



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:51 PM GMT

PDB ID : 4GF9
Title : Structural insights into the dual strategy of recognition of peptidoglycan recognition protein, PGRP-S: ternary complex of PGRP-S with LPS and fatty acid
Authors : Sharma, P.; Dube, D.; Sinha, M.; Yadav, S.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2012-08-03
Resolution : 2.80 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 (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

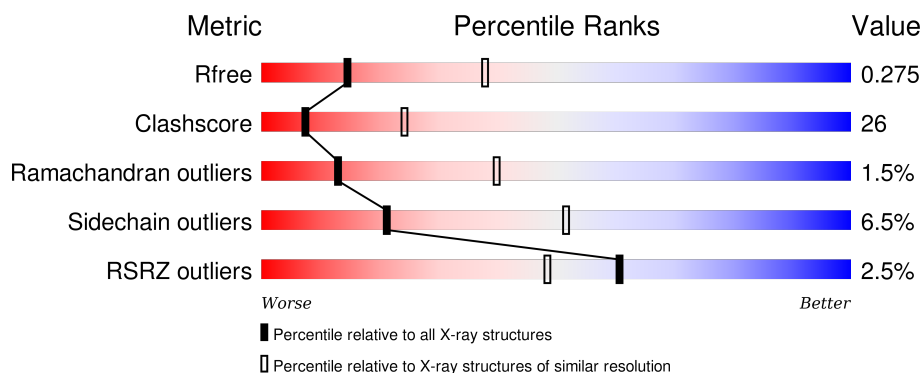
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 $\leq 5\%$. 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	171	<div> <div>4%</div> <div>53%</div> <div>43%</div> <div>5%</div> </div>
1	B	171	<div> <div>4%</div> <div>58%</div> <div>36%</div> <div>6%</div> </div>
1	C	171	<div> <div>%</div> <div>67%</div> <div>28%</div> <div>5%</div> </div>
1	D	171	<div> <div>2%</div> <div>64%</div> <div>31%</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	STE	B	201	-	-	X	-
3	LP5	C	501	-	-	-	X
4	GOL	D	201	-	-	-	X

2 Entry composition [i](#)

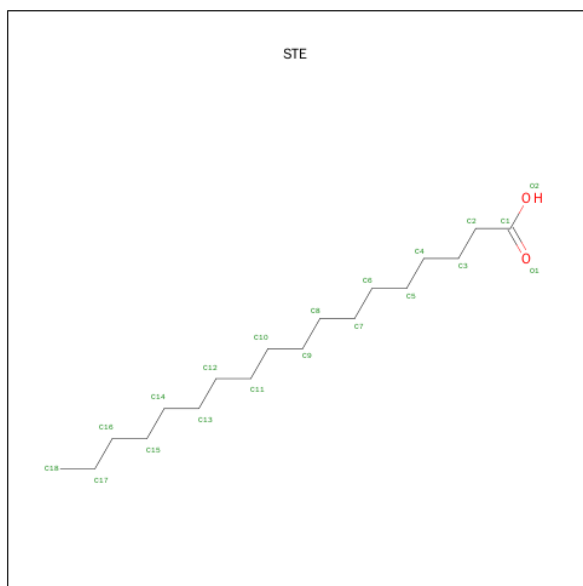
There are 5 unique types of molecules in this entry. The entry contains 5673 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Peptidoglycan recognition protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	0
			1336	834	254	240	8			
1	B	171	Total	C	N	O	S	0	0	0
			1336	834	254	240	8			
1	C	171	Total	C	N	O	S	0	0	0
			1336	834	254	240	8			
1	D	171	Total	C	N	O	S	0	0	0
			1336	834	254	240	8			

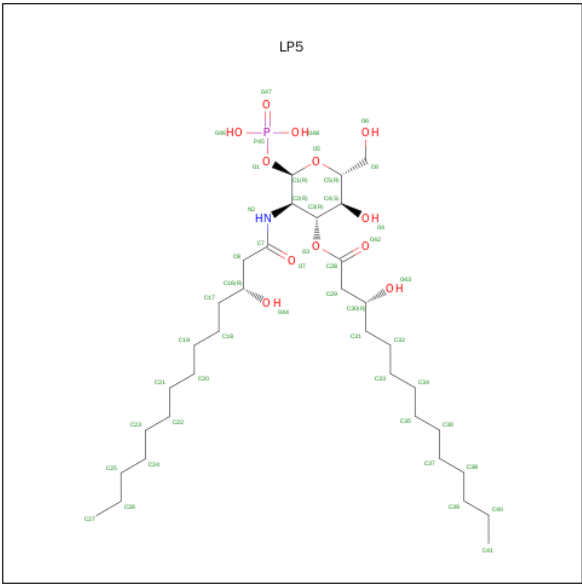
- Molecule 2 is STEARIC ACID (three-letter code: STE) (formula: C₁₈H₃₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			20	18	2		

