



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:49 PM GMT

PDB ID : 4AMV  
Title : E.COLI GLUCOSAMINE-6P SYNTHASE IN COMPLEX WITH FRUCTOSE-6P  
Authors : Mouilleron, S.; Golinelli-Pimpaneau, B.  
Deposited on : 2012-03-14  
Resolution : 2.05 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 (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

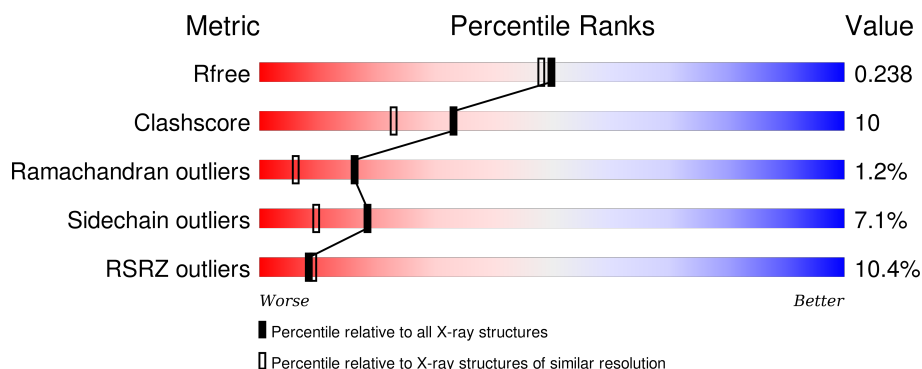
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	609	<div> <div>3%</div> <div>80%</div> <div>16%</div> <div>.</div> </div>
1	B	609	<div> <div>20%</div> <div>79%</div> <div>18%</div> <div>.</div> </div>
1	C	609	<div> <div>8%</div> <div>76%</div> <div>21%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	F6R	B	1609	X	-	-	-
2	F6R	C	1609	X	-	-	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 14225 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.

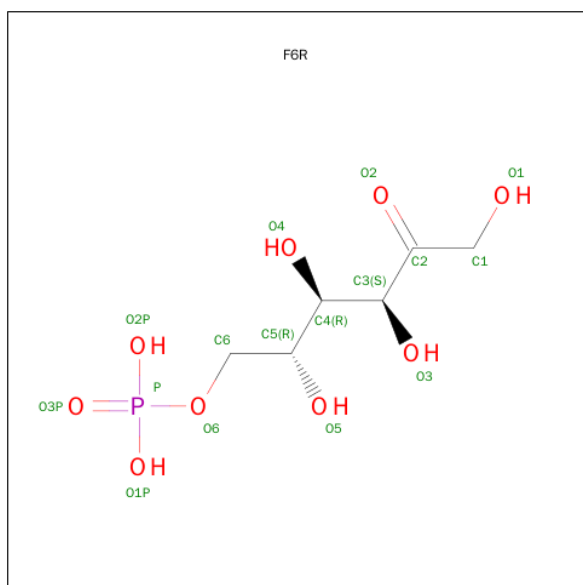
- Molecule 1 is a protein called GLUCOSAMINE--FRUCTOSE-6-PHOSPHATE AMINO-TRANSFERASE [ISOMER IZING].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	608	Total	C	N	O	S	0	0	0
			4679	2945	823	894	17			
1	B	608	Total	C	N	O	S	0	0	0
			4198	2618	740	825	15			
1	C	608	Total	C	N	O	S	0	0	0
			4606	2897	812	880	17			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	421	LYS	ARG	CONFLICT	UNP P17169
B	421	LYS	ARG	CONFLICT	UNP P17169
C	421	LYS	ARG	CONFLICT	UNP P17169

- Molecule 2 is FRUCTOSE -6-PHOSPHATE (three-letter code: F6R) (formula: C<sub>6</sub>H<sub>13</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		
2	B	1	Total	C	O	P	0	0
			16	6	9	1		
2	C	1	Total	C	O	P	0	0
			16	6	9	1		

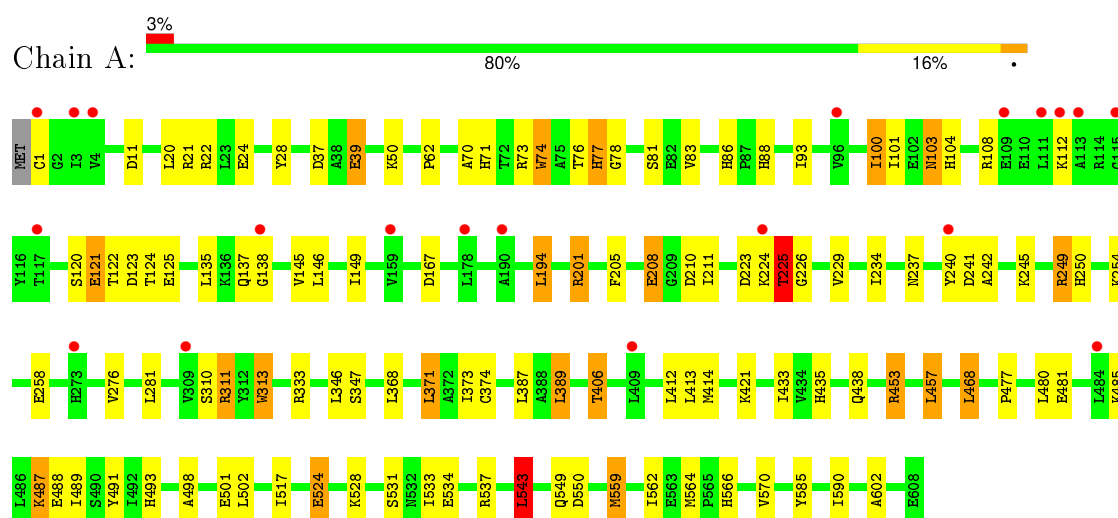
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	431	Total	O	0	0
			431	431		
3	B	53	Total	O	0	0
			53	53		
3	C	210	Total	O	0	0
			210	210		

