Fiber



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.35Å 87.36Å 217.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.76 – 2.39 54.76 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.9 (54.76-2.39) 99.9 (54.76-2.39)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.217 , 0.268 0.219 , 0.269	Depositor DCC
$R_{free}$ test set	2348 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.0	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 30.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9637	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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: EDO

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	0.83	3/1611 (0.2%)	0.96	4/2189 (0.2%)
1	B	0.73	0/1604	0.90	0/2179
1	C	0.71	0/1622	0.89	0/2204
1	D	0.68	0/1586	0.88	0/2156
1	E	0.69	0/1586	0.93	4/2156 (0.2%)
1	F	0.71	0/1621	0.91	0/2201
All	All	0.73	3/9630 (0.0%)	0.91	8/13085 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	D	0	2
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	238	GLU	CD-OE1	12.31	1.39	1.25
1	A	238	GLU	CD-OE2	6.12	1.32	1.25
1	A	242	GLY	C-O	5.17	1.31	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	191	THR	CA-CB-OG1	-6.84	94.63	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	THR	N-CA-CB	-6.83	97.33	110.30
1	E	190	THR	N-CA-C	-6.57	93.26	111.00
1	A	382	ASP	CB-CA-C	5.44	121.28	110.40
1	A	190	THR	OG1-CB-CG2	5.32	122.23	110.00
1	E	190	THR	CA-C-N	5.28	128.82	117.20
1	E	191	THR	CB-CA-C	5.25	125.77	111.60
1	A	303	ASN	C-N-CA	-5.06	111.67	122.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	242	GLY	Peptide
1	A	304	GLY	Peptide
1	B	302	ASN	Peptide
1	D	183	ASN	Peptide
1	D	242	GLY	Peptide

## 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	1577	0	1549	37	0
1	B	1570	0	1536	41	0
1	C	1588	0	1561	32	0
1	D	1552	0	1523	35	0
1	E	1552	0	1523	30	0
1	F	1587	0	1554	39	0
2	A	10	0	5	0	0
3	A	4	0	6	1	0
3	F	4	0	6	1	0
4	A	37	0	0	0	0
4	B	53	0	0	2	0
4	C	36	0	0	2	0
4	D	19	0	0	1	0
4	E	16	0	0	0	0
4	F	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9637	0	9263	181	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 10.

All (181) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ASN:HB3	1:B:279:VAL:CG2	1.54	1.36
1:B:272:ASN:HB3	1:B:279:VAL:HG23	1.21	1.09
1:A:190:THR:HG21	1:A:209:THR:HA	1.39	1.02
1:B:272:ASN:CB	1:B:279:VAL:CG2	2.42	0.96
1:B:190:THR:HG21	1:B:209:THR:HA	1.44	0.95
1:B:272:ASN:HB3	1:B:279:VAL:HG21	1.52	0.91
1:D:327:GLY:HA3	1:F:318:THR:HG21	1.54	0.88
1:A:276:LYS:O	1:A:276:LYS:HG3	1.76	0.83