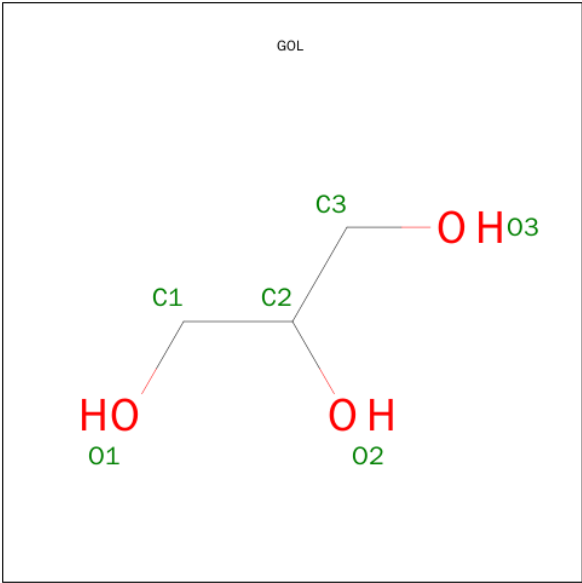
- Molecule 3 is (R)-((2R,3S,4R,5R,6R)-3-HYDROXY-2-(HYDROXYMETHYL)-5-((R)-3-HYDROXYTETRADECANAMIDO)-6-(PHOSPHONOOXY)TETRAHYDRO-2H-

PYRAN-4-YL) 3-HYDROXYTETRADECANOATE (three-letter code: LP5) (formula: C₃₄H₆₆NO₁₂P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			48	34	1	12	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

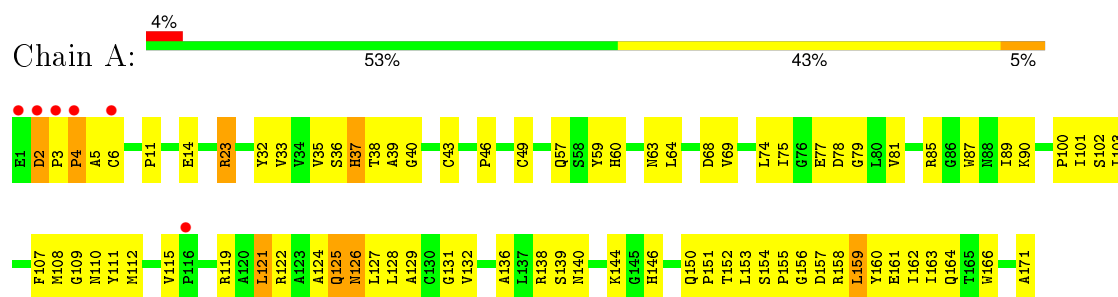
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	69	Total 69	O 69	0	0
5	B	60	Total 60	O 60	0	0
5	C	61	Total 61	O 61	0	0
5	D	65	Total 65	O 65	0	0

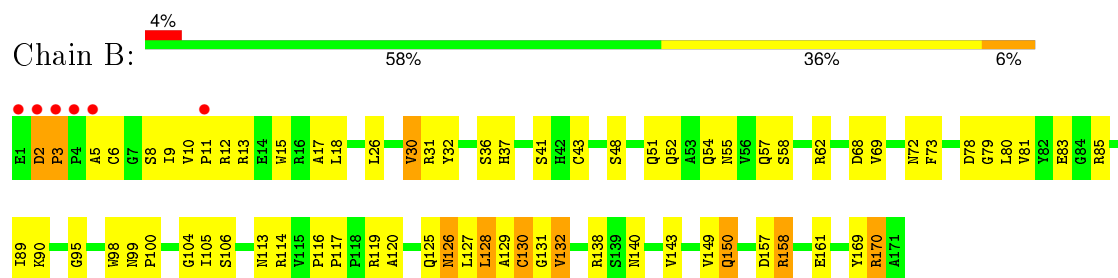
3 Residue-property plots

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.

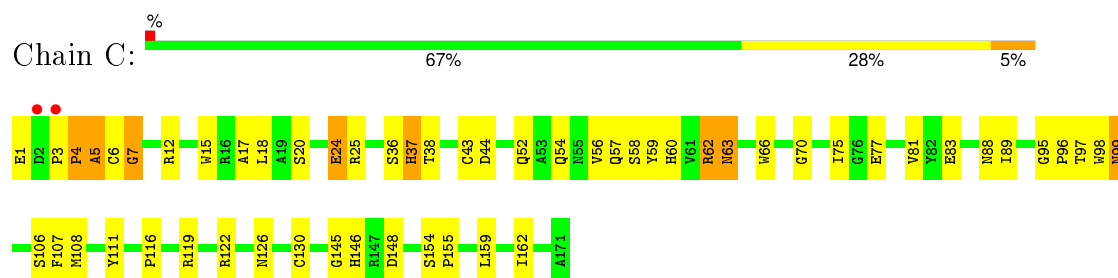
• Molecule 1: Peptidoglycan recognition protein 1



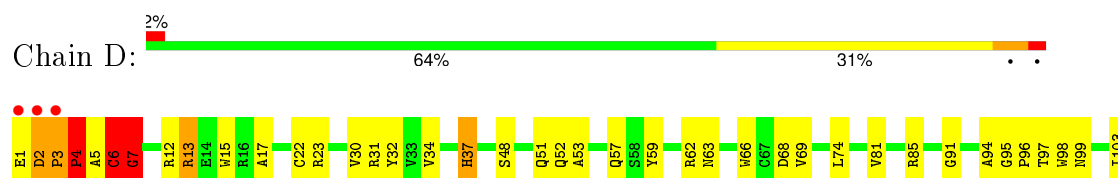
• Molecule 1: Peptidoglycan recognition protein 1



