



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 2, 2026 – 12:07 AM EDT

PDB ID : 9NS8 / pdb\_00009ns8  
Title : Crystal Structure of Side-VI IG1 Domain  
Authors : Olechwier, A.M.; Ozkan, E.  
Deposited on : 2025-03-16  
Resolution : 2.51 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

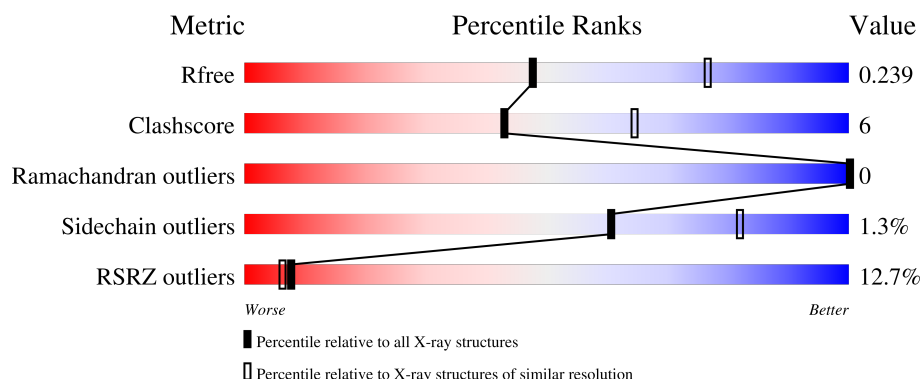
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.51 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))
$R_{free}$	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 of 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	135	
1	B	135	
1	C	135	
1	D	135	
1	E	135	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	135	<div><div></div><div>10%</div><div>70%</div><div>14%</div><div>16%</div></div>
1	G	135	<div><div></div><div>11%</div><div>70%</div><div>17%</div><div>12%</div></div>
1	H	135	<div><div></div><div>10%</div><div>73%</div><div>12%</div><div>15%</div></div>
1	I	135	<div><div></div><div>7%</div><div>73%</div><div>13%</div><div>13%</div></div>
1	J	135	<div><div></div><div>11%</div><div>70%</div><div>16%</div><div>13%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9432 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 Sidestep VI, isoform B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	115	Total	C	N	O	S	0	0	0
			915	573	165	175	2			
1	B	115	Total	C	N	O	S	0	0	0
			915	573	165	175	2			
1	C	117	Total	C	N	O	S	0	0	0
			931	584	168	177	2			
1	D	119	Total	C	N	O	S	0	0	0
			946	593	170	181	2			
1	E	118	Total	C	N	O	S	0	0	0
			938	587	169	180	2			
1	F	114	Total	C	N	O	S	0	0	0
			908	568	164	174	2			
1	G	119	Total	C	N	O	S	0	0	0
			946	593	170	181	2			
1	H	115	Total	C	N	O	S	0	0	0
			915	573	165	175	2			
1	I	117	Total	C	N	O	S	0	1	0
			937	590	167	178	2			
1	J	117	Total	C	N	O	S	0	0	0
			931	584	168	177	2			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLY	-	expression tag	UNP Q0KI85
B	18	GLY	-	expression tag	UNP Q0KI85
C	18	GLY	-	expression tag	UNP Q0KI85
D	18	GLY	-	expression tag	UNP Q0KI85
E	18	GLY	-	expression tag	UNP Q0KI85
F	18	GLY	-	expression tag	UNP Q0KI85
G	18	GLY	-	expression tag	UNP Q0KI85
H	18	GLY	-	expression tag	UNP Q0KI85
I	18	GLY	-	expression tag	UNP Q0KI85

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	18	GLY	-	expression tag	UNP Q0KI85

