Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:08 pm GMT

PDB ID	:	2J6H
Title	:	E. COLI GLUCOSAMINE-6-P SYNTHASE IN COMPLEX WITH GLUCOSE-6P AND 5-OXO-L-NORLEUCINE
Authors	:	Mouilleron, S.; Golinelli-Pimpaneau, B.
Deposited on	:	2006-09-28
Resolution	:	2.35 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*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

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 2.35 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.
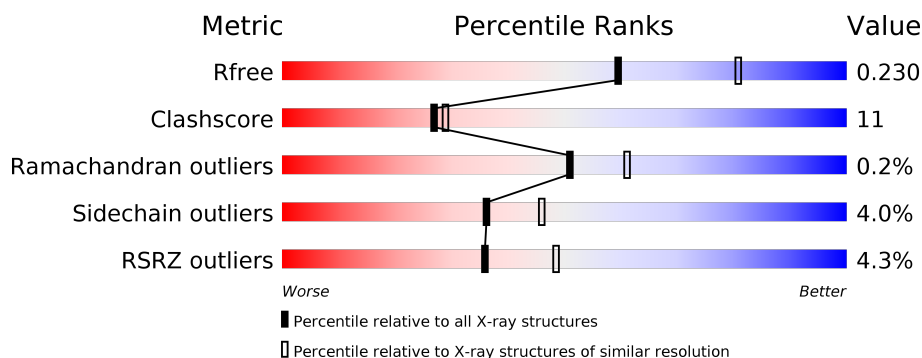
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

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 >=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 <=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	608	
1	B	608	

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	ONL	A	1609	-	-	-	X
2	ONL	B	1609	-	-	-	X

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 9826 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	608	Total	C	N	O	S	0	0	0
			4697	2953	831	896	17			
1	B	608	Total	C	N	O	S	0	0	0
			4692	2950	829	896	17			

- Molecule 2 is 5-OXO-L-NORLEUCINE (three-letter code: ONL) (formula: $C_6H_{11}NO_3$).
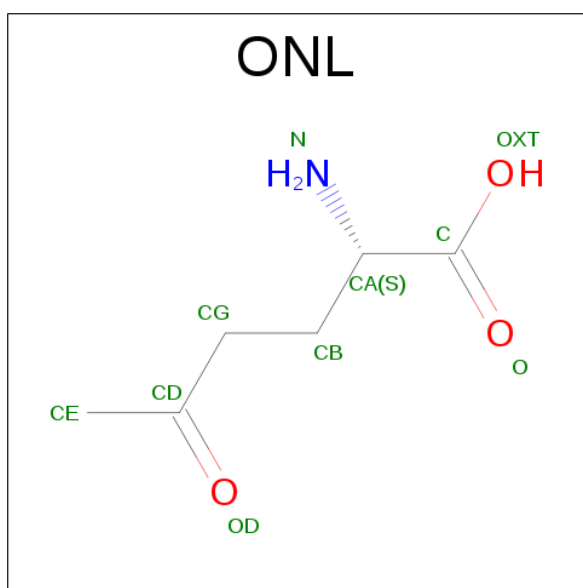
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	1	3		
2	B	1	Total	C	N	O	0	0
			10	6	1	3		

- Molecule 3 is SUGAR (GLUCOSE-6-PHOSPHATE) (three-letter code: G6Q) (formula: $C_6H_{13}O_9P$).
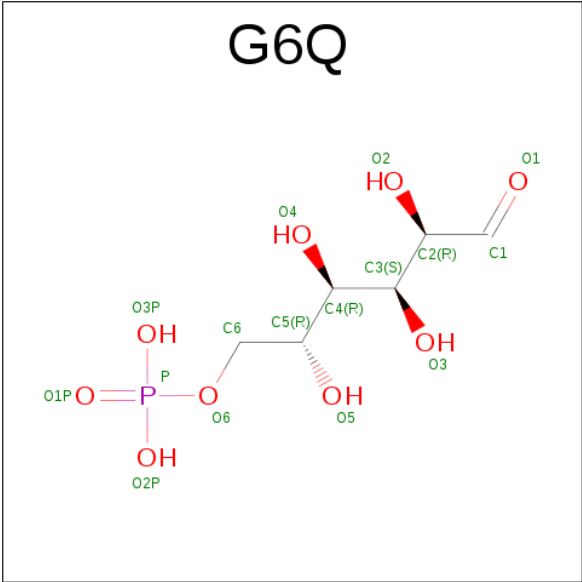
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total C O P				0	0
			16 6 9 1					
3	B	1	Total C O P				0	0
			16 6 9 1					

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	255	Total O		0	0
			255 255			
4	B	130	Total O		0	0
			130 130			