1:A:318:THR:HG21	1:B:327:GLY:HA3	1.60	0.83
1:A:295:THR:HG22	1:B:193:ASP:HB2	1.66	0.78
1:D:327:GLY:CA	1:F:318:THR:HG21	2.13	0.77
1:B:272:ASN:CB	1:B:279:VAL:HG21	2.12	0.77
1:A:382:ASP:OD1	1:A:383:LYS:N	2.15	0.77
1:B:293:ASN:HD22	1:B:296:ALA:H	1.35	0.74
1:F:234:ASN:ND2	1:F:363:ASN:HA	2.02	0.74
1:E:318:THR:HG21	1:F:327:GLY:HA3	1.70	0.73
1:D:318:THR:HG21	1:E:327:GLY:HA3	1.68	0.72
1:B:318:THR:HG21	1:C:327:GLY:HA3	1.70	0.72
1:D:293:ASN:HD22	1:D:296:ALA:H	1.37	0.72
1:B:237:ASN:HD21	1:B:357:TRP:HE1	1.39	0.71
1:C:293:ASN:HD22	1:C:296:ALA:H	1.37	0.71
1:C:237:ASN:HD21	1:C:357:TRP:HE1	1.39	0.71
1:C:303:ASN:ND2	4:C:401:HOH:O	2.21	0.71
1:A:293:ASN:HD22	1:A:296:ALA:H	1.37	0.70
1:E:227:VAL:HG13	1:E:366:PHE:HB3	1.71	0.70
1:F:293:ASN:HD22	1:F:296:ALA:H	1.38	0.70
1:A:318:THR:HG21	1:B:327:GLY:CA	2.22	0.70
1:B:227:VAL:HG13	1:B:366:PHE:HB3	1.72	0.70
1:E:293:ASN:HD22	1:E:296:ALA:H	1.37	0.70
1:C:227:VAL:HG13	1:C:366:PHE:HB3	1.74	0.70
1:E:237:ASN:HD21	1:E:357:TRP:HE1	1.40	0.70
1:D:227:VAL:HG13	1:D:366:PHE:HB3	1.72	0.70
1:A:276:LYS:CG	1:A:276:LYS:O	2.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ILE:HG13	1:B:312:LYS:HG3	1.74	0.69
1:D:193:ASP:HB2	1:F:295:THR:HG22	1.73	0.69
1:D:237:ASN:HD21	1:D:357:TRP:HE1	1.40	0.69
1:B:301:ILE:CG1	1:B:312:LYS:HG3	2.22	0.69
1:F:237:ASN:HD21	1:F:357:TRP:HE1	1.39	0.68
1:A:237:ASN:HD21	1:A:357:TRP:HE1	1.41	0.68
1:A:227:VAL:HG13	1:A:366:PHE:HB3	1.73	0.68
1:F:243:GLU:H	1:F:243:GLU:CD	1.96	0.68
1:A:327:GLY:HA3	1:C:318:THR:HG21	1.74	0.67
1:F:227:VAL:HG13	1:F:366:PHE:HB3	1.76	0.67
1:A:293:ASN:HD21	1:A:295:THR:HB	1.59	0.66
1:B:293:ASN:HD21	1:B:295:THR:HB	1.60	0.66
1:C:300:ILE:HD13	1:C:301:ILE:H	1.59	0.66
1:A:327:GLY:CA	1:C:318:THR:HG21	2.25	0.65
1:F:293:ASN:HD21	1:F:295:THR:HB	1.60	0.65
1:D:318:THR:HG21	1:E:327:GLY:CA	2.27	0.64
1:A:193:ASP:HB2	1:C:295:THR:HG22	1.78	0.64
1:D:293:ASN:HD21	1:D:295:THR:HB	1.61	0.64
1:E:318:THR:HG21	1:F:327:GLY:CA	2.27	0.64
1:D:184:ASP:HB3	1:D:274:LYS:O	1.98	0.64
1:F:184:ASP:HB3	1:F:274:LYS:O	1.98	0.64
1:A:380:ALA:O	1:A:384:ASN:ND2	2.31	0.63
1:E:295:THR:HG22	1:F:193:ASP:HB2	1.80	0.63
1:D:191:THR:HG23	1:D:192:PRO:HD2	1.81	0.63
1:B:304:GLY:O	1:B:305:THR:HG22	1.99	0.63
1:C:300:ILE:HD13	1:C:301:ILE:N	2.14	0.62
1:D:209:THR:HG21	1:F:316:LYS:NZ	2.14	0.62
1:B:318:THR:HG21	1:C:327:GLY:CA	2.30	0.61
1:E:293:ASN:HD21	1:E:295:THR:HB	1.64	0.61
1:D:299:LYS:HD3	1:D:343:THR:HG22	1.83	0.61
1:E:183:ASN:HB3	1:E:275:ASN:HA	1.83	0.60
1:A:224:SER:HB3	3:A:402:EDO:H11	1.84	0.58
1:D:207:LYS:NZ	1:F:311:LYS:O	2.35	0.58
1:E:215:CYS:O	1:F:213:THR:HG21	2.04	0.58
1:F:234:ASN:HD21	1:F:363:ASN:CA	2.17	0.57
