



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:39 PM GMT

PDB ID : 1BUI  
Title : Structure of the ternary microplasmin-staphylokinase-microplasmin complex:  
a proteinase-cofactor-substrate complex in action  
Authors : Parry, M.A.A.; Fernandez-Catalan, C.; Bergner, A.; Huber, R.; Hopfner, K.;  
Schlott, B.; Guehrs, K.; Bode, W.  
Deposited on : 1998-09-04  
Resolution : 2.65 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.

---

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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

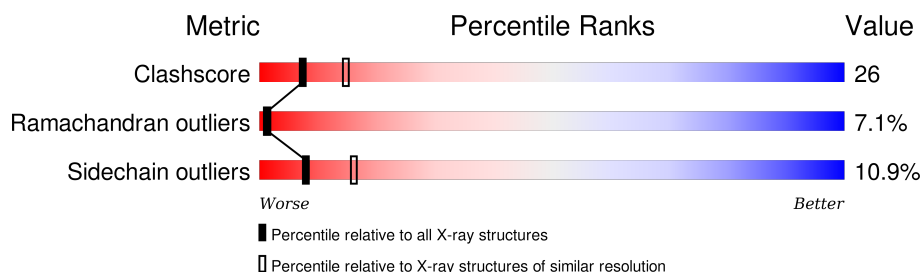
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 Å.


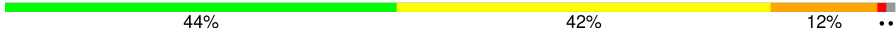

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	250	
1	B	250	
2	C	128	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5017 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 Plasmin light chain B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			1866	1181	326	345	14			
1	B	248	Total	C	N	O	S	0	0	0
			1856	1178	330	334	14			

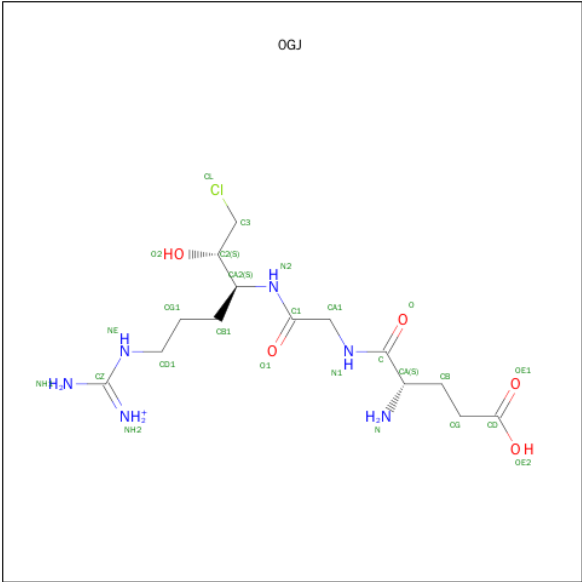
- Molecule 2 is a protein called Staphylokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	122	Total	C	N	O	S	0	0	0
			957	624	145	187	1			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	9	VAL	TYR	CONFLICT	UNP P15240
C	10	LEU	LYS	CONFLICT	UNP P15240
C	34	SER	GLY	CONFLICT	UNP P15240
C	36	GLY	ARG	CONFLICT	UNP P15240
C	43	HIS	ARG	CONFLICT	UNP P15240

- Molecule 3 is L-ALPHA-GLUTAMYL-N-{(1S)-4-{{[AMINO(IMINIO)METHYL]AMINO}-1-[(1S)-2-CHLORO-1-HYDROXYETHYL]BUTYL}GLYCINAMIDE (three-letter code: 0GJ) (formula: C<sub>14</sub>H<sub>28</sub>ClN<sub>6</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			25	14	6	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	146	Total	O	0	0
			146	146		
4	B	109	Total	O	0	0
			109	109		
4	C	58	Total	O	0	0
			58	58		