• Molecule 1: Peptidoglycan recognition protein 1



• Molecule 1: Peptidoglycan recognition protein 1



S106	F107	M108
M112	N113	R114
V115	P116	L127
C130	E142	V143
K144	Y149	Q150
P151	P155	G156
D157	R158	L159
I163	Q164	T165
W166	Y169	R170
A171		

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	89.62Å 101.88Å 163.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.01 – 2.80 48.01 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.01-2.80) 98.3 (48.01-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.43 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.227 , 0.265 0.241 , 0.275	Depositor DCC
R_{free} test set	948 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 18594 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5673	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GOL, LP5, STE

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	0.77	1/1373 (0.1%)	0.91	0/1871
1	B	0.89	1/1373 (0.1%)	0.96	1/1871 (0.1%)
1	C	0.83	0/1373	0.88	2/1871 (0.1%)
1	D	0.78	0/1373	0.88	2/1871 (0.1%)
All	All	0.82	2/5492 (0.0%)	0.91	5/7484 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	132	VAL	CA-C	5.63	1.67	1.52
1	A	49	CYS	CB-SG	-5.31	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	99	ASN	CB-CG-OD1	-6.17	109.26	121.60
1	C	7	GLY	N-CA-C	5.93	127.94	113.10
1	D	7	GLY	N-CA-C	5.67	127.27	113.10
1	D	3	PRO	C-N-CD	-5.58	108.33	120.60
1	B	170	ARG	NE-CZ-NH2	-5.29	117.66	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	6	CYS	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1336	0	1288	74	0
1	B	1336	0	1288	79	0
1	C	1336	0	1288	50	0
1	D	1336	0	1288	63	0
2	B	20	0	35	11	0
3	C	48	0	64	12	0
4	D	6	0	8	0	0
5	A	69	0	0	0	0
5	B	60	0	0	0	0
5	C	61	0	0	0	0
5	D	65	0	0	0	0
All	All	5673	0	5259	273	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 26.