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 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: GLUCOSAMINE-FRUCTOSE-6-PHOSPHATE AMINOTRANSFERASE
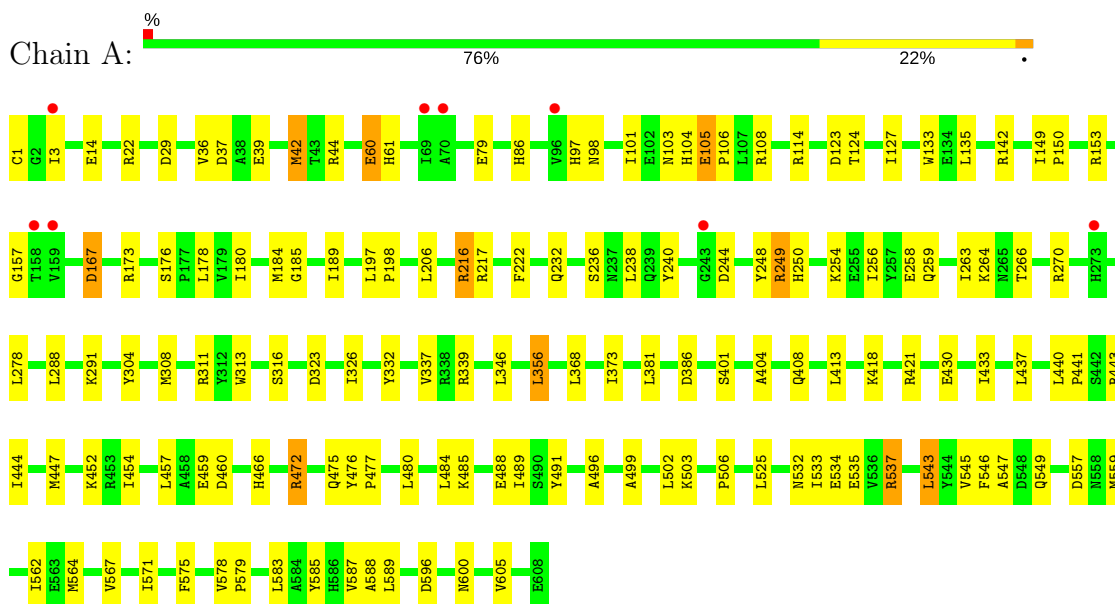
Chain A:

• Molecule 1: GLUCOSAMINE-FRUCTOSE-6-PHOSPHATE AMINOTRANSFERASE

Chain B:
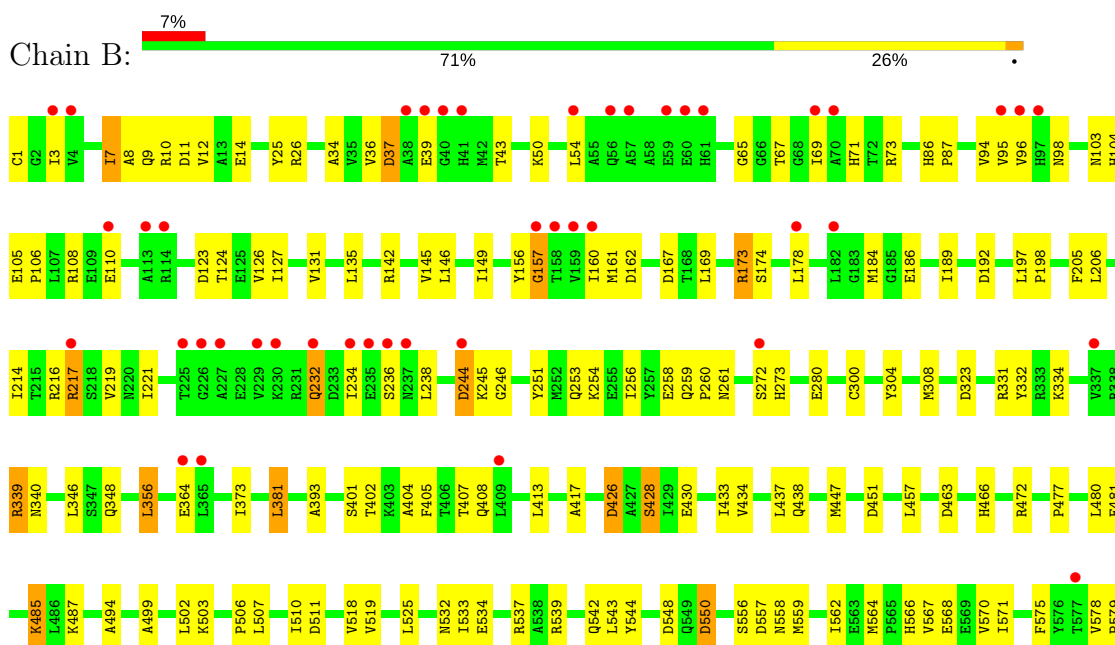
L582 Y585 H586 L589 I590 D594 P598 L601 V605 T606 V607 E608