A85	K86	I87	E88	Y89	Y92	D93	K94	I95	K96	K97	K98	E99	E100	T101	K102	S103	F104	P105	I106	V113	I120	P123	G124	F125	N126	V131	V132	I133	E134	K135	K136
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.14Å 76.14Å 324.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.65	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.65)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.204 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5017	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0GJ

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	0.50	0/1914	0.79	1/2607 (0.0%)
1	B	0.46	0/1903	0.78	0/2587
2	C	0.53	0/982	0.82	1/1335 (0.1%)
All	All	0.49	0/4799	0.79	2/6529 (0.0%)

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	18	PHE	N-CA-C	6.49	128.51	111.00
1	A	1(D)	PRO	N-CA-CB	5.77	110.22	103.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	228	TYR	Sidechain
1	B	228	TYR	Sidechain



## 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	1866	0	1800	70	0
1	B	1856	0	1803	119	0
2	C	957	0	929	59	0
3	A	25	0	24	0	0
4	A	146	0	0	0	0
4	B	109	0	0	2	0
4	C	58	0	0	2	0
All	All	5017	0	4556	238	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 (238) 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)
2:C:76:PHE:HA	2:C:135:LYS:HA	1.26	1.16
1:B:81:GLN:HE22	1:B:113:VAL:H	0.99	0.94
1:A:35:THR:HG23	1:A:38:GLY:HA3	1.49	0.92
2:C:24:TYR:HE2	2:C:26:MET:HB2	1.35	0.91
1:A:81:GLN:HE22	1:A:113:VAL:H	1.20	0.90
1:B:74:VAL:HG23	1:B:75:ASN:H	1.40	0.85
2:C:24:TYR:CE2	2:C:26:MET:HB2	2.11	0.85
2:C:76:PHE:HA	2:C:135:LYS:CA	2.10	0.81
2:C:32:VAL:HG12	2:C:38:GLU:HA	1.63	0.80
1:A:91:GLU:HG2	1:A:101:LYS:HB2	1.64	0.79
1:B:189:ASP:HB3	1:B:221:ALA:HA	1.63	0.78
2:C:76:PHE:CA	2:C:135:LYS:HA	2.10	0.77
1:A:17:VAL:HG22	1:A:144:THR:HA	1.66	0.77
1:B:7:GLU:HG3	2:C:46:GLU:HG3	1.67	0.77
1:A:77:GLU:HG2	1:A:80:VAL:HG23	1.66	0.76
1:B:90:LEU:HD21	1:B:94:ARG:HD3	1.67	0.75
1:A:115:THR:OG1	1:A:117:LYS:HG3	1.87	0.73
1:B:71:HIS:HE1	4:B:348:HOH:O	1.73	0.72
1:A:131:ALA:HB3	1:A:134:THR:HG23	1.71	0.72
2:C:42:PRO:HA	2:C:71:THR:HG21	1.69	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:81:LEU:HA	2:C:131:VAL:HG23	1.70	0.72
1:A:34:ARG:HG2	1:A:40:HIS:HA	1.71	0.71
1:B:14:GLY:O	1:B:14:GLY:CA	2.39	0.71
1:B:169:ASN:HD21	1:B:176:VAL:H	1.39	0.70
1:B:138:ILE:HD13	1:B:199:LEU:HD23	1.75	0.69