All (273) 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:D:4:PRO:CB	1:D:5:ALA:HA	1.40	1.38
1:B:85:ARG:CB	1:B:89:ILE:HD11	1.69	1.23
1:B:85:ARG:HB3	1:B:89:ILE:CD1	1.67	1.22
1:B:5:ALA:HB1	1:B:6:CYS:HA	1.16	1.15
1:B:158:ARG:HG2	1:B:158:ARG:HH21	1.04	1.13
1:A:5:ALA:HB1	1:A:6:CYS:HA	1.16	1.10
1:D:114:ARG:HH11	1:D:114:ARG:HG3	1.06	1.10
1:D:4:PRO:CB	1:D:5:ALA:CA	2.30	1.09
2:B:201:STE:H91	2:B:201:STE:H52	1.18	1.08
1:D:4:PRO:HB3	1:D:5:ALA:CA	1.90	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:CYS:O	1:A:77:GLU:HB2	1.62	0.99
3:C:501:LP5:H2	1:D:96:PRO:HD2	1.46	0.98
2:B:201:STE:H91	2:B:201:STE:C5	1.82	0.96
1:C:4:PRO:CB	1:C:5:ALA:HB2	1.96	0.96
1:B:78:ASP:OD1	1:B:79:GLY:N	2.00	0.94
1:D:4:PRO:HB3	1:D:5:ALA:HA	0.95	0.93
1:D:62:ARG:HG2	1:D:62:ARG:HH21	1.31	0.93
1:A:5:ALA:HB1	1:A:6:CYS:CA	1.98	0.93
1:A:129:ALA:HB2	2:B:201:STE:H122	1.50	0.90
1:C:4:PRO:HB2	1:C:5:ALA:HB2	1.53	0.90
1:D:4:PRO:HB2	1:D:5:ALA:HA	1.52	0.90
1:B:85:ARG:HB3	1:B:89:ILE:HD11	0.88	0.88
1:B:5:ALA:HB1	1:B:6:CYS:CA	2.04	0.87
1:D:52:GLN:HA	1:D:52:GLN:OE1	1.73	0.87
1:A:158:ARG:O	1:A:161:GLU:HB2	1.74	0.87
3:C:501:LP5:O4	3:C:501:LP5:H291	1.73	0.87
1:A:5:ALA:CB	1:A:6:CYS:HA	2.01	0.85
1:B:5:ALA:HB1	2:B:201:STE:H92	1.58	0.85
1:D:114:ARG:NH1	1:D:114:ARG:HG3	1.81	0.82
1:B:158:ARG:HH21	1:B:158:ARG:CG	1.92	0.81
1:C:62:ARG:CG	1:C:62:ARG:HH11	1.94	0.80
1:C:155:PRO:HB2	1:C:159:LEU:HD23	1.64	0.80
1:B:158:ARG:NH2	1:B:158:ARG:HG2	1.85	0.80
1:B:5:ALA:CB	1:B:6:CYS:HA	2.03	0.79
1:D:48:SER:O	1:D:51:GLN:HB3	1.83	0.79
1:D:112:MET:CE	1:D:156:GLY:HA2	2.16	0.75
1:C:43:CYS:O	1:C:77:GLU:HB2	1.87	0.74
1:A:40:GLY:O	1:A:109:GLY:HA2	1.86	0.73
1:B:81:VAL:HG11	1:B:127:LEU:HD13	1.69	0.73
1:B:26:LEU:HD22	1:B:100:PRO:O	1.89	0.72
1:B:12:ARG:HB3	1:B:17:ALA:HB3	1.71	0.72
1:D:112:MET:HE2	1:D:156:GLY:HA2	1.69	0.72
1:B:125:GLN:O	1:B:128:LEU:HB2	1.90	0.70
1:D:22:CYS:SG	1:D:68:ASP:HB2	2.30	0.70
1:A:160:TYR:CE2	1:A:164:GLN:NE2	2.59	0.70
1:D:74:LEU:HD22	1:D:108:MET:CE	2.23	0.69
1:C:58:SER:O	1:C:62:ARG:HB2	1.93	0.69
1:A:79:GLY:HA3	1:A:119:ARG:HD2	1.75	0.68
1:B:95:GLY:HA3	1:B:150:GLN:HE22	1.58	0.68
1:B:58:SER:O	1:B:62:ARG:HB2	1.91	0.68
1:B:89:ILE:HD12	1:B:89:ILE:O	1.93	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:PRO:HA	1:A:78:ASP:OD2	1.95	0.67
1:A:157:ASP:O	1:A:161:GLU:HG3	1.95	0.67
1:B:125:GLN:HA	1:B:128:LEU:CD2	2.25	0.66
1:B:9:ILE:HG13	1:B:9:ILE:O	1.95	0.66
1:D:6:CYS:SG	1:D:7:GLY:N	2.69	0.66
1:D:53:ALA:N	1:D:108:MET:HE1	2.10	0.66
1:C:36:SER:OG	1:C:106:SER:HB2	1.94	0.65
1:C:62:ARG:HG2	1:C:62:ARG:HH11	1.61	0.65
1:D:142:GLU:OE1	1:D:170:ARG:HD3	1.95	0.65
3:C:501:LP5:C29	3:C:501:LP5:O4	2.45	0.65
1:A:36:SER:HA	1:A:155:PRO:HB3	1.80	0.64
1:B:26:LEU:HG	1:B:90:LYS:HA	1.80	0.64
1:A:115:VAL:HG13	1:A:158:ARG:HD3	1.79	0.64
1:C:75:ILE:HD13	1:C:81:VAL:HG22	1.79	0.64
1:C:24:GLU:O	1:C:89:ILE:HG23	1.98	0.64
1:D:30:VAL:HG11	1:D:103:ILE:HG12	1.79	0.63
1:D:53:ALA:CA	1:D:108:MET:HE1	2.29	0.63
1:C:37:HIS:CD2	1:C:155:PRO:HA	2.34	0.63
1:C:4:PRO:HB3	1:C:5:ALA:HB2	1.82	0.62
1:B:89:ILE:HD12	1:B:89:ILE:C	2.20	0.62
1:D:74:LEU:HD22	1:D:108:MET:HE2	1.82	0.62
3:C:501:LP5:H273	1:D:99:ASN:HD21	1.66	0.61
1:D:53:ALA:HA	1:D:108:MET:CE	2.30	0.61
1:B:126:ASN:C	1:B:128:LEU:N	2.49	0.60
1:B:95:GLY:CA	1:B:150:GLN:HE22	2.15	0.60
1:C:38:THR:CG2	1:C:108:MET:HA	2.32	0.60
1:B:143:VAL:HB	1:B:169:TYR:HA	1.84	0.60
1:B:5:ALA:CB	2:B:201:STE:H92	2.30	0.60
1:D:22:CYS:SG	1:D:68:ASP:CB	2.90	0.60
1:B:95:GLY:HA3	1:B:150:GLN:NE2	2.16	0.59
1:D:6:CYS:SG	1:D:7:GLY:HA2	2.42	0.59
1:A:121:LEU:O	1:A:125:GLN:HB2	2.03	0.59
1:D:4:PRO:HB2	1:D:5:ALA:CA	2.18	0.59
1:D:62:ARG:CG	1:D:62:ARG:HH21	2.11	0.59
1:A:39:ALA:HA	1:A:110:ASN:HB2	1.83	0.59
1:D:53:ALA:HA	1:D:108:MET:HE1	1.83	0.59
1:D:62:ARG:NH2	1:D:62:ARG:HG2	2.08	0.59
1:C:4:PRO:HB2	1:C:5:ALA:CB	2.32	0.58
1:C:52:GLN:O	1:C:56:VAL:HG23	2.03	0.58
1:B:157:ASP:O	1:B:161:GLU:HG3	2.04	0.58
1:B:128:LEU:O	1:B:132:VAL:HG23	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:MET:CE	1:A:153:LEU:HD13	2.33	0.58