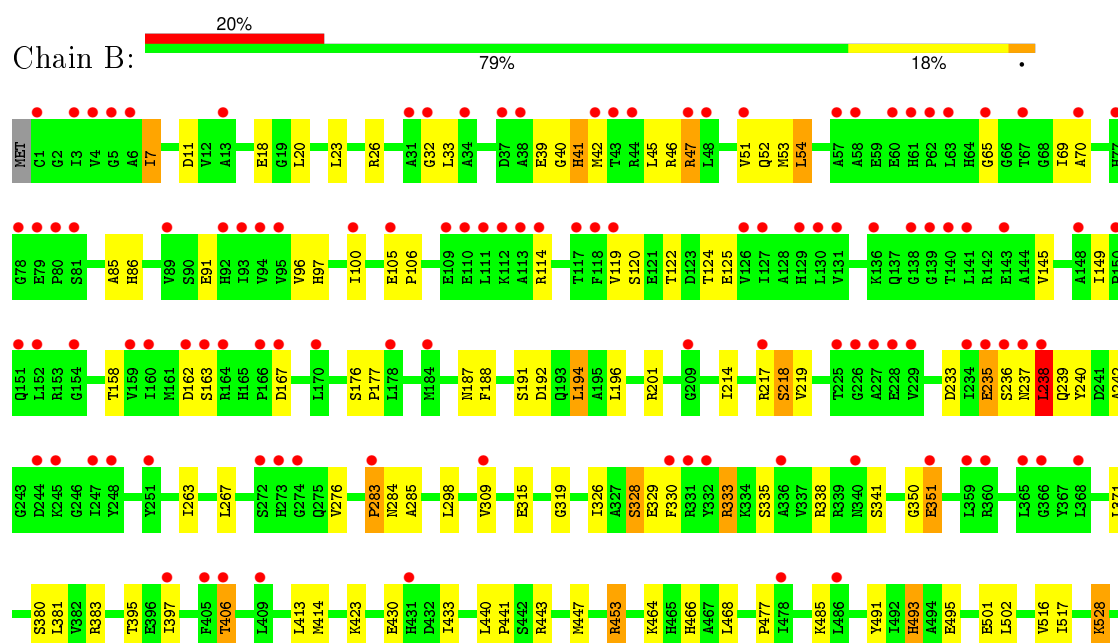
### 3 Residue-property plots

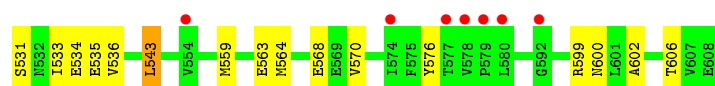
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: GLUCOSAMINE--FRUCTOSE-6-PHOSPHATE AMINOTRANSFERASE [ISOMER IZING]

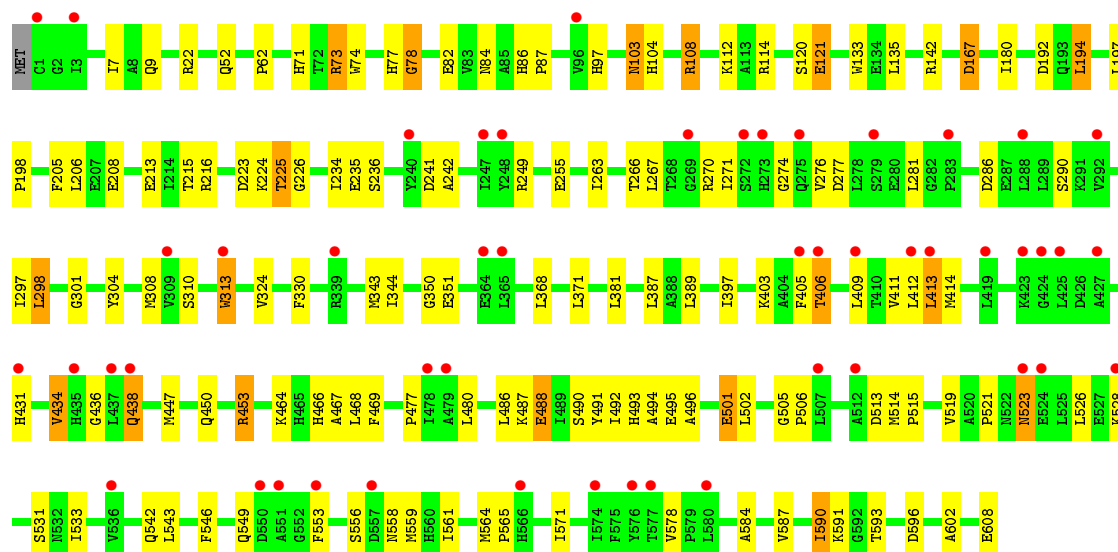
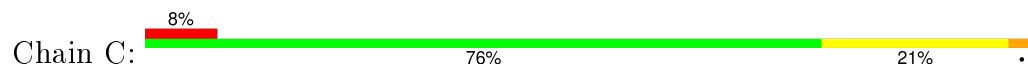


- Molecule 1: GLUCOSAMINE--FRUCTOSE-6-PHOSPHATE AMINOTRANSFERASE [ISOMER IZING]





- Molecule 1: GLUCOSAMINE--FRUCTOSE-6-PHOSPHATE AMINOTRANSFERASE [ISOMER IZING]



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.20 Å   109.68 Å   176.33 Å 90.00°   97.11°   90.00°	Depositor
Resolution (Å)	15.00 – 2.05 29.71 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.5 (15.00-2.05) 98.6 (29.71-2.05)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 2.04 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.206   ,   0.240 0.205   ,   0.238	Depositor DCC
$R_{free}$ test set	7769 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 51.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 154048 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14225	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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: F6R

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	0.96	3/4760 (0.1%)	1.02	16/6448 (0.2%)
1	B	0.72	8/4258 (0.2%)	0.75	5/5780 (0.1%)
1	C	0.79	3/4685 (0.1%)	0.86	4/6353 (0.1%)
All	All	0.83	14/13703 (0.1%)	0.89	25/18581 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	167	ASP	C-O	13.82	1.49	1.23
1	B	39	GLU	C-N	-12.14	1.11	1.33
1	B	167	ASP	C-N	9.81	1.56	1.34
1	B	39	GLU	N-CA	9.59	1.65	1.46
1	B	42	MET	N-CA	8.73	1.63	1.46
1	B	41	HIS	C-N	7.51	1.51	1.34
1	A	524	GLU	CD-OE1	7.27	1.33	1.25
1	B	39	GLU	C-O	6.90	1.36	1.23
1	B	40	GLY	N-CA	-6.30	1.36	1.46
1	C	488	GLU	CD-OE1	6.05	1.32	1.25
1	A	74	TRP	CD2-CE2	5.22	1.47	1.41
1	C	133	TRP	CD2-CE2	5.18	1.47	1.41
1	A	313	TRP	CD2-CE2	5.10	1.47	1.41
1	C	313	TRP	CD2-CE2	5.10	1.47	1.41