1:B:81:GLN:NE2	1:B:113:VAL:H	1.83	0.69
1:B:189:ASP:HB3	1:B:221:ALA:CA	2.22	0.69
1:B:165:ASN:HD22	1:B:165:ASN:H	1.41	0.69
2:C:135:LYS:HE3	4:C:154:HOH:O	1.92	0.68
1:B:229:VAL:HG23	1:B:234:PHE:HE2	1.58	0.68
1:B:81:GLN:HE22	1:B:113:VAL:N	1.83	0.67
2:C:81:LEU:O	2:C:82:ASP:HB2	1.96	0.66
1:A:138:ILE:HD13	1:A:228:TYR:OH	1.96	0.66
1:B:90:LEU:HD12	1:B:104:ALA:HB2	1.79	0.65
1:B:229:VAL:HG23	1:B:234:PHE:CE2	2.31	0.64
1:A:5:GLN:HG2	1:A:116:ASP:HB2	1.79	0.64
1:B:165:ASN:N	1:B:165:ASN:HD22	1.97	0.63
1:B:171:PHE:HA	1:B:224:LYS:HZ1	1.63	0.63
1:A:21:VAL:HA	1:A:156:LYS:HA	1.83	0.61
1:A:77:GLU:H	1:A:77:GLU:CD	2.03	0.60
1:A:36:ARG:HD2	1:A:62:SER:O	2.01	0.60
2:C:88:GLU:HA	2:C:103:SER:HA	1.82	0.60
1:A:76:LEU:HD12	1:A:80:VAL:HG11	1.83	0.59
1:A:131:ALA:HB3	1:A:134:THR:CG2	2.32	0.59
1:A:126:PRO:HA	1:A:235:VAL:HG11	1.83	0.59
1:A:76:LEU:HB3	1:A:80:VAL:HG21	1.85	0.59
1:B:170(A):TYR:HA	1:B:173:ASN:OD1	2.03	0.58
1:B:24:PRO:O	2:C:66:TRP:CZ3	2.56	0.58
1:B:6:VAL:HG13	1:B:26:SER:HB3	1.84	0.58
1:A:83:ILE:HD11	1:A:112:ALA:HA	1.86	0.57
1:A:72:GLN:O	1:A:76:LEU:HD22	2.04	0.57
1:B:31:VAL:HG12	1:B:32:SER:N	2.20	0.57
1:A:76:LEU:CD1	1:A:80:VAL:HG11	2.34	0.57
1:B:91:GLU:HB3	1:B:103:ILE:O	2.05	0.57
2:C:96:LYS:HB3	2:C:98:LYS:HE3	1.86	0.56
1:B:138:ILE:CD1	1:B:199:LEU:HD23	2.34	0.56
1:A:14:GLY:HA2	1:A:184(A):HIS:CE1	2.41	0.56
2:C:33:ASP:OD2	2:C:37:ASN:HB2	2.05	0.56
1:B:144:THR:C	1:B:146:GLY:H	2.09	0.56
2:C:134:GLU:O	2:C:135:LYS:HB3	2.04	0.56
1:A:170(A):TYR:HE2	2:C:99:GLU:CD	2.09	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:PRO:HG3	1:B:71:HIS:CE1	2.41	0.55
1:B:50:GLU:HG2	1:B:111:PRO:HA	1.87	0.55
1:A:138:ILE:HD12	1:A:160:LEU:HD12	1.87	0.55
1:A:36:ARG:O	1:A:37:PHE:CD1	2.60	0.55
1:A:46:LEU:HD13	1:A:68:LEU:HD21	1.89	0.55
1:B:90:LEU:HG	1:B:91:GLU:N	2.22	0.55
2:C:49:ILE:HD11	2:C:125:PHE:CD1	2.42	0.55
1:B:27:TRP:CD1	1:B:139:THR:HG21	2.42	0.54
1:B:139:THR:HG22	1:B:157:GLU:HB3	1.88	0.54
1:A:35:THR:HG23	1:A:38:GLY:CA	2.29	0.54
1:B:151:GLY:C	1:B:153:GLY:H	2.11	0.54
1:B:188(A):THR:H	1:B:221:ALA:HB1	1.72	0.54
1:B:151:GLY:HA2	1:B:156:LYS:HZ3	1.73	0.54
2:C:76:PHE:CD1	2:C:133:ILE:HD12	2.43	0.54
1:B:179:THR:HA	1:B:233:ARG:HG3	1.88	0.54
1:B:24:PRO:O	2:C:66:TRP:HZ3	1.91	0.54
1:A:83:ILE:HG21	1:A:110:SER:O	2.09	0.53
1:A:60(D):ARG:NH2	1:B:145:GLN:HG2	2.23	0.53
1:B:163:ILE:O	1:B:164:GLU:HB2	2.07	0.53