1:B:18:LEU:H	1:B:57:GLN:HE22	1.51	0.58
1:B:9:ILE:O	1:B:11:PRO:HD3	2.04	0.57
1:A:68:ASP:HB3	1:A:85:ARG:HE	1.70	0.57
1:A:60:HIS:HA	1:A:64:LEU:HD12	1.86	0.57
1:B:130:CYS:SG	1:B:130:CYS:O	2.62	0.57
1:B:125:GLN:HA	1:B:128:LEU:HD23	1.87	0.56
1:A:5:ALA:CB	1:A:6:CYS:CA	2.71	0.56
1:A:112:MET:HE3	1:A:153:LEU:HD13	1.86	0.56
1:C:6:CYS:SG	1:C:7:GLY:N	2.77	0.56
1:A:81:VAL:HG11	1:A:127:LEU:HD22	1.87	0.56
1:C:122:ARG:O	1:C:126:ASN:HB2	2.05	0.56
1:A:37:HIS:CD2	1:A:37:HIS:C	2.80	0.55
1:C:15:TRP:CZ2	1:C:17:ALA:HB2	2.42	0.55
1:C:116:PRO:HG3	1:C:159:LEU:HD13	1.88	0.55
1:A:37:HIS:HD2	1:A:37:HIS:O	1.90	0.55
1:A:144:LYS:NZ	1:A:171:ALA:HA	2.21	0.54
1:C:18:LEU:HB2	1:C:57:GLN:NE2	2.21	0.54
1:D:115:VAL:HG12	1:D:158:ARG:HB3	1.90	0.54
1:A:23:ARG:CG	1:A:23:ARG:HH21	2.21	0.54
1:C:12:ARG:NH2	1:C:20:SER:HB2	2.23	0.53
1:A:35:VAL:O	1:A:146:HIS:HB2	2.08	0.53
1:B:125:GLN:HA	1:B:128:LEU:HD22	1.91	0.53
1:D:1:GLU:O	1:D:2:ASP:CB	2.56	0.53
1:A:110:ASN:OD1	1:A:111:TYR:N	2.42	0.53
1:C:12:ARG:HA	1:C:15:TRP:NE1	2.23	0.53
1:A:75:ILE:O	1:A:108:MET:HG3	2.09	0.53
1:A:90:LYS:HD2	1:A:100:PRO:HA	1.91	0.53
1:D:74:LEU:HD22	1:D:108:MET:HE3	1.92	0.52
1:A:110:ASN:C	1:A:110:ASN:OD1	2.48	0.52
3:C:501:LP5:H292	1:D:97:THR:HB	1.90	0.52
1:B:98:TRP:NE1	1:B:149:VAL:HB	2.24	0.52
1:B:99:ASN:N	1:B:100:PRO:HD2	2.24	0.52
2:B:201:STE:H132	2:B:201:STE:H52	1.92	0.52
1:C:62:ARG:HG3	1:C:62:ARG:HH11	1.72	0.52
1:D:116:PRO:HG2	1:D:159:LEU:HD13	1.91	0.52
1:B:31:ARG:O	1:B:31:ARG:CG	2.57	0.52
1:C:6:CYS:HB3	1:C:130:CYS:HA	1.92	0.51
1:B:43:CYS:HB2	1:B:48:SER:OG	2.10	0.51
1:D:6:CYS:SG	1:D:7:GLY:CA	2.98	0.51
1:D:34:VAL:HA	1:D:144:LYS:O	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ASN:HB2	1:B:104:GLY:O	2.11	0.51
1:B:30:VAL:HG13	1:B:31:ARG:N	2.26	0.51
1:A:150:GLN:HB3	1:A:151:PRO:HD2	1.93	0.51
1:C:145:GLY:O	1:C:148:ASP:HB2	2.11	0.51
1:B:140:ASN:O	1:B:140:ASN:OD1	2.29	0.51
1:D:62:ARG:CG	1:D:62:ARG:NH2	2.73	0.50
1:A:33:VAL:HA	1:A:103:ILE:O	2.12	0.50
1:A:38:THR:HG23	1:A:108:MET:HA	1.93	0.50
1:A:140:ASN:HB3	3:C:501:LP5:H341	1.93	0.50
1:A:74:LEU:C	1:A:75:ILE:HD12	2.32	0.50
1:B:98:TRP:C	1:B:100:PRO:HD2	2.32	0.49
1:D:15:TRP:CZ2	1:D:17:ALA:HB2	2.46	0.49
1:A:11:PRO:HD2	1:A:14:GLU:HB2	1.94	0.49
1:D:52:GLN:O	1:D:53:ALA:C	2.51	0.49
1:D:48:SER:O	1:D:51:GLN:CB	2.58	0.49
1:B:57:GLN:HG3	1:B:58:SER:N	2.27	0.49
1:B:6:CYS:HA	2:B:201:STE:H92	1.94	0.49
1:A:166:TRP:CD1	1:A:166:TRP:N	2.78	0.49
1:A:154:SER:HA	1:A:156:GLY:H	1.76	0.49
1:B:95:GLY:N	1:B:150:GLN:HE22	2.10	0.49
1:C:60:HIS:O	1:C:66:TRP:HB2	2.13	0.49
1:D:1:GLU:C	1:D:3:PRO:HD3	2.32	0.49
1:D:149:VAL:O	1:D:150:GLN:HG2	2.13	0.49
1:A:87:TRP:CE3	1:A:103:ILE:HD13	2.48	0.48
1:B:5:ALA:CB	1:B:6:CYS:CA	2.77	0.48
1:B:98:TRP:CD1	1:B:149:VAL:HB	2.49	0.48
1:C:38:THR:HG23	1:C:107:PHE:O	2.13	0.48
1:B:68:ASP:OD1	1:B:69:VAL:N	2.40	0.48
1:A:129:ALA:CB	2:B:201:STE:H122	2.34	0.48
1:C:38:THR:HG21	1:C:108:MET:HG2	1.95	0.48
1:A:36:SER:CA	1:A:155:PRO:HB3	2.43	0.48
1:B:125:GLN:OE1	1:B:128:LEU:HD23	2.14	0.48
3:C:501:LP5:H292	1:D:97:THR:CB	2.43	0.48
1:C:62:ARG:CG	1:C:62:ARG:NH1	2.64	0.48
1:B:31:ARG:HA	1:B:138:ARG:HG3	1.95	0.48
1:C:63:ASN:N	1:C:63:ASN:OD1	2.46	0.48
1:D:2:ASP:O	1:D:2:ASP:OD1	2.32	0.47
1:B:126:ASN:C	1:B:128:LEU:H	2.18	0.47
1:D:57:GLN:HG3	1:D:69:VAL:HB	1.96	0.47
1:B:15:TRP:CZ2	1:B:17:ALA:HB2	2.50	0.47
1:B:68:ASP:OD1	1:B:69:VAL:HG12	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:TYR:HB2	1:A:102:SER:HB3	1.96	0.47
1:A:154:SER:HA	1:A:156:GLY:N	2.30	0.47
1:B:89:ILE:C	1:B:89:ILE:CD1	2.82	0.47
1:D:74:LEU:HA	1:D:106:SER:O	2.15	0.47
1:C:15:TRP:CH2	1:C:17:ALA:HB2	2.50	0.47
1:D:81:VAL:HG11	1:D:127:LEU:HD13	1.95	0.47
1:B:169:TYR:CD2	1:B:169:TYR:C	2.88	0.47
1:B:158:ARG:N	1:B:158:ARG:HD3	2.30	0.47
1:B:113:ASN:HA	1:B:158:ARG:NH2	2.30	0.47
1:B:117:PRO:O	1:B:120:ALA:HB3	2.15	0.47
1:A:81:VAL:CG1	1:A:127:LEU:HD22	2.45	0.46
1:D:85:ARG:HD2	1:D:91:GLY:HA2	1.97	0.46