1:C:293:ASN:HD21	1:C:295:THR:HB	1.70	0.57
1:E:249:SER:HB2	1:E:354:ASP:OD1	2.05	0.56
1:E:315:ALA:O	1:E:318:THR:HB	2.05	0.56
1:B:190:THR:HG23	1:B:191:THR:O	2.05	0.56
1:B:249:SER:HB2	1:B:354:ASP:OD1	2.05	0.56
1:A:315:ALA:O	1:A:318:THR:HB	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:ALA:O	1:C:318:THR:HB	2.05	0.55
1:F:315:ALA:O	1:F:318:THR:HB	2.07	0.55
1:A:209:THR:CG2	1:A:224:SER:HB3	2.36	0.55
1:A:215:CYS:O	1:B:213:THR:HG21	2.08	0.54
1:D:315:ALA:O	1:D:318:THR:HB	2.07	0.54
1:E:189:TRP:C	1:E:190:THR:O	2.40	0.53
1:B:190:THR:CG2	1:B:191:THR:O	2.57	0.53
1:B:315:ALA:O	1:B:318:THR:HB	2.08	0.53
1:E:227:VAL:HG22	1:E:233:ALA:HA	1.91	0.53
1:B:295:THR:HG22	1:C:193:ASP:HB2	1.90	0.53
1:B:304:GLY:HA2	4:B:448:HOH:O	2.08	0.53
1:E:285:GLU:OE2	1:E:286:ASN:N	2.42	0.52
1:A:293:ASN:ND2	1:A:295:THR:HB	2.25	0.52
1:E:303:ASN:C	1:E:303:ASN:HD22	2.13	0.51
1:D:213:THR:HG21	1:F:215:CYS:O	2.10	0.51
1:C:331:GLN:NE2	4:C:402:HOH:O	2.34	0.51
1:A:301:ILE:CD1	1:A:317:LYS:HD2	2.41	0.51
1:B:360:THR:HG22	4:B:410:HOH:O	2.11	0.50
1:B:318:THR:HG23	1:B:320:VAL:HG23	1.93	0.50
1:E:183:ASN:CB	1:E:275:ASN:HA	2.41	0.50
1:C:346:ASN:N	1:C:346:ASN:HD22	2.08	0.50
1:F:293:ASN:ND2	1:F:295:THR:HB	2.26	0.50
1:B:293:ASN:ND2	1:B:295:THR:HB	2.26	0.50
1:C:180:ASN:CB	1:C:275:ASN:HD21	2.24	0.49
1:D:327:GLY:HA2	1:F:318:THR:HG21	1.95	0.49
1:D:227:VAL:HG22	1:D:233:ALA:HA	1.95	0.49
1:D:293:ASN:ND2	1:D:295:THR:HB	2.28	0.48
1:E:189:TRP:CD1	1:E:190:THR:O	2.67	0.48
1:D:295:THR:HG22	1:E:193:ASP:HB2	1.96	0.48
1:A:183:ASN:HB2	1:A:280:ILE:CD1	2.44	0.48
1:A:190:THR:CG2	1:A:191:THR:O	2.61	0.48
1:A:327:GLY:HA2	1:C:318:THR:HG21	1.96	0.48
1:A:227:VAL:HG22	1:A:233:ALA:HA	1.97	0.47
1:B:305:THR:O	1:B:305:THR:HG23	2.14	0.47
1:D:209:THR:HG21	1:F:316:LYS:CE	2.44	0.47
1:F:227:VAL:HG22	1:F:233:ALA:HA	1.97	0.47
1:A:190:THR:HG22	1:A:191:THR:O	2.13	0.47
1:B:227:VAL:HG22	1:B:233:ALA:HA	1.96	0.47
1:D:215:CYS:O	1:E:213:THR:HG21	2.14	0.47
1:F:234:ASN:ND2	1:F:363:ASN:CA	2.73	0.47
1:B:272:ASN:HB2	1:B:279:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:THR:HG23	4:D:415:HOH:O	2.14	0.47
1:B:215:CYS:O	1:C:213:THR:HG21	2.15	0.46
1:E:293:ASN:ND2	1:E:295:THR:HB	2.30	0.46
1:B:298:PRO:HB2	1:B:301:ILE:HD13	1.97	0.46
1:D:193:ASP:CB	1:F:295:THR:HG22	2.45	0.46
1:B:382:ASP:HB3	1:B:385:GLU:OXT	2.16	0.46
1:D:202:GLU:OE1	1:D:202:GLU:HA	2.16	0.45
1:C:183:ASN:HB2	1:C:280:ILE:CD1	2.47	0.45
1:A:183:ASN:HB3	1:A:275:ASN:HD22	1.81	0.45
1:F:318:THR:HG23	1:F:320:VAL:HG23	1.99	0.45
1:C:184:ASP:OD1	1:C:274:LYS:HB3	2.17	0.44
1:A:295:THR:CG2	1:B:193:ASP:HB2	2.43	0.44