1:A:79:HIS:O	1:A:117:LYS:HE2	2.09	0.53
2:C:64:VAL:HG21	2:C:81:LEU:HD21	1.91	0.53
1:B:55:ALA:O	1:B:58:CYS:HB2	2.09	0.52
2:C:55:LEU:HD23	2:C:60:ILE:HD11	1.92	0.52
1:B:219:GLY:O	1:B:220:CYS:HB2	2.10	0.52
1:A:223:ASN:O	1:A:224:LYS:HD3	2.10	0.52
1:B:215:TRP:CZ2	1:B:227:VAL:HB	2.45	0.51
1:A:180:GLU:HA	1:A:228:TYR:O	2.11	0.51
2:C:25:LEU:HD12	2:C:125:PHE:O	2.09	0.51
1:A:114:ILE:HD12	1:A:120:PRO:HD3	1.93	0.51
1:B:89:PHE:CE2	1:B:245:ASN:HB3	2.45	0.51
1:B:132:ASP:OD1	1:B:164:GLU:HB2	2.12	0.50
1:B:171:PHE:HA	1:B:224:LYS:NZ	2.25	0.50
1:A:126:PRO:HA	1:A:235:VAL:CG1	2.40	0.50
1:A:81:GLN:HE22	1:A:113:VAL:N	2.00	0.50
1:A:221(A):ARG:HD3	1:A:222:PRO:HD2	1.92	0.50
2:C:87:ILE:HA	2:C:126:ASN:O	2.11	0.50
1:B:171:PHE:CD2	1:B:223:ASN:HB3	2.46	0.49
1:B:145:GLN:H	1:B:150:PHE:HB2	1.76	0.49
1:A:31:VAL:HG22	1:A:68:LEU:HD23	1.93	0.49
2:C:104:PHE:CD1	2:C:104:PHE:N	2.80	0.49
1:A:167:VAL:O	1:A:170:ARG:HB2	2.11	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:THR:HG22	1:B:157:GLU:CB	2.43	0.49
2:C:60:ILE:HG13	2:C:106:ILE:HD12	1.94	0.49
1:B:169:ASN:ND2	1:B:176:VAL:HB	2.28	0.49
1:A:199:LEU:HD23	1:A:199:LEU:O	2.12	0.49
1:B:187:GLY:HA3	1:B:221(A):ARG:O	2.13	0.49
1:A:171:PHE:HA	1:A:223:ASN:O	2.12	0.48
1:B:77:GLU:HB2	1:B:78:PRO:HD2	1.93	0.48
1:B:136:CYS:SG	1:B:162:VAL:HG23	2.53	0.48
1:B:30:GLN:HE22	1:B:198:PRO:HD2	1.78	0.48
1:B:208:ILE:N	1:B:208:ILE:HD12	2.27	0.48
1:B:74:VAL:HG23	1:B:75:ASN:N	2.20	0.48
1:A:31:VAL:HG12	1:A:32:SER:N	2.29	0.48
1:A:83:ILE:HG22	1:A:84:GLU:N	2.28	0.48
1:B:60(A):LYS:O	1:B:60(B):SER:HB3	2.13	0.48
1:B:200:VAL:O	1:B:200:VAL:HG23	2.14	0.48
2:C:87:ILE:O	2:C:87:ILE:HG23	2.14	0.48
1:B:7:GLU:HG2	2:C:46:GLU:O	2.14	0.47
1:B:56:ALA:CB	1:B:90:LEU:HD11	2.44	0.47
2:C:94:LYS:HG3	2:C:95:ASN:OD1	2.14	0.47
2:C:120:ILE:CG2	2:C:123:PRO:HB3	2.43	0.47
1:B:215:TRP:CE2	1:B:227:VAL:HB	2.49	0.47
1:A:29:TRP:O	1:A:45:THR:HA	2.14	0.47
1:A:33:LEU:HD21	1:A:106:LEU:HD11	1.97	0.47
1:A:31:VAL:CG1	1:A:32:SER:N	2.78	0.47
1:A:200:VAL:HG13	1:A:207:TYR:CD1	2.50	0.47
1:A:200:VAL:HG13	1:A:207:TYR:HD1	1.79	0.47
2:C:62:TYR:O	2:C:66:TRP:HB2	2.15	0.47
1:B:130:VAL:HG21	1:B:210:GLN:HB3	1.97	0.47
1:B:152:ALA:C	1:B:154:LEU:H	2.19	0.46
1:A:160:LEU:HD23	1:A:184(A):HIS:CE1	2.49	0.46
2:C:96:LYS:NZ	2:C:98:LYS:NZ	2.63	0.46
2:C:134:GLU:O	2:C:135:LYS:CB	2.63	0.46