1:B:26:LEU:CD2	1:B:100:PRO:O	2.63	0.46
1:A:144:LYS:HZ3	1:A:171:ALA:HA	1.79	0.46
1:B:126:ASN:O	1:B:127:LEU:C	2.54	0.46
1:C:146:HIS:HB3	1:C:154:SER:O	2.16	0.46
1:A:159:LEU:O	1:A:162:ILE:N	2.45	0.46
2:B:201:STE:H41	2:B:201:STE:O2	2.16	0.46
1:B:99:ASN:N	1:B:100:PRO:CD	2.79	0.46
1:D:98:TRP:CD1	1:D:149:VAL:HB	2.51	0.46
1:A:37:HIS:CD2	1:A:37:HIS:O	2.69	0.46
3:C:501:LP5:H171	3:C:501:LP5:H201	1.65	0.46
1:C:37:HIS:CD2	1:C:154:SER:HA	2.51	0.46
1:A:138:ARG:HE	1:A:138:ARG:HB3	1.69	0.46
1:D:149:VAL:C	1:D:150:GLN:HG2	2.36	0.45
1:A:89:ILE:N	1:A:89:ILE:HD12	2.31	0.45
1:A:32:TYR:CD1	1:A:101:ILE:HD13	2.52	0.45
1:A:3:PRO:HA	1:A:4:PRO:HD3	1.73	0.45
1:D:95:GLY:HA3	1:D:150:GLN:HE22	1.81	0.45
1:A:128:LEU:O	1:A:132:VAL:HG23	2.17	0.45
1:A:23:ARG:NH2	1:A:23:ARG:CG	2.80	0.45
1:B:52:GLN:O	1:B:55:ASN:HB2	2.17	0.45
1:B:31:ARG:O	1:B:31:ARG:HG3	2.18	0.45
1:D:59:TYR:O	1:D:63:ASN:HB2	2.17	0.44
1:B:2:ASP:HB2	1:B:3:PRO:HD3	1.98	0.44
1:A:163:ILE:HG13	1:A:163:ILE:H	1.59	0.44
1:C:95:GLY:H	3:C:501:LP5:H82	1.81	0.44
1:A:150:GLN:HB3	1:A:151:PRO:CD	2.48	0.44
1:C:146:HIS:ND1	1:C:154:SER:HB3	2.32	0.44
1:A:159:LEU:O	1:A:160:TYR:C	2.56	0.44
1:C:59:TYR:CE2	1:D:151:PRO:HA	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ASN:O	1:A:129:ALA:HB3	2.18	0.43
1:B:85:ARG:HB3	1:B:89:ILE:CG1	2.43	0.43
1:C:77:GLU:OE2	1:C:111:TYR:HE2	2.01	0.43
1:D:4:PRO:HB2	1:D:5:ALA:CB	2.47	0.43
1:C:99:ASN:HB2	3:C:501:LP5:O46	2.18	0.43
1:D:52:GLN:CA	1:D:52:GLN:OE1	2.50	0.43
1:C:60:HIS:CE1	1:C:70:GLY:H	2.35	0.43
1:A:57:GLN:HG3	1:A:69:VAL:HB	2.00	0.43
1:A:89:ILE:HG22	1:A:90:LYS:N	2.34	0.43
1:A:68:ASP:HB3	1:A:85:ARG:NE	2.34	0.43
1:B:30:VAL:HG13	1:B:32:TYR:H	1.83	0.43
1:A:87:TRP:HE3	1:A:103:ILE:HD13	1.83	0.43
1:C:38:THR:HG21	1:C:108:MET:HA	2.01	0.43
1:C:60:HIS:ND1	1:C:70:GLY:N	2.65	0.43
1:A:132:VAL:HG13	1:A:139:SER:HA	2.01	0.43
1:B:26:LEU:HD23	1:B:90:LYS:HB2	2.00	0.42
1:A:122:ARG:O	1:A:126:ASN:HB2	2.19	0.42
1:C:97:THR:HG22	1:C:98:TRP:CD1	2.53	0.42
1:D:127:LEU:O	1:D:130:CYS:HB3	2.18	0.42
1:B:73:PHE:HB2	1:B:105:ILE:HG22	2.00	0.42
1:B:26:LEU:HG	1:B:89:ILE:O	2.19	0.42
1:A:122:ARG:HD2	1:B:8:SER:HA	2.02	0.42
1:B:12:ARG:HA	1:B:15:TRP:NE1	2.33	0.42
1:D:31:ARG:HB3	1:D:32:TYR:CE1	2.55	0.42
1:C:6:CYS:HB2	1:C:130:CYS:HB2	1.63	0.42
1:B:57:GLN:CB	1:B:69:VAL:HB	2.49	0.42
1:C:96:PRO:HA	3:C:501:LP5:O46	2.20	0.42
1:C:36:SER:O	1:C:106:SER:HA	2.20	0.42
1:C:6:CYS:CB	1:C:130:CYS:HA	2.49	0.42
1:A:121:LEU:HD23	1:A:121:LEU:H	1.84	0.41
1:A:2:ASP:H	1:A:3:PRO:HD3	1.84	0.41
1:B:36:SER:O	1:B:106:SER:HA	2.20	0.41
1:D:164:GLN:HG2	1:D:169:TYR:CE2	2.55	0.41
3:C:501:LP5:H332	3:C:501:LP5:H371	2.02	0.41
1:C:77:GLU:OE2	1:C:111:TYR:CE2	2.73	0.41
1:B:129:ALA:O	1:B:131:GLY:N	2.52	0.41
1:C:18:LEU:HB2	1:C:57:GLN:HE22	1.86	0.41
1:D:66:TRP:N	1:D:66:TRP:CD1	2.88	0.41
1:B:116:PRO:HA	1:B:117:PRO:HD2	1.79	0.41
1:D:37:HIS:CD2	1:D:155:PRO:HA	2.55	0.41
1:A:59:TYR:O	1:A:63:ASN:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:ARG:HG2	1:C:88:ASN:O	2.20	0.41
1:D:163:ILE:O	1:D:166:TRP:HB2	2.21	0.41
1:C:12:ARG:HG3	1:C:83:GLU:HG2	2.02	0.41
1:A:38:THR:CG2	1:A:108:MET:HA	2.50	0.41
1:A:2:ASP:H	1:A:3:PRO:CD	2.34	0.41
1:B:78:ASP:O	1:B:119:ARG:NE	2.53	0.41
1:A:146:HIS:CD2	1:A:152:THR:HG21	2.55	0.41
1:B:10:VAL:O	1:B:83:GLU:HB2	2.20	0.41
1:B:98:TRP:O	1:B:99:ASN:C	2.60	0.40
1:A:126:ASN:ND2	2:B:201:STE:H101	2.36	0.40
1:A:124:ALA:O	1:A:127:LEU:HB3	2.22	0.40
1:A:37:HIS:HA	1:A:107:PHE:O	2.20	0.40
1:D:94:ALA:O	1:D:98:TRP:HB2	2.21	0.40
1:D:12:ARG:O	1:D:13:ARG:C	2.60	0.40
1:B:18:LEU:HG	1:B:57:GLN:HE22	1.86	0.40
1:A:131:GLY:HA2	1:A:136:ALA:HB3	2.01	0.40
2:B:201:STE:H172	2:B:201:STE:H142	1.22	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	169/171 (99%)	155 (92%)	12 (7%)	2 (1%)	16	47
1	B	169/171 (99%)	147 (87%)	20 (12%)	2 (1%)	16	47
1	C	169/171 (99%)	157 (93%)	9 (5%)	3 (2%)	11	34
1	D	169/171 (99%)	152 (90%)	14 (8%)	3 (2%)	11	34
All	All	676/684 (99%)	611 (90%)	55 (8%)	10 (2%)	13	40