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	ARG	NE-CZ-NH1	-9.71	115.45	120.30
1	A	414	MET	CG-SD-CE	-8.38	86.79	100.20
1	B	167	ASP	O-C-N	7.65	134.94	122.70
1	A	1	CYS	CA-CB-SG	-6.85	101.67	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	543	LEU	CA-CB-CG	-6.49	100.38	115.30
1	A	194	LEU	CB-CG-CD2	-6.46	100.02	111.00
1	A	333	ARG	CG-CD-NE	-6.43	98.30	111.80
1	B	371	LEU	CA-CB-CG	6.00	129.10	115.30
1	A	406	THR	CA-CB-CG2	5.99	120.78	112.40
1	B	39	GLU	C-N-CA	-5.78	110.17	122.30
1	C	114	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	A	468	LEU	CB-CG-CD1	5.59	120.50	111.00
1	A	208	GLU	OE1-CD-OE2	-5.53	116.67	123.30
1	A	421	LYS	CD-CE-NZ	5.51	124.37	111.70
1	B	39	GLU	O-C-N	5.49	132.53	123.20
1	A	406	THR	OG1-CB-CG2	5.34	122.29	110.00
1	A	210	ASP	CB-CG-OD1	5.33	123.09	118.30
1	B	167	ASP	CA-C-N	-5.26	105.64	117.20
1	C	308	MET	CG-SD-CE	-5.25	91.80	100.20
1	A	241	ASP	N-CA-CB	-5.24	101.17	110.60
1	A	406	THR	N-CA-CB	-5.22	100.37	110.30
1	A	21	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	C	298	LEU	CB-CG-CD1	-5.12	102.30	111.00
1	A	311	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	C	216	ARG	CB-CA-C	-5.05	100.30	110.40

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	4679	0	4689	94	1
1	B	4198	0	3876	88	0
1	C	4606	0	4563	121	1
2	A	16	0	8	0	0
2	B	16	0	11	0	0
2	C	16	0	11	0	0
3	A	431	0	0	10	0
3	B	53	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	210	0	0	15	0
All	All	14225	0	13158	276	1