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		

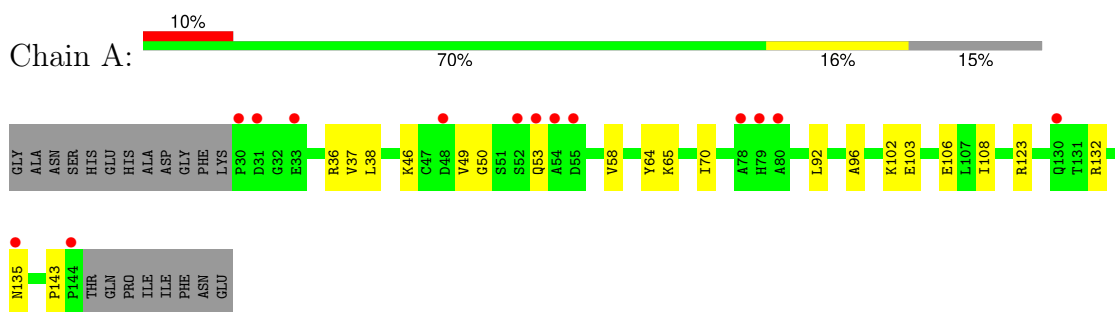
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		
4	B	10	Total	O	0	0
			10	10		
4	C	16	Total	O	0	0
			16	16		
4	D	11	Total	O	0	0
			11	11		
4	E	14	Total	O	0	0
			14	14		
4	F	8	Total	O	0	0
			8	8		
4	G	13	Total	O	0	0
			13	13		
4	H	16	Total	O	0	0
			16	16		
4	I	15	Total	O	0	0
			15	15		
4	J	10	Total	O	0	0
			10	10		

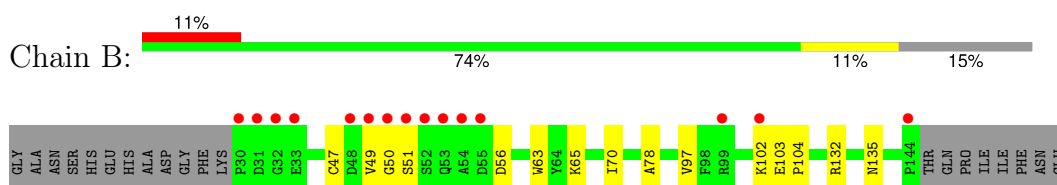
### 3 Residue-property plots

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.

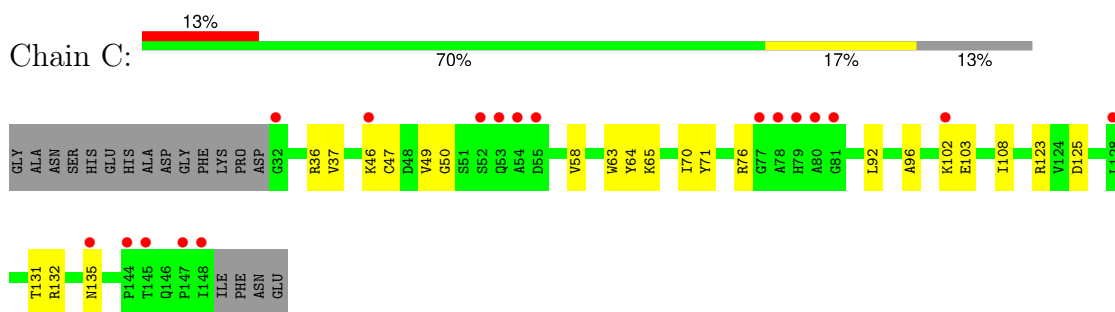
- Molecule 1: Sidestep VI, isoform B



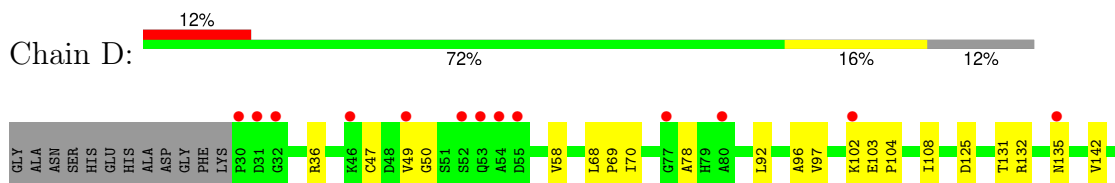
- Molecule 1: Sidestep VI, isoform B

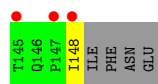


- Molecule 1: Sidestep VI, isoform B

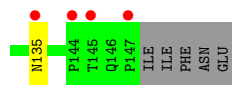
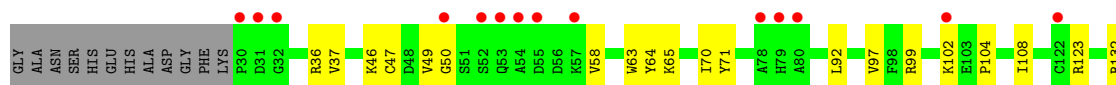