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	C	3	PRO
1	D	2	ASP
1	D	4	PRO
1	D	7	GLY
1	A	2	ASP
1	B	2	ASP
1	C	4	PRO
1	B	3	PRO
1	C	5	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	139/139 (100%)	133 (96%)	6 (4%)	35	70
1	B	139/139 (100%)	125 (90%)	14 (10%)	9	27
1	C	139/139 (100%)	130 (94%)	9 (6%)	21	52
1	D	139/139 (100%)	132 (95%)	7 (5%)	30	64
All	All	556/556 (100%)	520 (94%)	36 (6%)	21	52

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	37	HIS
1	A	121	LEU
1	A	125	GLN
1	A	126	ASN
1	A	159	LEU
1	B	13	ARG
1	B	30	VAL
1	B	37	HIS
1	B	41	SER
1	B	51	GLN
1	B	54	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	80	LEU
1	B	114	ARG
1	B	126	ASN
1	B	128	LEU
1	B	130	CYS
1	B	150	GLN
1	B	158	ARG
1	B	170	ARG
1	C	1	GLU
1	C	24	GLU
1	C	37	HIS
1	C	44	ASP
1	C	54	GLN
1	C	62	ARG
1	C	63	ASN
1	C	119	ARG
1	C	162	ILE
1	D	4	PRO
1	D	6	CYS
1	D	13	ARG
1	D	23	ARG
1	D	37	HIS
1	D	114	ARG
1	D	150	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	164	GLN
1	B	54	GLN
1	B	57	GLN
1	B	113	ASN
1	B	126	ASN
1	B	150	GLN
1	C	37	HIS
1	C	57	GLN
1	C	113	ASN
1	C	150	GLN
1	D	54	GLN
1	D	63	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	STE	B	201	-	16,19,19	0.17	0	16,19,19	0.80	0
3	LP5	C	501	-	47,48,48	1.19	3 (6%)	54,60,60	2.22	13 (24%)
4	GOL	D	201	-	5,5,5	0.83	0	5,5,5	0.39	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	STE	B	201	-	-	0/15/17/17	0/0/0/0
3	LP5	C	501	-	-	1/44/65/65	0/1/1/1
4	GOL	D	201	-	-	0/4/4/4	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	LP5	C2-N2	2.42	1.49	1.45
3	C	501	LP5	C1-C2	3.36	1.59	1.53
3	C	501	LP5	O3-C28	5.00	1.49	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	LP5	O7-C7-C8	-3.72	115.88	121.30
3	C	501	LP5	O42-C28-C29	-2.54	118.85	124.69
3	C	501	LP5	C17-C16-C8	-2.30	104.39	112.10
3	C	501	LP5	O3-C3-C2	2.49	112.68	108.21
3	C	501	LP5	C8-C7-N2	2.66	119.62	116.33
3	C	501	LP5	C1-O5-C5	2.90	119.37	113.75
3	C	501	LP5	O4-C4-C3	3.21	117.47	109.87
3	C	501	LP5	C1-C2-N2	3.71	117.98	111.01
3	C	501	LP5	C3-O3-C28	4.36	125.48	117.75
3	C	501	LP5	O3-C28-C29	4.63	120.52	111.54
3	C	501	LP5	O3-C3-C4	5.88	120.82	107.76
3	C	501	LP5	C2-N2-C7	6.07	132.51	123.05
3	C	501	LP5	O1-C1-C2	7.48	122.19	108.42