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.30Å 91.23Å 184.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.35 29.31 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-2.35) 96.0 (29.31-2.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.185 , 0.237 0.184 , 0.230	Depositor DCC
R_{free} test set	2876 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	34.7	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 35.2	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9826	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: G6Q, ONL

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	1.04	4/4778 (0.1%)	0.99	17/6470 (0.3%)
1	B	0.93	2/4772 (0.0%)	0.97	13/6462 (0.2%)
All	All	0.98	6/9550 (0.1%)	0.98	30/12932 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	GLU	CD-OE1	6.75	1.33	1.25
1	A	105	GLU	CD-OE2	6.53	1.32	1.25
1	A	105	GLU	CD-OE1	6.42	1.32	1.25
1	A	42	MET	SD-CE	6.02	2.11	1.77
1	B	364	GLU	CD-OE1	5.03	1.31	1.25
1	B	534	GLU	CD-OE2	5.02	1.31	1.25

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	550	ASP	CB-CG-OD2	9.84	127.15	118.30
1	B	167	ASP	CB-CG-OD2	7.97	125.47	118.30
1	A	123	ASP	CB-CG-OD2	7.58	125.12	118.30
1	B	244	ASP	CB-CG-OD2	7.37	124.93	118.30
1	A	217	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	323	ASP	CB-CG-OD2	7.03	124.63	118.30
1	B	463	ASP	CB-CG-OD2	6.89	124.50	118.30
1	B	37	ASP	CB-CG-OD2	6.81	124.43	118.30
1	A	153	ARG	NE-CZ-NH1	-6.78	116.91	120.30
1	B	557	ASP	CB-CG-OD2	6.61	124.25	118.30
1	B	192	ASP	CB-CG-OD2	6.58	124.22	118.30
1	B	323	ASP	CB-CG-OD2	6.42	124.08	118.30
1	A	311	ARG	NE-CZ-NH2	-6.39	117.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	596	ASP	CB-CG-OD2	6.21	123.89	118.30
1	A	167	ASP	CB-CG-OD2	6.15	123.84	118.30
1	A	244	ASP	CB-CG-OD2	6.05	123.75	118.30
1	B	511	ASP	CB-CG-OD2	5.93	123.63	118.30
1	A	557	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	29	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	157	GLY	N-CA-C	-5.65	98.97	113.10
1	A	386	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	44	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	B	157	GLY	N-CA-C	-5.36	99.71	113.10
1	B	594	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	472	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	B	426	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	216	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	162	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	37	ASP	CB-CG-OD1	5.02	122.82	118.30
1	A	537	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	4697	0	4714	105	0
1	B	4692	0	4709	126	0
2	A	10	0	9	2	0
2	B	10	0	9	5	0
3	A	16	0	11	2	0
3	B	16	0	11	1	0
4	A	255	0	0	5	0
4	B	130	0	0	1	0
All	All	9826	0	9463	217	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 11.