- Molecule 1: Sidestep VI, isoform B

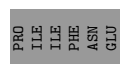
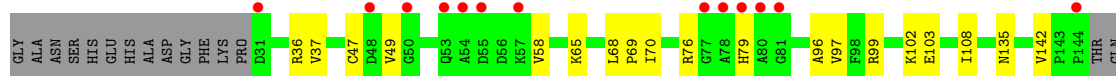




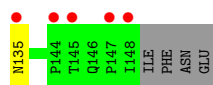
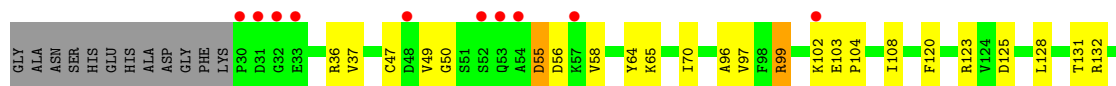
- Molecule 1: Sidestep VI, isoform B



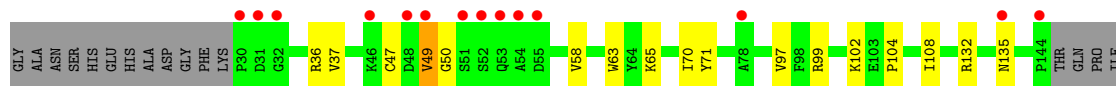
- Molecule 1: Sidestep VI, isoform B



- Molecule 1: Sidestep VI, isoform B



- Molecule 1: Sidestep VI, isoform B



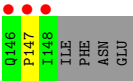
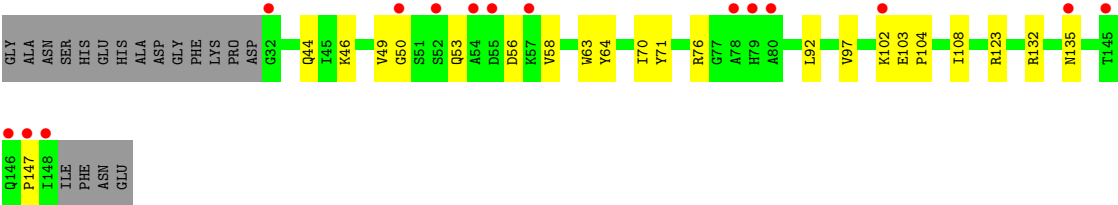
- Molecule 1: Sidestep VI, isoform B







● Molecule 1: Sidestep VI, isoform B



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.77Å 181.42Å 300.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.51 – 2.51 46.51 – 2.51	Depositor EDS
% Data completeness (in resolution range)	97.7 (46.51-2.51) 97.8 (46.51-2.51)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.97 (at 2.51Å)	Xtriage
Refinement program	PHENIX 2.0rc1_5617	Depositor
R, $R_{free}$	0.208 , 0.238 0.209 , 0.239	Depositor DCC
$R_{free}$ test set	1953 reflections (2.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.3	Xtriage
Anisotropy	0.770	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 48.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9432	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.22	0/934	0.42	0/1269
1	B	0.24	0/934	0.42	0/1269
1	C	0.21	0/950	0.40	0/1292
1	D	0.20	0/966	0.40	0/1314
1	E	0.21	0/958	0.40	0/1303
1	F	0.22	0/926	0.40	0/1258
1	G	0.20	0/966	0.38	0/1314
1	H	0.26	0/934	0.43	0/1269
1	I	0.20	0/958	0.37	0/1298
1	J	0.20	0/950	0.40	0/1292
All	All	0.22	0/9476	0.40	0/12878

There are no bond length outliers.

There are no bond angle outliers.