1:F:243:GLU:CD	1:F:243:GLU:N	2.68	0.44
1:A:209:THR:HG21	1:C:316:LYS:HE3	2.00	0.44
1:E:189:TRP:CG	1:E:190:THR:O	2.71	0.44
1:C:227:VAL:HG22	1:C:233:ALA:HA	2.00	0.44
1:A:303:ASN:HD21	1:A:312:LYS:H	1.66	0.44
1:B:301:ILE:HG12	1:B:312:LYS:HG3	1.96	0.44
1:D:348:VAL:HG22	1:D:349:TYR:CD2	2.53	0.43
1:B:288:VAL:HB	1:B:289:PRO:HD3	2.00	0.43
1:F:224:SER:HB2	3:F:401:EDO:O1	2.18	0.43
1:A:318:THR:HG23	1:A:320:VAL:HG23	2.01	0.43
1:E:183:ASN:N	1:E:274:LYS:O	2.51	0.43
1:A:348:VAL:HG22	1:A:349:TYR:CD2	2.53	0.43
1:A:288:VAL:N	1:A:289:PRO:CD	2.82	0.43
1:B:219:ILE:O	1:B:374:SER:HA	2.19	0.43
1:A:272:ASN:HB3	1:A:279:VAL:HB	2.01	0.43
1:D:288:VAL:N	1:D:289:PRO:CD	2.83	0.42
1:A:288:VAL:HB	1:A:289:PRO:HD3	2.00	0.42
1:E:272:ASN:HB3	1:E:279:VAL:HB	2.02	0.42
1:D:209:THR:HG21	1:F:316:LYS:HZ1	1.84	0.42
1:D:348:VAL:CG2	1:D:349:TYR:CE2	3.02	0.42
1:F:238:GLU:OE2	1:F:362:LYS:HG2	2.20	0.42
1:D:272:ASN:HB3	1:D:279:VAL:HB	2.00	0.42
1:D:235:ILE:HG12	1:D:364:VAL:O	2.20	0.42
1:F:272:ASN:HB3	1:F:279:VAL:HB	2.02	0.42
1:D:190:THR:O	1:D:191:THR:HB	2.20	0.42
1:D:288:VAL:HB	1:D:289:PRO:HD3	2.01	0.42
1:C:288:VAL:N	1:C:289:PRO:CD	2.83	0.42
1:C:293:ASN:ND2	1:C:295:THR:HB	2.34	0.42
1:C:272:ASN:HB3	1:C:279:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:288:VAL:N	1:E:289:PRO:CD	2.82	0.42
1:F:189:TRP:CH2	1:F:274:LYS:HE2	2.55	0.42
1:F:288:VAL:HB	1:F:289:PRO:HD3	2.02	0.42
1:C:235:ILE:HG12	1:C:364:VAL:O	2.19	0.41
1:C:183:ASN:HB3	1:C:275:ASN:HD22	1.84	0.41
1:C:180:ASN:HB3	1:C:275:ASN:HD21	1.85	0.41
1:F:235:ILE:HG12	1:F:364:VAL:O	2.20	0.41
1:B:301:ILE:CG2	1:B:301:ILE:O	2.69	0.41
1:E:288:VAL:HB	1:E:289:PRO:HD3	2.02	0.41
1:F:308:PRO:HA	1:F:311:LYS:HG3	2.03	0.41
1:B:288:VAL:N	1:B:289:PRO:CD	2.83	0.41
1:F:303:ASN:HD21	1:F:312:LYS:H	1.67	0.41
1:C:318:THR:HG23	1:C:320:VAL:HG23	2.01	0.41
1:E:318:THR:HG21	1:F:327:GLY:HA2	2.03	0.41
1:A:260:LEU:HA	1:A:260:LEU:HD23	1.97	0.41
1:B:298:PRO:HG2	1:B:301:ILE:HG21	2.03	0.41
1:C:288:VAL:HB	1:C:289:PRO:HD3	2.03	0.41
1:A:348:VAL:CG2	1:A:349:TYR:CE2	3.04	0.40
1:D:299:LYS:CD	1:D:343:THR:HG22	2.51	0.40
1:E:280:ILE:HG21	1:E:280:ILE:HD13	1.94	0.40
1:E:301:ILE:HD12	1:E:301:ILE:N	2.36	0.40
1:F:288:VAL:N	1:F:289:PRO:CD	2.84	0.40
1:C:180:ASN:ND2	1:C:275:ASN:HD21	2.20	0.40
1:D:318:THR:HG23	1:D:320:VAL:HG23	2.02	0.40
1:F:219:ILE:O	1:F:374:SER:HA	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	202/208 (97%)	190 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	201/208 (97%)	190 (94%)	11 (6%)	0	100	100
1	C	204/208 (98%)	193 (95%)	10 (5%)	1 (0%)	29	41
1	D	199/208 (96%)	187 (94%)	12 (6%)	0	100	100