All (217) 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:184:MET:SD	1:A:184:MET:CE	2.03	1.47
1:A:42:MET:CE	1:A:42:MET:SD	2.11	1.38
1:B:1:CYS:N	2:B:1609:ONL:HE1	1.63	1.09
1:B:7:ILE:HD11	1:B:169:LEU:HG	1.39	1.04
1:A:443:ARG:HD2	1:A:567:VAL:HG12	1.42	0.98
1:A:3:ILE:HD11	1:A:178:LEU:HD21	1.46	0.96
1:B:1:CYS:H3	2:B:1609:ONL:HE1	1.22	0.96
1:A:488:GLU:OE2	3:A:1610:G6Q:H1	1.72	0.90
1:A:443:ARG:CD	1:A:567:VAL:HG12	2.06	0.86
1:A:503:LYS:HD2	1:B:605:VAL:HG11	1.57	0.85
1:B:567:VAL:HG21	1:B:575:PHE:CD2	2.11	0.85
1:A:472:ARG:HH21	1:A:532:ASN:HD21	1.24	0.83
1:B:487:LYS:HE3	1:B:494:ALA:O	1.79	0.83
1:A:525:LEU:HD21	1:B:332:TYR:HB3	1.63	0.81
1:B:7:ILE:HD11	1:B:169:LEU:CG	2.09	0.81
1:A:421:ARG:HD2	1:A:430:GLU:OE1	1.82	0.80
1:B:346:LEU:HD23	1:B:373:ILE:HB	1.65	0.79
1:A:457:LEU:HD22	1:A:562:ILE:HD11	1.64	0.78
1:B:451:ASP:OD2	1:B:582:LEU:HD22	1.85	0.76
1:B:7:ILE:CD1	1:B:169:LEU:HG	2.15	0.76
1:B:1:CYS:H1	2:B:1609:ONL:HE1	1.51	0.75
1:A:14:GLU:HG2	4:A:2009:HOH:O	1.87	0.74
1:B:131:VAL:HG21	1:B:160:ILE:HD13	1.70	0.74
1:B:71:HIS:HE1	1:B:73:ARG:HB2	1.52	0.73
1:A:278:LEU:HD12	1:A:418:LYS:HG2	1.71	0.73
1:A:1:CYS:N	2:A:1609:ONL:HE1	2.05	0.72
1:B:356:LEU:HD13	1:B:381:LEU:HD22	1.70	0.72
1:B:507:LEU:HD12	1:B:510:ILE:HD12	1.71	0.71
1:A:356:LEU:HD13	1:A:381:LEU:HG	1.73	0.71
1:B:404:ALA:O	1:B:408:GLN:HG3	1.90	0.70
1:B:507:LEU:HD12	1:B:510:ILE:CD1	2.21	0.70
1:A:104:HIS:HD2	1:A:108:ARG:HH12	1.38	0.70
1:A:480:LEU:HD23	1:A:496:ALA:HB3	1.72	0.70
1:A:316:SER:HA	1:B:334:LYS:HD2	1.72	0.69
1:A:3:ILE:HD11	1:A:178:LEU:CD2	2.23	0.68
1:A:600:ASN:ND2	1:B:539:ARG:HD2	2.09	0.68
1:A:149:ILE:HB	1:A:150:PRO:HD3	1.75	0.67
1:A:332:TYR:HB3	1:B:525:LEU:HD21	1.77	0.67
1:B:123:ASP:O	1:B:126:VAL:HG22	1.96	0.65
1:A:583:LEU:O	1:A:587:VAL:HG23	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ILE:CD1	1:A:178:LEU:HD21	2.26	0.64
1:B:413:LEU:HG	1:B:433:ILE:HG23	1.80	0.64
1:A:562:ILE:HD12	1:A:562:ILE:N	2.12	0.64
1:B:586:HIS:O	1:B:590:ILE:HG12	1.97	0.64
1:B:562:ILE:HD12	1:B:562:ILE:N	2.14	0.63
1:B:244:ASP:O	1:B:254:LYS:HD3	1.98	0.63
1:A:421:ARG:HH11	1:A:421:ARG:HG2	1.63	0.63
1:A:401:SER:O	1:A:485:LYS:HE3	1.99	0.62
1:A:288:LEU:HD11	1:A:368:LEU:HB3	1.81	0.62
1:A:502:LEU:HD12	1:A:506:PRO:HB2	1.80	0.62
1:B:244:ASP:OD1	1:B:245:LYS:N	2.30	0.62
1:A:178:LEU:HD13	1:A:189:ILE:HD11	1.82	0.61
1:B:457:LEU:HD21	1:B:562:ILE:HD11	1.82	0.61
1:A:447:MET:CE	1:A:564:MET:SD	2.88	0.61
1:B:26:ARG:CZ	1:B:606:THR:HG21	2.30	0.61
1:B:477:PRO:HA	1:B:480:LEU:HD12	1.82	0.61
1:B:11:ASP:HA	1:B:65:GLY:O	2.01	0.61
1:A:101:ILE:HD11	1:A:127:ILE:HD11	1.83	0.60
1:B:537:ARG:HG2	1:B:543:LEU:HD12	1.82	0.60
1:B:567:VAL:HG21	1:B:575:PHE:CE2	2.37	0.60
1:B:71:HIS:CE1	1:B:73:ARG:HB2	2.36	0.60
1:B:103:ASN:O	1:B:106:PRO:HD2	2.02	0.59
1:A:443:ARG:HD2	1:A:567:VAL:CG1	2.26	0.59
1:B:104:HIS:HD2	1:B:108:ARG:HH12	1.51	0.58
1:A:466:HIS:CE1	1:B:466:HIS:CE1	2.91	0.58
1:A:562:ILE:HG22	1:A:564:MET:HE2	1.86	0.58
1:B:447:MET:CE	1:B:564:MET:SD	2.92	0.58
1:B:556:SER:HB3	1:B:559:MET:HB3	1.86	0.58
1:A:1:CYS:H1	2:A:1609:ONL:HE1	1.67	0.57
1:A:256:ILE:O	1:A:259:GLN:HG3	2.03	0.57
1:B:548:ASP:OD2	1:B:566:HIS:HD2	1.87	0.57
1:B:567:VAL:HG21	1:B:575:PHE:CG	2.40	0.56
1:A:605:VAL:HG11	1:B:503:LYS:HD2	1.88	0.56
1:B:173:ARG:NH1	1:B:206:LEU:O	2.30	0.56