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 (276) 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:240:TYR:HB3	1:C:235:GLU:CG	1.81	1.10
1:A:240:TYR:HB3	1:C:235:GLU:HG2	1.29	1.05
1:A:240:TYR:CB	1:C:235:GLU:HG2	1.86	1.05
1:B:453:ARG:HG2	1:B:453:ARG:HH11	1.18	1.02
1:C:104:HIS:CE1	1:C:108:ARG:HH21	1.76	1.02
1:A:201:ARG:HH12	1:A:240:TYR:HD1	1.07	0.94
1:B:534:GLU:HG2	3:B:2005:HOH:O	1.73	0.88
1:C:596:ASP:HB2	3:C:2161:HOH:O	1.72	0.88
1:B:453:ARG:CG	1:B:453:ARG:HH11	1.86	0.88
1:B:466:HIS:HD2	1:C:493:HIS:CD2	1.91	0.88
1:B:466:HIS:HD2	1:C:493:HIS:HD2	1.19	0.86
1:C:103:ASN:H	1:C:103:ASN:HD22	1.23	0.85
1:B:466:HIS:CD2	1:C:493:HIS:HD2	1.97	0.83
1:C:270:ARG:HB3	1:C:414:MET:CE	2.09	0.82
1:B:263:ILE:HD11	1:B:406:THR:HG23	1.59	0.82
1:C:593:THR:HG21	3:C:2194:HOH:O	1.80	0.82
1:C:270:ARG:HB3	1:C:414:MET:HE1	1.62	0.82
1:A:533:ILE:HG23	1:A:543:LEU:HD22	1.61	0.81
1:A:104:HIS:CE1	1:A:108:ARG:HD2	2.16	0.81
1:B:351:GLU:HG3	1:B:606:THR:CG2	2.11	0.81
1:B:351:GLU:HG3	1:B:606:THR:HG22	1.61	0.80
1:A:225:THR:OG1	1:A:226:GLY:N	2.13	0.80
1:A:240:TYR:CB	1:C:235:GLU:CG	2.55	0.79
1:A:103:ASN:HD22	1:A:103:ASN:H	1.30	0.79
1:B:120:SER:OG	1:B:122:THR:HG22	1.81	0.79
1:B:453:ARG:NH1	1:B:453:ARG:HG2	1.93	0.78
1:A:281:LEU:HD21	1:A:389:LEU:HD13	1.67	0.76
1:B:493:HIS:HE1	1:C:495:GLU:OE1	1.68	0.76
1:A:240:TYR:HB3	1:C:235:GLU:CD	2.06	0.76
1:B:122:THR:HG23	1:B:125:GLU:H	1.52	0.74
1:B:447:MET:HE1	1:B:564:MET:SD	2.28	0.74
1:C:205:PHE:HE2	1:C:234:ILE:HD11	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ARG:HH11	1:A:453:ARG:HG3	1.51	0.73
1:C:194:LEU:HD21	1:C:397:ILE:HD11	1.71	0.73
1:A:11:ASP:H	1:C:9:GLN:NE2	1.87	0.72
1:C:492:ILE:HD12	3:C:2196:HOH:O	1.87	0.72
1:B:447:MET:CE	1:B:564:MET:SD	2.76	0.72
1:A:240:TYR:CD2	1:C:235:GLU:HG3	2.25	0.72
1:A:104:HIS:HE1	1:A:108:ARG:HD2	1.52	0.72
1:B:217:ARG:O	1:B:218:SER:HB3	1.89	0.71
1:B:47:ARG:HG2	1:B:53:MET:CG	2.21	0.71
1:B:430:GLU:HB3	3:B:2022:HOH:O	1.90	0.69
1:A:39:GLU:CD	1:A:39:GLU:N	2.46	0.68
1:A:201:ARG:NH1	1:A:240:TYR:CD1	2.58	0.68
1:C:108:ARG:HH22	1:C:121:GLU:HA	1.58	0.68
1:A:122:THR:HG23	1:A:125:GLU:H	1.59	0.67
1:B:350:GLY:HA2	1:B:381:LEU:HD12	1.76	0.67
1:B:491:TYR:CZ	1:B:599:ARG:HG2	2.30	0.67
1:C:453:ARG:HG2	1:C:453:ARG:HH11	1.60	0.67
1:A:201:ARG:NH1	3:A:2161:HOH:O	2.28	0.67
1:B:466:HIS:CD2	1:C:493:HIS:CD2	2.78	0.67
1:C:103:ASN:HD22	1:C:103:ASN:N	1.93	0.67
1:B:263:ILE:HD11	1:B:406:THR:CG2	2.25	0.66
1:C:180:ILE:HD12	1:C:206:LEU:HD21	1.77	0.66
1:C:71:HIS:CE1	1:C:73:ARG:HB3	2.30	0.66
1:A:205:PHE:HE2	1:A:234:ILE:HD11	1.60	0.66
1:C:298:LEU:HD11	1:C:330:PHE:CD2	2.31	0.65
1:A:240:TYR:HB2	1:C:235:GLU:HG2	1.77	0.65
1:A:39:GLU:CD	1:A:39:GLU:H	1.99	0.65
1:C:490:SER:HA	3:C:2194:HOH:O	1.96	0.65
1:C:205:PHE:CE2	1:C:234:ILE:HD11	2.31	0.65
1:A:11:ASP:H	1:C:9:GLN:HE22	1.44	0.65
1:A:120:SER:OG	1:A:122:THR:HG22	1.97	0.65
1:B:535:GLU:OE1	3:B:2048:HOH:O	2.13	0.65
1:C:453:ARG:HG2	1:C:453:ARG:NH1	2.12	0.65
1:B:495:GLU:OE1	1:C:493:HIS:HE1	1.79	0.65
1:A:93:ILE:HD11	1:A:135:LEU:HD12	1.79	0.64
1:A:76:THR:HG22	1:A:77:HIS:N	2.13	0.64
1:A:550:ASP:OD2	1:A:566:HIS:CE1	2.51	0.64
1:C:104:HIS:CE1	1:C:108:ARG:NH2	2.60	0.64
1:C:225:THR:OG1	1:C:226:GLY:N	2.30	0.64
1:C:591:LYS:NZ	3:C:2205:HOH:O	2.12	0.64
1:C:310:SER:HB3	1:C:412:LEU:HD13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:GLN:O	1:C:9:GLN:HG2	1.97	0.63
1:C:549:GLN:HG3	1:C:564:MET:O	1.97	0.63
1:B:145:VAL:O	1:B:149:ILE:HG12	2.00	0.62
1:A:537:ARG:HG2	1:A:543:LEU:HD13	1.81	0.62
1:B:443:ARG:NH1	1:B:568:GLU:OE1	2.31	0.62
1:A:223:ASP:O	1:A:225:THR:O	2.18	0.62
1:B:267:LEU:HD23	1:B:414:MET:HE1	1.82	0.62
1:B:440:LEU:HB3	1:B:441:PRO:HD3	1.81	0.61
1:A:223:ASP:OD1	1:A:225:THR:HG23	2.00	0.61
1:B:395:THR:HA	3:B:2017:HOH:O	2.00	0.61
1:C:350:GLY:HA2	1:C:381:LEU:HD12	1.83	0.60
1:C:492:ILE:HD11	1:C:591:LYS:HE3	1.83	0.60
1:B:194:LEU:HD21	1:B:397:ILE:HD11	1.83	0.60
1:C:270:ARG:HB3	1:C:414:MET:HE3	1.84	0.60
1:C:223:ASP:O	1:C:225:THR:O	2.20	0.59
1:A:453:ARG:NH1	1:A:457:LEU:HD13	2.17	0.59
1:C:542:GLN:HA	1:C:558:ASN:HB3	1.84	0.59