2:C:101:THR:HG22	2:C:101:THR:O	2.15	0.46
1:B:25:HIS:HB2	2:C:66:TRP:HH2	1.80	0.46
1:B:185:LEU:CD2	1:B:223:ASN:HA	2.46	0.46
1:B:1(C):SER:O	1:B:1(B):PHE:CD1	2.67	0.46
1:A:138:ILE:HG21	1:A:190:SER:HB3	1.97	0.46
1:B:192:GLN:C	1:B:194:ASP:H	2.19	0.46
2:C:32:VAL:HG12	2:C:38:GLU:CA	2.42	0.45
1:A:34:ARG:HG2	1:A:40:HIS:CA	2.43	0.45
1:B:87:ARG:HB3	1:B:89:PHE:CE1	2.50	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:PHE:N	1:B:89:PHE:CD1	2.84	0.45
1:B:25:HIS:HB2	2:C:66:TRP:CH2	2.51	0.45
1:B:145:GLN:HB2	1:B:150:PHE:CG	2.51	0.45
2:C:84:SER:HB3	2:C:86:LYS:HE2	1.98	0.45
2:C:81:LEU:O	2:C:82:ASP:CB	2.63	0.45
1:B:220:CYS:O	1:B:221:ALA:HB3	2.15	0.45
1:B:228:TYR:CD1	1:B:228:TYR:N	2.84	0.45
1:B:9:LYS:HB2	1:B:23:HIS:CE1	2.52	0.45
1:A:86:SER:HB2	1:A:109:SER:HA	1.99	0.45
2:C:75:GLU:HG3	2:C:135:LYS:NZ	2.32	0.45
1:B:213:THR:HA	1:B:228:TYR:CD2	2.52	0.45
1:A:1:CYS:O	1:A:122:CYS:SG	2.74	0.45
1:B:185:LEU:HD23	1:B:223:ASN:HA	1.97	0.45
1:B:6:VAL:O	1:B:8:PRO:HD3	2.17	0.45
1:B:19:GLY:HA3	1:B:157:GLU:O	2.17	0.45
1:A:215:TRP:CZ2	1:A:227:VAL:HG21	2.52	0.45
1:B:187:GLY:HA3	1:B:221(A):ARG:CA	2.47	0.44
1:A:144:THR:OG1	1:A:145:GLN:N	2.49	0.44
2:C:120:ILE:HG21	2:C:123:PRO:HB3	1.98	0.44
1:B:76:LEU:HG	1:B:80:VAL:HG11	1.99	0.44
1:B:10:LYS:HE3	2:C:18:PHE:HB2	1.99	0.44
1:B:77:GLU:HG2	1:B:80:VAL:HG23	2.00	0.44
1:A:60(B):SER:HA	1:A:60(C):PRO:HD3	1.72	0.44
2:C:89:VAL:HG13	2:C:102:LYS:HB2	2.00	0.44
1:B:170:ARG:O	1:B:170(B):GLU:N	2.51	0.44
1:A:126:PRO:CA	1:A:235:VAL:HG11	2.48	0.44
1:A:27:TRP:CZ3	1:A:200:VAL:HG11	2.54	0.43
2:C:30:THR:HG22	2:C:32:VAL:HG13	2.00	0.43
1:B:1:CYS:O	1:B:122:CYS:SG	2.76	0.43
1:B:212:VAL:HG23	1:B:231:VAL:CG2	2.48	0.43
2:C:75:GLU:HG2	2:C:76:PHE:CD2	2.53	0.43
1:B:91:GLU:O	1:B:94:ARG:HB2	2.18	0.43
1:B:184(A):HIS:ND1	1:B:185:LEU:N	2.60	0.43
1:B:50:GLU:HG2	1:B:111:PRO:CA	2.47	0.43
1:B:101:LYS:O	1:B:102:ASP:HB2	2.18	0.43
2:C:76:PHE:H	2:C:136:LYS:H	1.64	0.43
1:B:11:CYS:HA	1:B:13:PRO:HD3	1.79	0.43
1:B:173:ASN:O	1:B:175:ARG:N	2.52	0.43
2:C:92:TYR:HA	2:C:99:GLU:HG3	2.00	0.43
1:B:134:THR:O	1:B:161:PRO:HA	2.19	0.43
1:A:76:LEU:HD23	1:A:76:LEU:N	2.34	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:HIS:O	1:B:154:LEU:HA	2.18	0.43
1:A:8:PRO:HA	1:A:26:SER:HB2	2.01	0.43
1:B:46:LEU:O	1:B:120:PRO:HA	2.19	0.43
1:B:144:THR:C	1:B:146:GLY:N	2.72	0.43
1:A:33:LEU:HD21	1:A:106:LEU:CD1	2.48	0.43