1:A:533:ILE:HG23	1:A:543:LEU:HD22	1.87	0.56
1:B:3:ILE:HD13	1:B:157:GLY:O	2.06	0.56
1:B:69:ILE:HD12	1:B:96:VAL:HG13	1.86	0.56
1:B:67:THR:HG22	1:B:161:MET:CE	2.35	0.56
1:A:104:HIS:CD2	1:A:108:ARG:HH12	2.19	0.56
1:B:95:VAL:HG22	1:B:160:ILE:HG12	1.86	0.55
1:B:161:MET:HB3	1:B:169:LEU:CD2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:LEU:HB3	1:A:441:PRO:HD3	1.88	0.55
1:A:346:LEU:HD23	1:A:373:ILE:HB	1.88	0.55
1:B:447:MET:HE3	1:B:564:MET:SD	2.47	0.55
1:A:447:MET:HE3	1:A:564:MET:SD	2.47	0.55
1:B:578:VAL:N	1:B:579:PRO:HD2	2.22	0.55
1:A:457:LEU:CD2	1:A:562:ILE:HD11	2.36	0.55
1:B:104:HIS:CD2	1:B:108:ARG:HH12	2.25	0.55
1:B:537:ARG:HG2	1:B:543:LEU:CD1	2.36	0.55
1:B:393:ALA:HB2	1:B:407:THR:HG21	1.89	0.54
1:A:326:ILE:HG12	4:A:2150:HOH:O	2.07	0.54
1:A:197:LEU:N	1:A:198:PRO:CD	2.71	0.53
1:A:22:ARG:HG2	1:A:240:TYR:CZ	2.43	0.53
1:B:232:GLN:HE21	1:B:232:GLN:H	1.55	0.53
1:B:161:MET:CE	1:B:169:LEU:HD21	2.39	0.52
1:B:253:GLN:HB2	1:B:585:TYR:CZ	2.44	0.52
1:A:216:ARG:NH1	4:A:2115:HOH:O	2.38	0.52
1:B:178:LEU:HD22	1:B:189:ILE:HD11	1.90	0.52
1:A:503:LYS:HE2	1:B:608:GLU:C	2.31	0.52
1:A:567:VAL:HG11	1:A:575:PHE:CG	2.46	0.51
1:A:532:ASN:HA	1:A:535:GLU:OE1	2.11	0.51
1:A:104:HIS:HD2	1:A:108:ARG:NH1	2.06	0.51
1:B:434:VAL:O	1:B:438:GLN:HG3	2.10	0.51
1:B:598:PRO:HG2	1:B:601:LEU:HD12	1.91	0.51
1:B:256:ILE:HG13	1:B:402:THR:HG21	1.92	0.51
1:B:94:VAL:HB	1:B:161:MET:HG3	1.91	0.51
1:A:304:TYR:O	1:A:308:MET:HG2	2.11	0.51
1:A:476:TYR:HB3	1:A:477:PRO:HD3	1.92	0.51
1:A:491:TYR:N	1:A:491:TYR:CD1	2.77	0.51
1:B:156:TYR:CZ	1:B:174:SER:HB2	2.46	0.51
1:B:124:THR:HA	1:B:127:ILE:HD12	1.92	0.51
1:B:69:ILE:HD11	1:B:94:VAL:HG12	1.94	0.50
1:B:426:ASP:OD1	1:B:428:SER:HB3	2.12	0.50
1:A:232:GLN:HG3	4:A:2128:HOH:O	2.11	0.49
1:A:503:LYS:HD2	1:B:605:VAL:CG1	2.34	0.49
1:A:142:ARG:HD2	1:A:222:PHE:CE1	2.47	0.49
1:A:86:HIS:CD2	1:A:86:HIS:N	2.80	0.49
1:A:254:LYS:NZ	1:A:258:GLU:OE1	2.45	0.49
1:A:313:TRP:CD2	1:A:413:LEU:HD13	2.48	0.48
1:B:67:THR:HG22	1:B:161:MET:HE1	1.94	0.48
1:A:488:GLU:OE2	3:A:1610:G6Q:C1	2.54	0.48
1:A:440:LEU:O	1:A:441:PRO:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:GLN:HG3	1:A:564:MET:O	2.14	0.47
1:B:1:CYS:N	2:B:1609:ONL:CE	2.56	0.47
1:B:570:VAL:HG13	1:B:571:ILE:HG23	1.96	0.47
1:A:339:ARG:NH2	1:B:339:ARG:HH22	2.12	0.47
1:A:534:GLU:OE1	1:A:537:ARG:HD3	2.15	0.47
1:A:537:ARG:NH1	1:A:559:MET:HE2	2.30	0.47
1:B:272:SER:O	1:B:273:HIS:C	2.53	0.47
1:A:503:LYS:CD	1:B:605:VAL:HG11	2.38	0.47
1:B:86:HIS:CD2	1:B:86:HIS:N	2.83	0.47
1:A:562:ILE:HG22	1:A:564:MET:CE	2.45	0.47
1:A:605:VAL:HG11	1:B:503:LYS:CD	2.44	0.47
1:A:249:ARG:HG2	1:A:250:HIS:CD2	2.49	0.47
1:A:250:HIS:HD2	1:A:585:TYR:OH	1.98	0.47
1:B:537:ARG:HD2	1:B:558:ASN:ND2	2.30	0.46
1:A:413:LEU:HG	1:A:433:ILE:HG23	1.97	0.46
1:B:544:TYR:N	1:B:544:TYR:CD1	2.83	0.46
1:B:123:ASP:OD1	2:B:1609:ONL:N	2.49	0.46
1:B:161:MET:HE2	1:B:169:LEU:HD21	1.98	0.46
1:B:86:HIS:HA	1:B:87:PRO:C	2.36	0.46
1:A:105:GLU:HB2	1:A:106:PRO:HD3	1.98	0.46
1:A:185:GLY:O	1:A:216:ARG:HG2	2.16	0.46
1:A:472:ARG:NH2	1:A:532:ASN:HD21	2.03	0.46
1:B:206:LEU:HD23	1:B:221:ILE:HD13	1.98	0.45
1:A:525:LEU:CD2	1:B:332:TYR:HB3	2.41	0.45
1:B:537:ARG:HD2	1:B:558:ASN:HD21	1.80	0.45
1:B:502:LEU:HD12	1:B:506:PRO:HB2	1.98	0.45
1:B:417:ALA:HB1	1:B:430:GLU:HG3	1.98	0.45