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	915	0	901	16	0
1	B	915	0	901	10	0
1	C	931	0	922	16	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	946	0	934	15	0
1	E	938	0	923	14	0
1	F	908	0	893	13	0
1	G	946	0	934	16	0
1	H	915	0	901	10	0
1	I	937	0	932	14	0
1	J	931	0	922	14	0
2	B	4	0	3	0	0
2	D	4	0	3	0	0
2	G	4	0	3	0	0
2	H	4	0	3	0	0
3	D	6	0	8	0	0
3	G	6	0	8	1	0
4	A	9	0	0	0	0
4	B	10	0	0	0	0
4	C	16	0	0	0	0
4	D	11	0	0	0	0
4	E	14	0	0	0	0
4	F	8	0	0	0	0
4	G	13	0	0	0	0
4	H	16	0	0	0	0
4	I	15	0	0	0	0
4	J	10	0	0	0	0
All	All	9432	0	9191	115	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 6.

All (115) 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)
3:G:1002:GOL:HO3	3:G:1002:GOL:HO1	1.15	0.86
1:J:64:TYR:OH	1:J:123:ARG:NH1	2.24	0.71
1:H:50:GLY:O	1:H:132:ARG:NH1	2.24	0.70
1:E:50:GLY:O	1:E:132:ARG:NH1	2.21	0.69
1:G:99:ARG:HG3	1:G:108:ILE:HD13	1.74	0.69
1:J:50:GLY:O	1:J:132:ARG:NH1	2.26	0.69
1:I:70:ILE:HD12	1:I:92:LEU:HD11	1.75	0.68
1:C:50:GLY:O	1:C:132:ARG:NH1	2.26	0.68
1:H:49:VAL:HG12	1:H:58:VAL:HG21	1.76	0.66
1:G:49:VAL:HG12	1:G:58:VAL:HG21	1.79	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:TYR:OH	1:C:123:ARG:NH1	2.32	0.63
1:I:49:VAL:HG12	1:I:58:VAL:HG21	1.80	0.63
1:D:47:CYS:O	1:D:49:VAL:HG23	1.98	0.62
1:G:50:GLY:O	1:G:132:ARG:NH1	2.32	0.62
1:C:70:ILE:HD12	1:C:92:LEU:HD11	1.82	0.62
1:J:70:ILE:HD12	1:J:92:LEU:HD11	1.81	0.62
1:B:47:CYS:O	1:B:49:VAL:HG23	2.01	0.61
1:B:102:LYS:HG3	1:H:37:VAL:HG12	1.83	0.60
1:A:50:GLY:O	1:A:132:ARG:NH1	2.34	0.60
1:G:97:VAL:HG21	1:H:97:VAL:HG21	1.83	0.60
1:F:65:LYS:HB2	1:F:70:ILE:HD13	1.84	0.59
1:A:64:TYR:OH	1:A:123:ARG:NH1	2.36	0.59
1:G:55:ASP:OD1	1:G:55:ASP:N	2.28	0.58
1:A:49:VAL:HG12	1:A:49:VAL:O	2.04	0.58
1:B:50:GLY:O	1:B:132:ARG:NH1	2.37	0.57
1:A:37:VAL:HG12	1:C:102:LYS:HG3	1.87	0.57
1:B:51:SER:OG	1:B:56:ASP:HB3	2.05	0.57
1:H:47:CYS:O	1:H:49:VAL:HG23	2.05	0.56
1:E:70:ILE:HD12	1:E:92:LEU:HD11	1.86	0.56
1:D:49:VAL:HG12	1:D:58:VAL:HG21	1.88	0.56
1:G:125:ASP:OD1	1:G:131:THR:OG1	2.17	0.56
1:D:50:GLY:O	1:D:132:ARG:NH1	2.38	0.55
1:J:53:GLN:HB2	1:J:56:ASP:HB2	1.87	0.55
1:C:49:VAL:HG13	1:C:58:VAL:HG21	1.89	0.54
1:F:99:ARG:HG3	1:F:108:ILE:HD13	1.90	0.54
1:A:36:ARG:HB3	1:C:103:GLU:HB2	1.90	0.53