1:A:81:SER:OG	1:A:83:VAL:HG23	2.03	0.59
1:C:490:SER:CA	3:C:2194:HOH:O	2.49	0.58
1:C:468:LEU:HD13	1:C:514:MET:SD	2.43	0.58
1:C:180:ILE:CD1	1:C:206:LEU:HD21	2.33	0.58
1:B:267:LEU:HD23	1:B:414:MET:CE	2.34	0.58
1:C:301:GLY:O	1:C:304:TYR:HB3	2.03	0.58
1:A:537:ARG:CG	1:A:543:LEU:HD13	2.33	0.57
1:A:240:TYR:HB3	1:C:235:GLU:OE2	2.03	0.57
1:A:258:GLU:HG2	3:A:2195:HOH:O	2.05	0.57
1:B:351:GLU:CG	1:B:606:THR:HG22	2.33	0.57
1:A:346:LEU:HD23	1:A:373:ILE:HB	1.87	0.57
1:C:104:HIS:NE2	1:C:108:ARG:NH2	2.48	0.57
1:C:22:ARG:NH1	3:C:2026:HOH:O	2.38	0.57
1:B:493:HIS:HD2	1:C:466:HIS:ND1	2.03	0.56
1:B:20:LEU:HD11	1:B:70:ALA:HB1	1.87	0.56
1:C:263:ILE:O	1:C:267:LEU:HG	2.05	0.56
1:B:235:GLU:HG3	1:B:236:SER:N	2.20	0.56
1:C:313:TRP:CH2	1:C:413:LEU:HD22	2.41	0.56
1:B:69:ILE:HD12	1:B:96:VAL:HG22	1.87	0.56
1:B:447:MET:HE3	1:B:564:MET:SD	2.46	0.56
1:B:32:GLY:HA2	1:B:54:LEU:HD11	1.87	0.56
1:C:263:ILE:HD11	1:C:406:THR:HG23	1.87	0.56
1:C:84:ASN:HD22	1:C:120:SER:HB2	1.71	0.56
1:C:276:VAL:HG22	1:C:414:MET:HE2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:LYS:HA	3:B:2023:HOH:O	2.05	0.55
1:A:534:GLU:OE1	3:A:2395:HOH:O	2.18	0.55
1:B:517:ILE:HD12	1:B:517:ILE:N	2.21	0.55
1:A:250:HIS:HD2	1:A:585:TYR:OH	1.89	0.55
1:A:249:ARG:NE	3:A:2182:HOH:O	2.34	0.55
1:A:93:ILE:HD11	1:A:135:LEU:CD1	2.36	0.55
1:A:103:ASN:N	1:A:103:ASN:HD22	2.01	0.54
1:A:453:ARG:HH12	1:A:457:LEU:HD13	1.71	0.54
1:B:47:ARG:HG2	1:B:53:MET:HG2	1.88	0.54
1:A:194:LEU:HG	3:A:2037:HOH:O	2.07	0.54
1:C:313:TRP:CE3	1:C:413:LEU:HD13	2.41	0.54
1:A:201:ARG:NH1	1:A:240:TYR:HD1	1.91	0.54
1:C:477:PRO:HA	1:C:480:LEU:HD12	1.88	0.54
1:C:453:ARG:CG	1:C:453:ARG:HH11	2.21	0.54
1:A:74:TRP:CE3	1:A:602:ALA:HB3	2.43	0.54
1:A:240:TYR:HE2	1:C:236:SER:O	1.90	0.53
1:C:286:ASP:O	1:C:290:SER:HB2	2.08	0.53
1:B:495:GLU:OE1	1:C:493:HIS:CE1	2.61	0.53
1:C:523:ASN:HB2	3:C:2200:HOH:O	2.09	0.53
1:C:86:HIS:HB3	1:C:87:PRO:HA	1.91	0.53
1:A:28:TYR:HB2	1:A:50:LYS:HD3	1.90	0.53
1:B:267:LEU:CD2	1:B:414:MET:CE	2.87	0.52
1:C:142:ARG:NH1	1:C:213:GLU:OE1	2.42	0.52
1:C:103:ASN:H	1:C:103:ASN:ND2	1.99	0.52
1:C:447:MET:HG2	1:C:578:VAL:HB	1.91	0.52
1:C:297:ILE:HB	1:C:324:VAL:HG13	1.91	0.52
1:C:281:LEU:HD21	1:C:389:LEU:HD13	1.90	0.52
1:B:453:ARG:CG	1:B:453:ARG:NH1	2.57	0.52
1:B:298:LEU:HD11	1:B:330:PHE:CD2	2.44	0.52
1:C:71:HIS:HE1	1:C:73:ARG:HB3	1.75	0.51
1:A:537:ARG:HD2	1:A:559:MET:SD	2.50	0.51
1:A:517:ILE:N	1:A:517:ILE:HD12	2.26	0.51
1:C:298:LEU:HG	1:C:343:MET:SD	2.51	0.50
1:B:18:GLU:OE1	1:B:18:GLU:HA	2.11	0.50
1:B:192:ASP:OD2	1:B:194:LEU:HB2	2.10	0.50
1:A:22:ARG:NH1	3:A:2037:HOH:O	2.24	0.50
1:C:274:GLY:O	1:C:431:HIS:HD2	1.94	0.50
1:A:62:PRO:HD2	3:A:2065:HOH:O	2.11	0.50
1:B:283:PRO:O	1:B:285:ALA:N	2.45	0.49
1:C:297:ILE:HA	1:C:344:ILE:O	2.13	0.49
1:C:270:ARG:O	1:C:277:ASP:N	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ASP:OD1	1:C:225:THR:HG23	2.13	0.49
1:C:84:ASN:ND2	1:C:120:SER:HB2	2.28	0.49
1:C:513:ASP:O	1:C:515:PRO:HD3	2.13	0.49
1:A:108:ARG:HH12	1:A:121:GLU:HB3	1.78	0.49
1:B:188:PHE:HB3	1:B:196:LEU:HD22	1.93	0.49
1:B:32:GLY:HA3	1:B:86:HIS:O	2.13	0.48
1:C:466:HIS:NE2	3:C:2193:HOH:O	2.30	0.48
1:C:121:GLU:N	1:C:121:GLU:OE1	2.44	0.48
1:A:100:ILE:HD13	1:A:101:ILE:N	2.27	0.48
1:B:32:GLY:HA3	1:B:46:ARG:HG2	1.96	0.48
1:C:436:GLY:O	1:C:571:ILE:HD13	2.12	0.48
1:A:485:LYS:HD3	1:A:485:LYS:HA	1.66	0.48
1:C:7:ILE:HD13	1:C:215:THR:HA	1.94	0.48
1:B:267:LEU:CD2	1:B:414:MET:HE3	2.44	0.48
1:A:481:GLU:OE2	1:A:485:LYS:NZ	2.47	0.48
1:C:271:ILE:HG21	1:C:438:GLN:NE2	2.29	0.48
1:C:192:ASP:OD1	1:C:194:LEU:HB2	2.14	0.48
1:B:267:LEU:CD2	1:B:414:MET:HE1	2.44	0.47
1:C:255:GLU:HG2	1:C:403:LYS:HE2	1.96	0.47
1:C:371:LEU:HD23	1:C:387:LEU:HB2	1.97	0.47
1:A:240:TYR:CE2	1:C:236:SER:O	2.67	0.47
1:B:329:GLU:O	1:B:333:ARG:HG2	2.13	0.47
1:C:266:THR:O	1:C:270:ARG:HD2	2.14	0.47
1:C:389:LEU:HD23	1:C:411:VAL:HG13	1.96	0.47
1:B:466:HIS:HE1	3:B:2025:HOH:O	1.97	0.47
1:A:254:LYS:O	1:A:258:GLU:HG3	2.14	0.47
1:A:498:ALA:O	1:A:501:GLU:HG2	2.15	0.47
1:B:283:PRO:C	1:B:285:ALA:H	2.18	0.47
1:A:435:HIS:HB3	3:A:2325:HOH:O	2.15	0.47