1:B:169:ASN:HD21	1:B:176:VAL:N	2.12	0.42
1:B:171:PHE:HD2	1:B:223:ASN:HB3	1.84	0.42
1:B:165:ASN:N	1:B:165:ASN:ND2	2.66	0.42
1:A:206:LYS:HE2	1:A:208:ILE:HD11	2.01	0.42
1:A:31:VAL:HG13	1:A:66:VAL:HG13	2.01	0.42
1:B:188(A):THR:N	1:B:221:ALA:HB1	2.34	0.42
1:B:56:ALA:HB1	1:B:90:LEU:HD11	2.01	0.42
1:A:66:VAL:C	1:A:67:ILE:HD12	2.40	0.42
1:A:241:VAL:O	1:A:245:ASN:HB2	2.19	0.42
1:B:171:PHE:O	1:B:172:LEU:HB2	2.19	0.42
1:B:173:ASN:C	1:B:175:ARG:N	2.72	0.42
2:C:16:SER:HB3	2:C:18:PHE:CZ	2.54	0.42
1:B:124:PRO:O	1:B:235:VAL:HG21	2.20	0.42
1:B:222:PRO:HB2	1:B:223:ASN:H	1.67	0.42
1:B:51:TRP:CZ2	1:B:107:LYS:HG3	2.54	0.42
1:A:219:GLY:HA3	2:C:17:TYR:CB	2.49	0.42
1:B:180:GLU:O	1:B:230:ARG:NH1	2.53	0.42
2:C:23:PRO:HG2	2:C:51:PRO:HG3	2.01	0.42
2:C:88:GLU:HG2	2:C:103:SER:HB2	2.00	0.42
1:A:36:ARG:NH1	1:A:37:PHE:CZ	2.87	0.42
1:A:28:PRO:HB2	1:A:119:ILE:H	1.85	0.42
1:A:145:GLN:O	1:A:149:THR:HG23	2.20	0.42
1:A:1(A):ASP:HB3	1:A:1:CYS:H	1.71	0.42
1:B:77:GLU:HB2	1:B:78:PRO:CD	2.49	0.41
2:C:59:LYS:HG3	4:C:179:HOH:O	2.20	0.41
2:C:85:ALA:HB1	2:C:105:PRO:HA	2.01	0.41
2:C:47:PHE:HA	2:C:48:PRO:HD3	1.93	0.41
1:B:169:ASN:HD21	1:B:176:VAL:HB	1.85	0.41
2:C:79:VAL:HB	2:C:132:VAL:O	2.19	0.41
1:B:151:GLY:C	1:B:153:GLY:N	2.74	0.41
1:B:1(B):PHE:HB3	1:B:119:ILE:HG12	2.03	0.41
1:B:191:CYS:O	1:B:192:GLN:O	2.38	0.41
1:B:90:LEU:HG	1:B:91:GLU:H	1.83	0.41
1:B:106:LEU:N	1:B:106:LEU:HD12	2.36	0.41
1:B:128:TYR:HE1	4:B:274:HOH:O	2.03	0.41
1:B:139:THR:HA	1:B:157:GLU:HA	2.03	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60(B):SER:HG	1:A:60(D):ARG:HB2	1.86	0.41
1:B:167:VAL:O	1:B:170:ARG:HB3	2.21	0.41
2:C:29:VAL:HG21	2:C:64:VAL:HG13	2.02	0.41
1:B:170(A):TYR:C	1:B:171:PHE:H	2.24	0.41
2:C:51:PRO:HA	2:C:113:VAL:HG12	2.03	0.41
1:B:216:GLY:O	1:B:217:LEU:CB	2.69	0.41
2:C:135:LYS:HE2	2:C:135:LYS:HB2	1.96	0.41
1:A:73:GLU:HB2	1:A:141:TRP:CD1	2.56	0.41
1:B:150:PHE:HD1	1:B:150:PHE:H	1.69	0.40
1:B:200:VAL:HA	1:B:208:ILE:O	2.22	0.40
2:C:34:SER:C	2:C:36:GLY:H	2.24	0.40
1:B:47:ILE:HD12	1:B:123:LEU:HD21	2.03	0.40
1:B:215:TRP:CZ2	1:B:227:VAL:HG11	2.56	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	243/250 (97%)	203 (84%)	32 (13%)	8 (3%)	5	9
1	B	244/250 (98%)	178 (73%)	35 (14%)	31 (13%)	0	0
2	C	120/128 (94%)	99 (82%)	17 (14%)	4 (3%)	5	9
All	All	607/628 (97%)	480 (79%)	84 (14%)	43 (7%)	1	1