1:H:102:LYS:HE2	1:H:104:PRO:O	2.09	0.53
1:C:47:CYS:HB2	1:C:63:TRP:CZ2	2.44	0.53
1:D:142:VAL:HG11	1:D:148:ILE:HG22	1.91	0.53
1:H:65:LYS:HB2	1:H:70:ILE:HD13	1.91	0.52
1:C:125:ASP:OD1	1:C:131:THR:OG1	2.24	0.51
1:D:78:ALA:HA	1:J:76:ARG:NH1	2.26	0.51
1:G:47:CYS:O	1:G:49:VAL:HG23	2.11	0.50
1:I:50:GLY:O	1:I:132:ARG:NH1	2.45	0.50
1:I:65:LYS:HB2	1:I:70:ILE:HD13	1.93	0.50
1:B:65:LYS:HB2	1:B:70:ILE:HD13	1.94	0.49
1:E:36:ARG:HB3	1:J:103:GLU:HB2	1.94	0.49
1:D:125:ASP:OD1	1:D:131:THR:OG1	2.30	0.49
1:E:65:LYS:HB2	1:E:70:ILE:HD13	1.95	0.49
1:G:102:LYS:HE2	1:G:104:PRO:O	2.13	0.48
1:E:64:TYR:OH	1:E:123:ARG:NH1	2.47	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LEU:HD22	1:A:143:PRO:HG3	1.94	0.48
1:E:46:LYS:HE2	1:J:46:LYS:HE2	1.95	0.48
1:H:99:ARG:HG3	1:H:108:ILE:HD13	1.95	0.48
1:A:65:LYS:HB2	1:A:70:ILE:HD13	1.95	0.48
1:E:97:VAL:HG21	1:F:97:VAL:HG21	1.94	0.48
1:F:76:ARG:HE	1:F:79:HIS:CD2	2.31	0.48
1:B:102:LYS:HE2	1:B:104:PRO:O	2.14	0.48
1:B:97:VAL:HG21	1:D:97:VAL:HG21	1.95	0.47
1:I:47:CYS:O	1:I:49:VAL:HG23	2.14	0.47
1:A:102:LYS:HG3	1:C:37:VAL:HG12	1.95	0.47
1:J:102:LYS:HE2	1:J:104:PRO:O	2.14	0.47
1:D:103:GLU:HB2	1:G:36:ARG:HB3	1.96	0.47
1:E:99:ARG:HG3	1:E:108:ILE:HD13	1.97	0.47
1:A:103:GLU:HB2	1:C:36:ARG:HB3	1.96	0.47
1:C:65:LYS:HB2	1:C:70:ILE:HD13	1.97	0.47
1:G:64:TYR:OH	1:G:123:ARG:NH1	2.49	0.46
1:A:49:VAL:CG1	1:A:58:VAL:HG21	2.45	0.46
1:A:49:VAL:HG13	1:A:58:VAL:HG21	1.97	0.46
1:F:102:LYS:HG3	1:I:37:VAL:HG12	1.97	0.46
1:I:97:VAL:HG21	1:J:97:VAL:HG21	1.97	0.45
1:A:46:LYS:HG3	1:A:106:GLU:HG2	1.98	0.45
1:B:103:GLU:HB2	1:H:36:ARG:HB3	1.98	0.45
1:F:142:VAL:HG11	1:J:147:PRO:HD2	1.99	0.45
1:G:56:ASP:HA	1:G:128:LEU:HD23	1.99	0.44
1:I:38:LEU:O	1:I:41:SER:OG	2.32	0.44
1:I:36:ARG:HG3	1:I:139:GLU:HB3	2.00	0.44
1:C:49:VAL:CG1	1:C:58:VAL:HG21	2.48	0.43
1:D:36:ARG:HB3	1:G:103:GLU:HB2	2.00	0.43
1:I:29:LYS:HB2	1:I:29:LYS:HE3	1.73	0.43
1:D:102:LYS:HE2	1:D:104:PRO:O	2.18	0.43
1:F:49:VAL:CG1	1:F:58:VAL:HG21	2.49	0.43
1:J:49:VAL:CG1	1:J:58:VAL:HG21	2.49	0.43
1:C:63:TRP:HB2	1:C:71:TYR:HB3	2.00	0.43
1:E:49:VAL:CG1	1:E:58:VAL:HG21	2.48	0.43
1:B:78:ALA:HA	1:C:76:ARG:NH1	2.33	0.42
1:I:102[B]:LYS:HE2	1:I:102[B]:LYS:HB3	1.74	0.42
1:B:47:CYS:HB2	1:B:63:TRP:CZ2	2.54	0.42