1	E	199/208 (96%)	186 (94%)	13 (6%)	0	100	100
1	F	203/208 (98%)	191 (94%)	12 (6%)	0	100	100
All	All	1208/1248 (97%)	1137 (94%)	70 (6%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	305	THR

### 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	180/183 (98%)	164 (91%)	16 (9%)	9	14
1	B	179/183 (98%)	163 (91%)	16 (9%)	9	14
1	C	181/183 (99%)	162 (90%)	19 (10%)	7	9
1	D	177/183 (97%)	163 (92%)	14 (8%)	12	19
1	E	177/183 (97%)	158 (89%)	19 (11%)	6	9
1	F	181/183 (99%)	161 (89%)	20 (11%)	6	8
All	All	1075/1098 (98%)	971 (90%)	104 (10%)	8	12

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	TRP
1	A	190	THR
1	A	225	LEU
1	A	238	GLU
1	A	247	LYS

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Mol	Chain	Res	Type
1	A	253	LEU
1	A	260	LEU
1	A	276	LYS
1	A	294	SER
1	A	318	THR
1	A	325	LEU
1	A	348	VAL
1	A	359	LYS
1	A	360	THR
1	A	382	ASP
1	A	383	LYS
1	B	183	ASN
1	B	185	LYS
1	B	186	LEU
1	B	189	TRP
1	B	190	THR
1	B	225	LEU
1	B	227	VAL
1	B	249	SER
1	B	253	LEU
1	B	260	LEU
1	B	294	SER
1	B	305	THR
1	B	318	THR
1	B	325	LEU
1	B	360	THR
1	B	384	ASN
1	C	183	ASN
1	C	189	TRP
1	C	225	LEU
1	C	247	LYS
1	C	253	LEU
1	C	260	LEU
1	C	269	ASN
1	C	282	SER
1	C	294	SER
1	C	300	ILE
1	C	301	ILE
1	C	305	THR
1	C	310	ASP
1	C	318	THR
1	C	325	LEU

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Mol	Chain	Res	Type
1	C	346	ASN
1	C	359	LYS
1	C	360	THR
1	C	381	GLU
1	D	183	ASN
1	D	185	LYS
1	D	189	TRP
1	D	224	SER
1	D	225	LEU
1	D	227	VAL
1	D	253	LEU
1	D	260	LEU
1	D	269	ASN
1	D	294	SER
1	D	318	THR
1	D	325	LEU
1	D	348	VAL
1	D	360	THR
1	E	189	TRP
1	E	202	GLU
1	E	215	CYS
1	E	224	SER
1	E	225	LEU
1	E	238	GLU
1	E	243	GLU
1	E	249	SER
1	E	253	LEU
1	E	260	LEU
1	E	285	GLU
1	E	294	SER
1	E	299	LYS
1	E	303	ASN
1	E	305	THR
1	E	309	GLU
1	E	318	THR
1	E	325	LEU
1	E	360	THR
1	F	182	ASN
1	F	189	TRP
1	F	202	GLU
1	F	225	LEU
1	F	234	ASN

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Mol	Chain	Res	Type
1	F	247	LYS
1	F	253	LEU
1	F	260	LEU
1	F	294	SER
1	F	302	ASN
1	F	305	THR
1	F	318	THR
1	F	325	LEU
1	F	344	GLU
1	F	359	LYS
1	F	360	THR
1	F	381	GLU
1	F	383	LYS
1	F	384	ASN
1	F	385	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	ASN
1	A	218	GLN
1	A	237	ASN
1	A	275	ASN
1	A	293	ASN
1	A	302	ASN
1	A	303	ASN
1	A	363	ASN
1	B	218	GLN
1	B	237	ASN
1	B	293	ASN
1	B	303	ASN
1	B	363	ASN
1	C	180	ASN
1	C	218	GLN
1	C	237	ASN
1	C	269	ASN
1	C	275	ASN
1	C	293	ASN
1	C	346	ASN
1	C	363	ASN
1	D	218	GLN
1	D	237	ASN

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Mol	Chain	Res	Type
1	D	293	ASN
1	D	303	ASN
1	D	346	ASN
1	D	363	ASN