1:A:401:SER:O	1:A:485:LYS:CE	2.63	0.45
1:A:489:ILE:HG13	1:A:588:ALA:HB2	1.99	0.45
1:B:405:PHE:CE2	1:B:481:GLU:HG2	2.51	0.45
1:B:217:ARG:HH11	1:B:217:ARG:HB3	1.81	0.45
1:A:180:ILE:HD12	1:A:206:LEU:HD21	1.98	0.44
1:B:106:PRO:O	1:B:110:GLU:HG3	2.17	0.44
1:B:433:ILE:HG12	1:B:570:VAL:HG21	1.98	0.44
1:A:578:VAL:N	1:A:579:PRO:HD2	2.31	0.44
1:B:232:GLN:NE2	1:B:232:GLN:H	2.16	0.44
1:B:472:ARG:HH21	1:B:532:ASN:HD21	1.65	0.44
1:A:472:ARG:HG3	1:A:499:ALA:HB3	1.98	0.44
1:A:443:ARG:HD3	1:A:567:VAL:HG12	1.97	0.44
1:A:339:ARG:HH22	1:B:339:ARG:NH2	2.15	0.44
1:A:567:VAL:HG11	1:A:575:PHE:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:ALA:O	1:A:408:GLN:HB2	2.16	0.44
1:B:472:ARG:HG3	1:B:499:ALA:HB3	1.99	0.44
1:B:245:LYS:HE3	1:B:251:TYR:CE2	2.52	0.44
1:B:205:PHE:CE2	1:B:234:ILE:HD11	2.53	0.43
1:B:567:VAL:CG2	1:B:575:PHE:CE2	3.01	0.43
1:B:447:MET:HE1	1:B:564:MET:SD	2.59	0.43
1:B:567:VAL:HG12	1:B:568:GLU:N	2.33	0.43
1:B:550:ASP:OD1	1:B:566:HIS:NE2	2.51	0.43
1:B:457:LEU:CD2	1:B:562:ILE:HD11	2.48	0.43
1:B:304:TYR:O	1:B:308:MET:HG2	2.17	0.43
1:A:114:ARG:HD3	1:A:133:TRP:CD2	2.53	0.43
1:B:206:LEU:CD2	1:B:221:ILE:HD13	2.49	0.43
1:A:248:TYR:CD2	1:A:254:LYS:HB2	2.54	0.43
1:A:36:VAL:HG22	1:A:42:MET:HG3	2.00	0.43
1:B:156:TYR:O	1:B:174:SER:N	2.41	0.43
1:B:67:THR:HG22	1:B:161:MET:HE2	2.00	0.43
1:A:413:LEU:HD23	1:A:437:LEU:HD21	2.00	0.42
1:B:156:TYR:CE2	1:B:174:SER:HB2	2.54	0.42
1:B:10:ARG:NH2	1:B:186:GLU:OE2	2.50	0.42
1:A:266:THR:O	1:A:270:ARG:HD2	2.19	0.42
1:B:300:CYS:HB2	3:B:1610:G6Q:H62	2.01	0.42
1:B:339:ARG:HD3	1:B:340:ASN:ND2	2.34	0.42
1:B:197:LEU:N	1:B:198:PRO:CD	2.82	0.42
1:A:454:ILE:CD1	1:A:546:PHE:HE2	2.32	0.42
1:B:161:MET:HE3	1:B:169:LEU:HD21	2.00	0.42
1:B:8:ALA:HB3	1:B:12:VAL:CG1	2.49	0.42
1:A:472:ARG:O	1:A:475:GLN:HB2	2.18	0.42
1:A:484:LEU:O	1:A:488:GLU:HB2	2.20	0.42
1:B:25:TYR:HA	4:B:2010:HOH:O	2.18	0.42
1:B:105:GLU:HB2	1:B:106:PRO:HD3	2.02	0.42
1:B:413:LEU:HD23	1:B:437:LEU:HD21	2.02	0.42
1:B:145:VAL:O	1:B:149:ILE:HG12	2.20	0.42
1:B:214:ILE:HG23	1:B:219:VAL:HG22	2.02	0.42
1:B:401:SER:O	1:B:485:LYS:HE3	2.20	0.42
1:B:518:VAL:HG11	1:B:533:ILE:HD11	2.02	0.42
1:B:7:ILE:HD13	1:B:67:THR:HG23	2.01	0.41
1:A:114:ARG:HD3	1:A:133:TRP:CE3	2.55	0.41
1:B:142:ARG:O	1:B:146:LEU:HD12	2.20	0.41
1:B:236:SER:HB2	1:B:238:LEU:HD13	2.01	0.41
1:A:263:ILE:HD12	1:A:444:ILE:HD12	2.01	0.41
1:A:313:TRP:CE3	1:A:413:LEU:HD13	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:GLN:HE21	1:B:216:ARG:CZ	2.34	0.41
1:A:60:GLU:HG3	1:A:61:HIS:CD2	2.56	0.41
1:A:440:LEU:HD13	1:A:571:ILE:HD13	2.02	0.41
1:A:537:ARG:CG	1:A:543:LEU:HD13	2.50	0.41
1:A:545:VAL:HG12	1:A:547:ALA:HB2	2.02	0.40
1:A:79:GLU:HG2	4:A:2074:HOH:O	2.22	0.40
1:A:173:ARG:HG3	1:A:176:SER:O	2.21	0.40
1:A:97:HIS:HB3	1:A:124:THR:HG23	2.02	0.40
1:B:245:LYS:O	1:B:246:GLY:C	2.58	0.40
1:B:254:LYS:HE2	1:B:258:GLU:OE1	2.21	0.40
1:B:259:GLN:N	1:B:260:PRO:CD	2.85	0.40
1:B:34:ALA:HB2	1:B:87:PRO:HG2	2.03	0.40
1:A:103:ASN:O	1:A:106:PRO:HD2	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	606/608 (100%)	591 (98%)	14 (2%)	1 (0%)	51	61
1	B	606/608 (100%)	580 (96%)	25 (4%)	1 (0%)	51	61
All	All	1212/1216 (100%)	1171 (97%)	39 (3%)	2 (0%)	51	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	337	VAL
1	B	280	GLU