1:D:49:VAL:CG1	1:D:58:VAL:HG21	2.49	0.42
1:E:102:LYS:HE2	1:E:104:PRO:O	2.19	0.42
1:A:49:VAL:O	1:A:49:VAL:CG1	2.67	0.42
1:D:102:LYS:HG3	1:G:37:VAL:HG12	2.02	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:LEU:HD12	1:D:69:PRO:HD2	2.01	0.42
1:E:63:TRP:HB2	1:E:71:TYR:HB3	2.02	0.42
1:G:65:LYS:HB2	1:G:70:ILE:HD13	2.01	0.42
1:F:37:VAL:HG12	1:I:102[B]:LYS:HG2	2.01	0.42
1:J:63:TRP:HB2	1:J:71:TYR:HB3	2.02	0.42
1:D:70:ILE:HD12	1:D:92:LEU:HD11	2.00	0.42
1:A:46:LYS:HE2	1:C:46:LYS:HE2	2.01	0.41
1:E:37:VAL:HG12	1:J:102:LYS:HG3	2.02	0.41
1:F:96:ALA:HA	1:F:108:ILE:O	2.19	0.41
1:J:44:GLN:HG2	1:J:108:ILE:HG13	2.02	0.41
1:F:103:GLU:HB2	1:I:36:ARG:HB3	2.02	0.41
1:D:96:ALA:HA	1:D:108:ILE:O	2.21	0.41
1:E:47:CYS:HB2	1:E:63:TRP:CZ2	2.55	0.41
1:F:36:ARG:HB3	1:I:103:GLU:HB2	2.02	0.41
1:C:96:ALA:HA	1:C:108:ILE:O	2.20	0.41
1:F:47:CYS:O	1:F:49:VAL:HG23	2.20	0.41
1:A:70:ILE:HD12	1:A:92:LEU:HD11	2.03	0.41
1:F:68:LEU:HD12	1:F:69:PRO:HD2	2.02	0.41
1:E:49:VAL:HG13	1:E:58:VAL:HG21	2.03	0.41
1:A:96:ALA:HA	1:A:108:ILE:O	2.21	0.40
1:G:64:TYR:O	1:G:120:PHE:HA	2.22	0.40
1:G:96:ALA:HA	1:G:108:ILE:O	2.21	0.40
1:H:63:TRP:HB2	1:H:71:TYR:HB3	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/135 (84%)	110 (97%)	3 (3%)	0	100	100
1	B	113/135 (84%)	110 (97%)	3 (3%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	115/135 (85%)	112 (97%)	3 (3%)	0	100	100
1	D	117/135 (87%)	114 (97%)	3 (3%)	0	100	100
1	E	116/135 (86%)	111 (96%)	5 (4%)	0	100	100
1	F	112/135 (83%)	108 (96%)	4 (4%)	0	100	100
1	G	117/135 (87%)	113 (97%)	4 (3%)	0	100	100
1	H	113/135 (84%)	108 (96%)	5 (4%)	0	100	100
1	I	114/135 (84%)	112 (98%)	2 (2%)	0	100	100
1	J	115/135 (85%)	114 (99%)	1 (1%)	0	100	100
All	All	1145/1350 (85%)	1112 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	103/119 (87%)	101 (98%)	2 (2%)	50	76
1	B	103/119 (87%)	102 (99%)	1 (1%)	68	86
1	C	105/119 (88%)	104 (99%)	1 (1%)	68	86
1	D	107/119 (90%)	106 (99%)	1 (1%)	70	87
1	E	106/119 (89%)	105 (99%)	1 (1%)	70	87
1	F	102/119 (86%)	101 (99%)	1 (1%)	68	86
1	G	107/119 (90%)	104 (97%)	3 (3%)	38	66
1	H	103/119 (87%)	101 (98%)	2 (2%)	50	76
1	I	106/119 (89%)	105 (99%)	1 (1%)	70	87
1	J	105/119 (88%)	104 (99%)	1 (1%)	68	86
All	All	1047/1190 (88%)	1033 (99%)	14 (1%)	61	82