1:A:347:SER:O	1:A:374:CYS:HA	2.15	0.47
1:B:338:ARG:O	1:B:341:SER:HB2	2.16	0.46
1:A:104:HIS:HE1	1:A:108:ARG:CD	2.26	0.46
1:C:486:LEU:HD13	1:C:584:ALA:HA	1.97	0.46
1:C:505:GLY:N	1:C:506:PRO:CD	2.78	0.46
1:B:47:ARG:CB	1:B:54:LEU:HD22	2.46	0.46
1:A:487:LYS:HG2	1:A:488:GLU:N	2.30	0.46
1:A:146:LEU:HD23	1:A:211:ILE:HD12	1.97	0.46
1:C:464:LYS:HE3	3:C:2192:HOH:O	2.16	0.46
1:B:564:MET:HG3	1:B:576:TYR:CE2	2.51	0.46
1:C:74:TRP:CE3	1:C:602:ALA:HB3	2.51	0.46
1:A:549:GLN:HG3	1:A:564:MET:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:VAL:CG2	1:B:477:PRO:HB2	2.46	0.45
1:A:311:ARG:NH1	3:A:2242:HOH:O	2.14	0.45
1:B:7:ILE:CD1	1:B:214:ILE:HG22	2.46	0.45
1:B:7:ILE:HD13	1:B:214:ILE:O	2.17	0.45
1:A:145:VAL:O	1:A:149:ILE:HG12	2.17	0.45
1:B:533:ILE:HG23	1:B:543:LEU:HD22	1.99	0.45
1:C:447:MET:O	1:C:450:GLN:HB2	2.17	0.45
1:C:521:PRO:O	1:C:526:LEU:HD13	2.16	0.45
1:B:351:GLU:HG3	1:B:606:THR:HG21	1.96	0.45
1:C:197:LEU:N	1:C:198:PRO:CD	2.79	0.45
1:B:485:LYS:HD3	1:B:485:LYS:HA	1.59	0.45
1:A:103:ASN:ND2	1:A:103:ASN:H	2.08	0.45
1:A:76:THR:CG2	1:A:77:HIS:N	2.81	0.44
1:A:457:LEU:HD21	1:A:562:ILE:HD11	1.99	0.44
1:A:88:HIS:NE2	1:A:122:THR:HG21	2.32	0.44
1:A:100:ILE:HD13	1:A:100:ILE:C	2.38	0.44
1:A:100:ILE:HD13	1:A:101:ILE:C	2.38	0.44
1:B:162:ASP:OD1	1:B:162:ASP:C	2.56	0.44
1:A:313:TRP:CD2	1:A:413:LEU:HD13	2.52	0.44
1:B:315:GLU:O	1:B:319:GLY:HA2	2.17	0.44
1:C:453:ARG:NH1	1:C:453:ARG:CG	2.81	0.44
1:B:533:ILE:HG21	1:B:559:MET:CE	2.47	0.44
1:C:590:ILE:HD12	1:C:590:ILE:HA	1.87	0.44
1:B:326:ILE:HD13	1:C:501:GLU:HB3	1.99	0.44
1:C:167:ASP:HB3	3:C:2132:HOH:O	2.17	0.44
1:A:310:SER:HB3	1:A:412:LEU:HD13	2.00	0.44
1:C:62:PRO:HB3	3:C:2069:HOH:O	2.17	0.44
1:C:467:ALA:O	1:C:494:ALA:HA	2.18	0.44
1:A:477:PRO:HA	1:A:480:LEU:HD12	1.99	0.43
1:B:237:ASN:O	1:B:238:LEU:CB	2.66	0.43
1:A:88:HIS:CD2	1:A:122:THR:HG21	2.53	0.43
1:A:371:LEU:HD23	1:A:387:LEU:HB2	2.00	0.43
1:C:241:ASP:O	1:C:242:ALA:C	2.55	0.43
1:B:46:ARG:NH1	1:B:85:ALA:O	2.46	0.43
1:A:37:ASP:OD1	1:A:37:ASP:C	2.57	0.43
1:A:240:TYR:CE2	1:C:236:SER:HB3	2.54	0.43
1:A:240:TYR:CD2	1:C:235:GLU:CG	3.00	0.43
1:B:47:ARG:HB2	1:B:54:LEU:HD22	2.00	0.43
1:C:553:PHE:HB3	1:C:561:ILE:HD12	2.01	0.43
1:C:469:PHE:O	1:C:496:ALA:HA	2.18	0.43
1:C:405:PHE:CE2	1:C:409:LEU:HD11	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:TYR:CG	1:C:235:GLU:CG	3.01	0.42
1:C:487:LYS:HG2	1:C:488:GLU:N	2.33	0.42
1:A:433:ILE:HG12	1:A:570:VAL:HG21	2.01	0.42
1:B:528:LYS:HA	1:B:528:LYS:HD2	1.76	0.42
1:A:104:HIS:HD2	1:A:123:ASP:OD1	2.01	0.42
1:B:493:HIS:CD2	1:C:466:HIS:ND1	2.85	0.42
1:A:453:ARG:HH12	1:A:457:LEU:CD1	2.32	0.42
1:C:533:ILE:HG23	1:C:543:LEU:HD22	2.01	0.42
1:B:201:ARG:O	1:B:236:SER:HB2	2.20	0.42
1:B:599:ARG:O	1:B:600:ASN:HB2	2.19	0.42
1:B:493:HIS:CE1	1:C:495:GLU:OE1	2.59	0.41
1:A:453:ARG:NH1	1:A:453:ARG:HG3	2.28	0.41
1:B:237:ASN:O	1:B:238:LEU:HB3	2.20	0.41
1:B:26:ARG:O	1:B:602:ALA:HB1	2.20	0.41
1:A:245:LYS:CE	3:A:2179:HOH:O	2.68	0.41
1:C:77:HIS:O	1:C:78:GLY:O	2.39	0.41
1:A:234:ILE:HD12	1:A:234:ILE:C	2.40	0.41
1:B:309:VAL:HG22	1:B:477:PRO:HB2	2.02	0.41
1:B:187:ASN:ND2	1:B:219:VAL:HG23	2.36	0.41
1:A:201:ARG:NH1	1:A:240:TYR:CE1	2.87	0.41
1:C:62:PRO:HA	3:C:2069:HOH:O	2.19	0.41
1:C:546:PHE:HD2	1:C:564:MET:CE	2.34	0.41
1:B:326:ILE:HG12	1:B:328:SER:OG	2.21	0.41
1:A:457:LEU:HD21	1:A:562:ILE:CG1	2.51	0.41
1:C:587:VAL:HG11	3:C:2196:HOH:O	2.20	0.41
1:B:23:LEU:HD21	1:B:192:ASP:HB3	2.03	0.41
1:A:71:HIS:HB3	1:A:86:HIS:HB2	2.03	0.41
1:B:516:VAL:HG21	1:B:536:VAL:HG11	2.03	0.41
1:B:433:ILE:HG12	1:B:570:VAL:HG21	2.03	0.41
1:B:528:LYS:HE2	1:C:608:GLU:OE1	2.21	0.41
1:B:11:ASP:HA	1:B:65:GLY:O	2.21	0.41
1:C:276:VAL:HG23	1:C:434:VAL:HG23	2.03	0.40
1:A:485:LYS:O	1:A:489:ILE:HG12	2.21	0.40
1:B:177:PRO:HB2	1:B:191:SER:O	2.22	0.40
1:A:88:HIS:CD2	1:A:124:THR:HB	2.57	0.40
1:A:20:LEU:HD11	1:A:70:ALA:HB1	2.04	0.40
1:C:549:GLN:NE2	1:C:565:PRO:HA	2.37	0.40
1:A:24:GLU:HG2	1:A:28:TYR:HB3	2.02	0.40
1:C:490:SER:C	3:C:2194:HOH:O	2.59	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLY:O	1:C:82:GLU:OE1[2_656]	1.92	0.28