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	500/500 (100%)	485 (97%)	15 (3%)	46	58
1	B	499/500 (100%)	474 (95%)	25 (5%)	28	35
All	All	999/1000 (100%)	959 (96%)	40 (4%)	36	46

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	98	ASN
1	A	135	LEU
1	A	167	ASP
1	A	236	SER
1	A	238	LEU
1	A	249	ARG
1	A	264	LYS
1	A	291	LYS
1	A	356	LEU
1	A	452	LYS
1	A	459	GLU
1	A	460	ASP
1	A	543	LEU
1	A	589	LEU
1	B	7	ILE
1	B	14	GLU
1	B	36	VAL
1	B	37	ASP
1	B	39	GLU
1	B	43	THR
1	B	50	LYS
1	B	54	LEU
1	B	98	ASN
1	B	135	LEU
1	B	173	ARG
1	B	184	MET

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Mol	Chain	Res	Type
1	B	217	ARG
1	B	232	GLN
1	B	261	ASN
1	B	331	ARG
1	B	339	ARG
1	B	348	GLN
1	B	356	LEU
1	B	381	LEU
1	B	428	SER
1	B	485	LYS
1	B	519	VAL
1	B	542	GLN
1	B	589	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	104	HIS
1	A	250	HIS
1	A	450	GLN
1	A	532	ASN
1	A	542	GLN
1	A	549	GLN
1	A	600	ASN
1	B	9	GLN
1	B	71	HIS
1	B	104	HIS
1	B	193	GLN
1	B	232	GLN
1	B	250	HIS
1	B	348	GLN
1	B	438	GLN
1	B	522	ASN
1	B	532	ASN
1	B	600	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	ONL	A	1609	1	4,9,9	1.15	0	5,11,11	1.96	2 (40%)
3	G6Q	A	1610	-	15,15,15	0.92	0	20,21,21	1.93	3 (15%)
2	ONL	B	1609	1	4,9,9	0.91	0	5,11,11	1.37	1 (20%)
3	G6Q	B	1610	-	15,15,15	0.84	1 (6%)	20,21,21	1.61	2 (10%)