All (14) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	53	GLN
1	A	135	ASN
1	B	135	ASN
1	C	135	ASN
1	D	135	ASN
1	E	135	ASN
1	F	135	ASN
1	G	55	ASP
1	G	99	ARG
1	G	135	ASN
1	H	49	VAL
1	H	135	ASN
1	I	135	ASN
1	J	135	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	B	40	ASN
1	B	44	GLN
1	B	119	ASN
1	B	135	ASN
1	C	44	GLN
1	D	44	GLN
1	D	119	ASN
1	D	135	ASN
1	E	44	GLN
1	F	79	HIS
1	F	119	ASN
1	F	137	ASN
1	G	44	GLN
1	G	146	GLN
1	H	44	GLN
1	J	44	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

6 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	GOL	D	1002	-	5,5,5	0.29	0	5,5,5	0.65	0
2	ACT	G	1001	-	3,3,3	1.12	0	3,3,3	1.25	0
3	GOL	G	1002	-	5,5,5	0.77	0	5,5,5	3.44	3 (60%)
2	ACT	D	1001	-	3,3,3	1.17	0	3,3,3	1.08	0
2	ACT	B	1001	-	3,3,3	1.16	0	3,3,3	1.08	0
2	ACT	H	1001	-	3,3,3	1.09	0	3,3,3	1.31	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	GOL	D	1002	-	-	0/4/4/4	-
3	GOL	G	1002	-	-	1/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1002	GOL	C3-C2-C1	-5.80	90.53	111.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1002	GOL	O1-C1-C2	-3.82	93.19	110.38
3	G	1002	GOL	O3-C3-C2	-3.01	96.84	110.38

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	1002	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1002	GOL	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	115/135 (85%)	0.58	14 (12%) 8 7	38, 55, 117, 130	0
1	B	115/135 (85%)	0.53	15 (13%) 7 6	37, 56, 99, 117	0
1	C	117/135 (86%)	0.58	18 (15%) 5 4	40, 56, 112, 138	0
1	D	119/135 (88%)	0.56	16 (13%) 7 5	41, 56, 106, 121	0
1	E	118/135 (87%)	0.57	18 (15%) 5 4	43, 55, 106, 140	0
1	F	114/135 (84%)	0.57	13 (11%) 10 8	41, 57, 115, 124	0
1	G	119/135 (88%)	0.62	15 (12%) 8 6	40, 56, 106, 121	0
1	H	115/135 (85%)	0.64	14 (12%) 8 7	35, 55, 97, 112	0
1	I	117/135 (86%)	0.46	10 (8%) 16 14	37, 54, 106, 127	1 (0%)
1	J	117/135 (86%)	0.61	15 (12%) 7 6	45, 58, 105, 139	0
All	All	1166/1350 (86%)	0.57	148 (12%) 8 6	35, 56, 107, 140	1 (0%)