## 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	606/609 (100%)	591 (98%)	11 (2%)	4 (1%)	26	15
1	B	606/609 (100%)	557 (92%)	33 (5%)	16 (3%)	7	1
1	C	606/609 (100%)	580 (96%)	25 (4%)	1 (0%)	52	43
All	All	1818/1827 (100%)	1728 (95%)	69 (4%)	21 (1%)	16	6

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	106	PRO
1	B	235	GLU
1	B	238	LEU
1	B	240	TYR
1	B	284	ASN
1	B	423	LYS
1	A	225	THR
1	B	105	GLU
1	C	78	GLY
1	A	78	GLY
1	A	224	LYS
1	A	242	ALA
1	B	91	GLU
1	B	163	SER
1	B	41	HIS
1	B	51	VAL
1	B	114	ARG
1	B	218	SER
1	B	283	PRO

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Mol	Chain	Res	Type
1	B	239	GLN
1	B	242	ALA

### 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	497/501 (99%)	464 (93%)	33 (7%)	21	11
1	B	388/501 (77%)	355 (92%)	33 (8%)	13	6
1	C	479/501 (96%)	448 (94%)	31 (6%)	21	11
All	All	1364/1503 (91%)	1267 (93%)	97 (7%)	18	10

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	73	ARG
1	A	77	HIS
1	A	100	ILE
1	A	103	ASN
1	A	112	LYS
1	A	121	GLU
1	A	137	GLN
1	A	167	ASP
1	A	208	GLU
1	A	225	THR
1	A	229	VAL
1	A	237	ASN
1	A	249	ARG
1	A	276	VAL
1	A	368	LEU
1	A	371	LEU
1	A	389	LEU
1	A	406	THR
1	A	438	GLN

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Mol	Chain	Res	Type
1	A	453	ARG
1	A	457	LEU
1	A	468	LEU
1	A	487	LYS
1	A	491	TYR
1	A	493	HIS
1	A	502	LEU
1	A	524	GLU
1	A	528	LYS
1	A	531	SER
1	A	543	LEU
1	A	559	MET
1	A	590	ILE
1	B	7	ILE
1	B	33	LEU
1	B	45	LEU
1	B	47	ARG
1	B	52	GLN
1	B	54	LEU
1	B	97	HIS
1	B	100	ILE
1	B	119	VAL
1	B	124	THR
1	B	158	THR
1	B	176	SER
1	B	194	LEU
1	B	233	ASP
1	B	238	LEU
1	B	276	VAL
1	B	328	SER
1	B	333	ARG
1	B	335	SER
1	B	351	GLU
1	B	380	SER
1	B	383	ARG
1	B	406	THR
1	B	413	LEU
1	B	453	ARG
1	B	468	LEU
1	B	493	HIS
1	B	501	GLU
1	B	502	LEU

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Mol	Chain	Res	Type
1	B	528	LYS
1	B	531	SER
1	B	543	LEU
1	B	563	GLU
1	C	52	GLN
1	C	73	ARG
1	C	97	HIS
1	C	103	ASN
1	C	108	ARG
1	C	112	LYS
1	C	121	GLU
1	C	135	LEU
1	C	167	ASP
1	C	194	LEU
1	C	208	GLU
1	C	224	LYS
1	C	225	THR
1	C	249	ARG
1	C	351	GLU
1	C	368	LEU
1	C	406	THR
1	C	413	LEU
1	C	434	VAL
1	C	438	GLN
1	C	453	ARG
1	C	491	TYR
1	C	501	GLU
1	C	502	LEU
1	C	519	VAL
1	C	523	ASN
1	C	528	LYS
1	C	531	SER
1	C	556	SER
1	C	559	MET
1	C	590	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	104	HIS
1	A	250	HIS

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Mol	Chain	Res	Type
1	A	265	ASN
1	A	542	GLN
1	B	86	HIS
1	B	250	HIS
1	B	265	ASN
1	B	466	HIS
1	B	493	HIS
1	B	542	GLN
1	B	600	ASN
1	C	9	GLN
1	C	84	ASN
1	C	86	HIS
1	C	103	ASN
1	C	250	HIS
1	C	265	ASN
1	C	431	HIS
1	C	438	GLN
1	C	493	HIS
1	C	523	ASN
1	C	542	GLN
1	C	600	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 carbohydrates 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	$\# Z  > 2$
2	F6R	A	1609	-	15,15,15	2.29	5 (33%)	14,21,21	2.69	5 (35%)
2	F6R	B	1609	-	15,15,15	0.88	0	14,21,21	2.67	8 (57%)
2	F6R	C	1609	-	15,15,15	1.17	1 (6%)	14,21,21	2.70	5 (35%)

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	F6R	A	1609	-	-	0/20/20/20	0/0/0/0
2	F6R	B	1609	-	2/2/5/5	0/20/20/20	0/0/0/0
2	F6R	C	1609	-	2/2/5/5	0/20/20/20	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1609	F6R	C6-C5	-4.97	1.44	1.51
2	A	1609	F6R	C5-C4	-3.99	1.45	1.53
2	A	1609	F6R	O4-C4	-3.45	1.34	1.43
2	C	1609	F6R	C6-C5	-2.79	1.47	1.51
2	A	1609	F6R	C4-C3	-2.15	1.48	1.53
2	A	1609	F6R	O2-C2	2.97	1.26	1.21

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1609	F6R	O3-C3-C4	-4.40	101.23	110.41
2	A	1609	F6R	O3-C3-C4	-4.38	101.29	110.41
2	C	1609	F6R	O3-C3-C4	-4.07	101.93	110.41
2	B	1609	F6R	O6-P-O3P	-2.68	100.33	107.14
2	B	1609	F6R	O3-C3-C2	-2.25	106.84	111.01
2	B	1609	F6R	O2P-P-O1P	2.02	115.07	107.38
2	B	1609	F6R	O5-C5-C6	2.10	114.77	110.19
2	B	1609	F6R	O5-C5-C4	2.83	116.14	109.02
2	C	1609	F6R	O5-C5-C6	2.95	116.61	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1609	F6R	O5-C5-C4	3.16	116.95	109.02
2	A	1609	F6R	O4-C4-C5	3.26	116.96	108.75
2	B	1609	F6R	O4-C4-C5	3.27	117.00	108.75
2	C	1609	F6R	O4-C4-C5	3.43	117.40	108.75
2	A	1609	F6R	O5-C5-C6	4.78	120.60	110.19
2	C	1609	F6R	O5-C5-C4	4.84	121.18	109.02
2	C	1609	F6R	O4-C4-C3	5.75	119.69	109.28
2	A	1609	F6R	O4-C4-C3	5.77	119.72	109.28
2	B	1609	F6R	O4-C4-C3	5.86	119.89	109.28

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1609	F6R	C5
2	B	1609	F6R	C4
2	C	1609	F6R	C5
2	C	1609	F6R	C4