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	ONL	A	1609	1	-	0/5/9/9	0/0/0/0
3	G6Q	A	1610	-	-	0/18/20/20	0/0/0/0
2	ONL	B	1609	1	-	0/5/9/9	0/0/0/0
3	G6Q	B	1610	-	-	0/18/20/20	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1610	G6Q	O4-C4	2.04	1.47	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1610	G6Q	O2-C2-C1	-5.22	97.90	110.30
3	A	1610	G6Q	O1-C1-C2	-4.42	113.10	125.13
3	B	1610	G6Q	O2-C2-C1	-4.18	100.38	110.30
3	B	1610	G6Q	O1-C1-C2	-3.48	115.64	125.13
2	B	1609	ONL	CB-CG-CD	-2.79	111.46	114.47
2	A	1609	ONL	CG-CB-CA	-2.66	107.64	113.84
2	A	1609	ONL	CE-CD-CG	-2.48	110.60	116.87
3	A	1610	G6Q	O3-C3-C2	2.69	114.10	109.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1609	ONL	2	0
3	A	1610	G6Q	2	0
2	B	1609	ONL	5	0
3	B	1610	G6Q	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, 95th 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^2)	Q<0.9
1	A	608/608 (100%)	-0.37	8 (1%)	77	85	19, 24, 30, 36	0
1	B	608/608 (100%)	0.14	44 (7%)	16	23	17, 23, 30, 37	0
All	All	1216/1216 (100%)	-0.12	52 (4%)	36	48	17, 24, 30, 37	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	113	ALA	5.2
1	B	234	ILE	4.4
1	B	38	ALA	4.2
1	B	225	THR	4.1
1	B	232	GLN	3.8
1	B	227	ALA	3.8
1	B	159	VAL	3.7
1	B	110	GLU	3.6
1	B	96	VAL	3.6
1	B	3	ILE	3.6
1	B	4	VAL	3.4
1	B	364	GLU	3.4
1	B	57	ALA	3.3
1	B	237	ASN	3.2
1	B	217	ARG	3.2
1	B	157	GLY	3.0
1	B	41	HIS	3.0
1	B	236	SER	3.0
1	B	272	SER	2.9
1	B	226	GLY	2.9
1	A	96	VAL	2.9
1	B	235	GLU	2.8
1	B	70	ALA	2.7
1	B	59	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	230	LYS	2.7
1	B	69	ILE	2.6
1	A	159	VAL	2.6
1	B	337	VAL	2.6
1	B	365	LEU	2.6
1	B	39	GLU	2.6
1	B	95	VAL	2.6
1	B	56	GLN	2.5
1	A	3	ILE	2.4
1	B	229	VAL	2.4
1	A	158	THR	2.4
1	A	273	HIS	2.4
1	B	160	ILE	2.3
1	B	244	ASP	2.3
1	B	60	GLU	2.3
1	B	409	LEU	2.3
1	A	70	ALA	2.3
1	B	97	HIS	2.2
1	B	114	ARG	2.2
1	B	178	LEU	2.2
1	A	243	GLY	2.2
1	B	54	LEU	2.1
1	B	182	LEU	2.1
1	B	61	HIS	2.1
1	A	69	ILE	2.1
1	B	158	THR	2.1
1	B	577	THR	2.0
1	B	40	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ONL	A	1609	10/10	0.97	0.30	4.06	24,24,28,29	0
2	ONL	B	1609	10/10	0.93	0.34	3.82	23,25,26,27	0
3	G6Q	B	1610	16/16	0.97	0.09	-1.10	22,27,39,39	0
3	G6Q	A	1610	16/16	0.98	0.08	-1.47	22,24,32,34	0

6.5 Other polymers ⓘ

There are no such residues in this entry.