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	80	ALA	7.3
1	G	148	ILE	6.8
1	C	148	ILE	6.4
1	D	30	PRO	6.3
1	J	148	ILE	6.3
1	I	145	THR	5.9
1	B	30	PRO	5.6
1	A	78	ALA	5.6
1	C	80	ALA	5.4
1	D	148	ILE	5.4
1	A	30	PRO	5.3
1	H	30	PRO	5.2
1	F	78	ALA	4.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	78	ALA	4.9
1	E	147	PRO	4.8
1	A	80	ALA	4.8
1	E	80	ALA	4.7
1	H	54	ALA	4.7
1	I	80	ALA	4.5
1	E	78	ALA	4.5
1	H	144	PRO	4.5
1	J	78	ALA	4.5
1	E	30	PRO	4.4
1	G	30	PRO	4.4
1	I	77	GLY	4.4
1	C	145	THR	4.3
1	F	79	HIS	4.3
1	A	79	HIS	4.2
1	G	54	ALA	4.2
1	B	52	SER	4.0
1	G	145	THR	3.9
1	B	53	GLN	3.9
1	G	144	PRO	3.9
1	J	80	ALA	3.9
1	H	53	GLN	3.9
1	E	54	ALA	3.8
1	B	50	GLY	3.8
1	H	55	ASP	3.8
1	B	144	PRO	3.8
1	E	79	HIS	3.7
1	B	48	ASP	3.7
1	C	79	HIS	3.7
1	G	102	LYS	3.7
1	J	79	HIS	3.6
1	G	53	GLN	3.6
1	A	144	PRO	3.6
1	J	135	ASN	3.6
1	G	48	ASP	3.4
1	E	145	THR	3.4
1	B	31	ASP	3.3
1	A	54	ALA	3.2
1	F	53	GLN	3.2
1	A	31	ASP	3.2
1	I	54	ALA	3.1
1	J	52	SER	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	57	LYS	3.0
1	C	54	ALA	3.0
1	D	80	ALA	3.0
1	A	55	ASP	3.0
1	J	147	PRO	3.0
1	I	48	ASP	3.0
1	F	77	GLY	3.0
1	J	54	ALA	2.9
1	D	49	VAL	2.9
1	D	102	LYS	2.9
1	H	32	GLY	2.9
1	D	32	GLY	2.9
1	H	49	VAL	2.9
1	B	54	ALA	2.9
1	F	54	ALA	2.9
1	H	31	ASP	2.9
1	G	32	GLY	2.8
1	H	78	ALA	2.8
1	C	128	LEU	2.8
1	F	144	PRO	2.8
1	F	55	ASP	2.8
1	D	31	ASP	2.7
1	J	55	ASP	2.7
1	H	135	ASN	2.7
1	C	144	PRO	2.7
1	C	102	LYS	2.7
1	A	52	SER	2.7
1	D	145	THR	2.6
1	C	55	ASP	2.6
1	F	50	GLY	2.6
1	J	32	GLY	2.6
1	C	53	GLN	2.6
1	C	77	GLY	2.5
1	H	52	SER	2.5
1	F	31	ASP	2.5
1	C	135	ASN	2.5
1	I	144	PRO	2.5
1	E	55	ASP	2.5
1	J	102	LYS	2.5
1	G	147	PRO	2.4
1	C	81	GLY	2.4
1	E	31	ASP	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	32	GLY	2.4
1	G	31	ASP	2.4
1	A	135	ASN	2.4
1	I	52	SER	2.4
1	E	50	GLY	2.4
1	D	55	ASP	2.4
1	B	49	VAL	2.4
1	F	57	LYS	2.4
1	H	46	LYS	2.4
1	J	57	LYS	2.4
1	B	99	ARG	2.3
1	E	122	CYS	2.3
1	A	48	ASP	2.3
1	H	51	SER	2.3
1	E	144	PRO	2.3
1	F	81	GLY	2.3
1	I	53	GLN	2.3
1	E	57	LYS	2.3
1	D	53	GLN	2.2
1	B	51	SER	2.2
1	D	52	SER	2.2
1	D	147	PRO	2.2
1	D	54	ALA	2.2
1	D	135	ASN	2.2
1	I	81	GLY	2.2
1	G	52	SER	2.2
1	C	147	PRO	2.2
1	G	135	ASN	2.2
1	B	32	GLY	2.2
1	A	33	GLU	2.2
1	G	33	GLU	2.2
1	A	53	GLN	2.1
1	J	50	GLY	2.1
1	C	52	SER	2.1
1	B	102	LYS	2.1
1	E	53	GLN	2.1
1	J	146	GLN	2.1
1	B	55	ASP	2.1
1	H	48	ASP	2.1
1	D	46	LYS	2.1
1	E	102	LYS	2.1
1	I	102[A]	LYS	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	46	LYS	2.1
1	A	130	GLN	2.1
1	E	135	ASN	2.1
1	E	52	SER	2.1
1	B	33	GLU	2.0
1	D	77	GLY	2.0
1	J	145	THR	2.0
1	F	48	ASP	2.0
1	E	32	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 oligosaccharides 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	ACT	B	1001	4/4	0.80	0.26	47,54,61,62	0
2	ACT	G	1001	4/4	0.80	0.20	57,58,60,64	0
2	ACT	D	1001	4/4	0.82	0.28	65,65,78,81	0
3	GOL	G	1002	6/6	0.82	0.27	73,79,95,98	0
3	GOL	D	1002	6/6	0.86	0.17	56,74,75,85	0
2	ACT	H	1001	4/4	0.89	0.19	43,49,59,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.