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	501	LP5	C3-O3-C28-C29

There are no ring outliers.

2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	201	STE	11	0
3	C	501	LP5	12	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	171/171 (100%)	0.41	6 (3%)	48	35	25, 45, 75, 129	0
1	B	171/171 (100%)	0.11	6 (3%)	48	35	22, 47, 91, 162	0
1	C	171/171 (100%)	-0.10	2 (1%)	81	73	22, 40, 58, 92	0
1	D	171/171 (100%)	-0.05	3 (1%)	71	61	20, 40, 72, 106	0
All	All	684/684 (100%)	0.09	17 (2%)	61	48	20, 42, 78, 162	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	PRO	8.6
1	A	2	ASP	8.2
1	B	3	PRO	6.9
1	D	2	ASP	6.1
1	B	4	PRO	5.1
1	B	5	ALA	5.0
1	A	4	PRO	5.0
1	B	1	GLU	4.9
1	A	1	GLU	4.6
1	C	2	ASP	4.4
1	C	3	PRO	4.2
1	D	1	GLU	3.9
1	B	2	ASP	3.8
1	D	3	PRO	3.1
1	A	116	PRO	2.3
1	A	6	CYS	2.3
1	B	11	PRO	2.1

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 [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, 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(\AA^2)	Q<0.9
3	LP5	C	501	48/48	0.70	0.39	6.44	46,56,61,62	0
4	GOL	D	201	6/6	0.89	0.29	5.37	72,76,78,81	0
2	STE	B	201	20/20	0.69	0.34	0.41	39,41,44,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.