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	608/609 (99%)	-0.05	20 (3%) 50 57	24, 37, 65, 89	0
1	B	608/609 (99%)	1.04	120 (19%) 1 1	46, 96, 163, 202	0
1	C	608/609 (99%)	0.38	50 (8%) 14 16	29, 61, 114, 141	0
All	All	1824/1827 (99%)	0.46	190 (10%) 8 9	24, 60, 139, 202	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	113	ALA	10.1
1	B	127	ILE	8.8
1	B	138	GLY	8.5
1	C	240	TYR	7.6
1	B	58	ALA	7.2
1	C	424	GLY	7.1
1	B	139	GLY	6.4
1	B	100	ILE	5.9
1	B	117	THR	5.8
1	B	148	ALA	5.7
1	B	114	ARG	5.7
1	B	62	PRO	5.4
1	B	580	LEU	5.3
1	C	423	LYS	5.3
1	B	80	PRO	5.2
1	B	237	ASN	5.2
1	B	140	THR	5.1
1	B	151	GLN	5.1
1	B	330	PHE	4.9
1	C	272	SER	4.9
1	B	63	LEU	4.9
1	A	113	ALA	4.8
1	B	248	TYR	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	227	ALA	4.6
1	B	274	GLY	4.6
1	B	51	VAL	4.6
1	B	229	VAL	4.6
1	B	152	LEU	4.5
1	B	368	LEU	4.4
1	B	57	ALA	4.3
1	B	110	GLU	4.3
1	B	43	THR	4.3
1	B	112	LYS	4.2
1	B	109	GLU	4.2
1	B	13	ALA	4.2
1	B	130	LEU	4.2
1	B	162	ASP	4.2
1	A	240	TYR	4.2
1	B	226	GLY	4.1
1	B	48	LEU	4.1
1	B	6	ALA	4.1
1	B	236	SER	4.1
1	B	143	GLU	4.0
1	B	126	VAL	4.0
1	B	129	HIS	4.0
1	C	438	GLN	4.0
1	B	131	VAL	4.0
1	B	154	GLY	4.0
1	C	273	HIS	4.0
1	C	283	PRO	4.0
1	B	118	PHE	3.8
1	B	81	SER	3.7
1	B	119	VAL	3.7
1	B	163	SER	3.7
1	B	272	SER	3.7
1	B	184	MET	3.7
1	B	93	ILE	3.7
1	B	141	LEU	3.6
1	B	283	PRO	3.6
1	B	31	ALA	3.6
1	C	247	ILE	3.5
1	A	3	ILE	3.5
1	C	288	LEU	3.5
1	B	478	ILE	3.5
1	B	225	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	577	THR	3.5
1	B	38	ALA	3.4
1	C	566	HIS	3.4
1	B	92	HIS	3.4
1	B	251	TYR	3.4
1	C	512	ALA	3.4
1	B	94	VAL	3.3
1	B	47	ARG	3.3
1	C	275	GLN	3.3
1	C	339	ARG	3.3
1	B	167	ASP	3.3
1	B	1	CYS	3.3
1	C	364	GLU	3.2
1	B	405	PHE	3.2
1	B	60	GLU	3.2
1	A	4	VAL	3.2
1	C	309	VAL	3.2
1	B	160	ILE	3.1
1	B	61	HIS	3.1
1	C	409	LEU	3.1
1	A	159	VAL	3.0
1	B	245	LYS	3.0
1	B	166	PRO	2.9
1	B	32	GLY	2.9
1	B	42	MET	2.9
1	B	70	ALA	2.9
1	B	247	ILE	2.9
1	C	3	ILE	2.9
1	B	5	GLY	2.8
1	B	65	GLY	2.8
1	A	273	HIS	2.7
1	C	524	GLU	2.7
1	B	78	GLY	2.7
1	C	528	LYS	2.7
1	C	412	LEU	2.7
1	C	478	ILE	2.7
1	B	34	ALA	2.7
1	A	409	LEU	2.7
1	B	89	VAL	2.6
1	C	557	ASP	2.6
1	B	170	LEU	2.6
1	C	365	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	95	VAL	2.6
1	B	217	ARG	2.6
1	B	228	GLU	2.6
1	A	224	LYS	2.6
1	B	366	GLY	2.6
1	B	431	HIS	2.6
1	C	419	LEU	2.5
1	B	574	ILE	2.5
1	B	244	ASP	2.5
1	B	340	ASN	2.5
1	C	313	TRP	2.5
1	B	3	ILE	2.5
1	B	159	VAL	2.5
1	B	578	VAL	2.4
1	B	486	LEU	2.4
1	C	580	LEU	2.4
1	B	150	PRO	2.4
1	B	273	HIS	2.4
1	B	238	LEU	2.4
1	B	209	GLY	2.4
1	B	554	VAL	2.4
1	C	292	VAL	2.4
1	C	427	ALA	2.4
1	B	351	GLU	2.4
1	C	1	CYS	2.4
1	B	67	THR	2.4
1	B	178	LEU	2.4
1	B	359	LEU	2.4
1	C	553	PHE	2.4
1	B	105	GLU	2.4
1	B	235	GLU	2.4
1	C	96	VAL	2.3
1	C	577	THR	2.3
1	C	550	ASP	2.3
1	B	409	LEU	2.3
1	C	523	ASN	2.3
1	B	111	LEU	2.3
1	B	44	ARG	2.3
1	B	79	GLU	2.3
1	B	164	ARG	2.3
1	C	269	GLY	2.3
1	B	4	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	111	LEU	2.3
1	A	178	LEU	2.3
1	C	576	TYR	2.2
1	B	406	THR	2.2
1	B	37	ASP	2.2
1	B	397	ILE	2.2
1	A	190	ALA	2.2
1	A	484	LEU	2.2
1	A	96	VAL	2.2
1	A	1	CYS	2.2
1	C	435	HIS	2.2
1	C	413	LEU	2.2
1	C	431	HIS	2.2
1	B	336	ALA	2.2
1	C	405	PHE	2.2
1	B	579	PRO	2.2
1	C	248	TYR	2.2
1	B	309	VAL	2.2
1	B	234	ILE	2.2
1	B	77	HIS	2.1
1	B	365	LEU	2.1
1	C	279	SER	2.1
1	A	112	LYS	2.1
1	B	136	LYS	2.1
1	C	536	VAL	2.1
1	A	138	GLY	2.1
1	C	507	LEU	2.1
1	A	115	GLY	2.1
1	A	109	GLU	2.1
1	C	574	ILE	2.1
1	C	425	LEU	2.1
1	B	331	ARG	2.0
1	B	360	ARG	2.0
1	C	437	LEU	2.0
1	A	117	THR	2.0
1	A	309	VAL	2.0
1	B	332	TYR	2.0
1	C	479	ALA	2.0
1	C	551	ALA	2.0
1	C	406	THR	2.0
1	B	592	GLY	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
2	F6R	B	1609	16/16	0.94	0.18	0.97	67,72,80,82	0
2	F6R	C	1609	16/16	0.97	0.17	0.79	52,55,61,62	0
2	F6R	A	1609	16/16	0.98	0.14	-0.19	25,27,28,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.