1	E	218	GLN
1	E	237	ASN
1	E	257	ASN
1	E	269	ASN
1	E	293	ASN
1	E	363	ASN
1	F	234	ASN
1	F	237	ASN
1	F	269	ASN
1	F	293	ASN
1	F	303	ASN
1	F	363	ASN
1	F	384	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 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
3	EDO	A	402	-	3,3,3	0.56	0	2,2,2	0.74	0
3	EDO	F	401	-	3,3,3	0.36	0	2,2,2	0.50	0
2	GLU	A	401	-	2,9,9	0.94	0	2,11,11	0.28	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
3	EDO	A	402	-	-	0/1/1/1	-
3	EDO	F	401	-	-	1/1/1/1	-
2	GLU	A	401	-	-	0/3/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	401	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	EDO	1	0
3	F	401	EDO	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	204/208 (98%)	0.01	2 (0%) 82 80	36, 50, 94, 131	0
1	B	203/208 (97%)	0.05	8 (3%) 39 38	34, 51, 104, 155	0
1	C	206/208 (99%)	0.21	14 (6%) 17 15	40, 59, 129, 174	0
1	D	201/208 (96%)	0.41	18 (8%) 9 8	35, 71, 138, 192	0
1	E	201/208 (96%)	0.30	14 (6%) 16 15	40, 65, 116, 153	0
1	F	205/208 (98%)	0.09	7 (3%) 45 44	34, 52, 95, 142	0
All	All	1220/1248 (97%)	0.18	63 (5%) 27 26	34, 57, 116, 192	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	305	THR	8.2
1	B	384	ASN	8.0
1	E	306	ALA	7.0
1	D	306	ALA	6.9
1	F	183	ASN	6.6
1	B	383	LYS	6.1
1	C	306	ALA	5.8
1	C	303	ASN	5.7
1	F	280	ILE	5.4
1	C	178	VAL	5.1
1	C	301	ILE	5.0
1	C	302	ASN	4.8
1	D	382	ASP	4.6
1	C	179	GLY	4.6
1	D	276	LYS	4.5
1	D	303	ASN	4.4
1	B	385	GLU	4.4
1	A	384	ASN	4.1
1	E	280	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	301	ILE	3.9
1	D	305	THR	3.7
1	F	182	ASN	3.7
1	D	304	GLY	3.6
1	F	385	GLU	3.5
1	D	301	ILE	3.4
1	B	304	GLY	3.4
1	E	279	VAL	3.3
1	D	358	ASN	3.3
1	C	305	THR	3.1
1	C	382	ASP	2.9
1	D	279	VAL	2.9
1	D	307	ASN	2.8
1	C	304	GLY	2.7
1	B	305	THR	2.7
1	E	304	GLY	2.7
1	C	200	VAL	2.7
1	D	300	ILE	2.6
1	D	308	PRO	2.6
1	B	280	ILE	2.6
1	D	184	ASP	2.6
1	D	381	GLU	2.5
1	E	183	ASN	2.5
1	E	273	TYR	2.4
1	F	290	PHE	2.4
1	D	380	ALA	2.3
1	C	241	PRO	2.3
1	E	184	ASP	2.3
1	C	180	ASN	2.3
1	B	183	ASN	2.3
1	D	270	TYR	2.2
1	E	309	GLU	2.2
1	A	239	THR	2.2
1	E	194	PRO	2.2
1	D	310	ASP	2.2
1	C	383	LYS	2.1
1	E	225	LEU	2.1
1	E	277	ASP	2.1
1	F	184	ASP	2.1
1	C	262	THR	2.1
1	E	382	ASP	2.0
1	F	181	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	281	GLY	2.0
1	E	208	LEU	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 monosaccharides 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	GLU	A	401	10/10	0.41	0.28	136,142,146,150	0
3	EDO	F	401	4/4	0.89	0.23	59,61,63,67	0
3	EDO	A	402	4/4	0.91	0.34	52,54,56,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.