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	ALA
1	A	150	PHE
1	B	1(A)	ASP
1	B	78	PRO

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	102	ASP
1	B	143	GLU
1	B	144	THR
1	B	163	ILE
1	B	164	GLU
1	B	170(A)	TYR
1	B	170(B)	GLU
1	B	192	GLN
1	B	217	LEU
1	B	220	CYS
1	B	221(A)	ARG
1	B	222	PRO
2	C	82	ASP
1	A	9	LYS
1	A	143	GLU
1	A	152	ALA
1	B	40	HIS
1	B	41	PHE
1	B	142	GLY
1	B	170	ARG
1	B	188(A)	THR
1	B	216	GLY
2	C	18	PHE
1	B	74	VAL
1	B	171	PHE
1	A	1	CYS
1	A	25	HIS
1	A	60(A)	LYS
1	B	13	PRO
1	B	60(B)	SER
1	B	76	LEU
1	B	79	HIS
1	B	186	ALA
2	C	76	PHE
2	C	135	LYS
1	B	151	GLY
1	B	165	ASN
1	B	223	ASN
1	B	80	VAL



### 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	202/210 (96%)	174 (86%)	28 (14%)	4	9
1	B	198/210 (94%)	181 (91%)	17 (9%)	13	26
2	C	105/116 (90%)	95 (90%)	10 (10%)	11	22
All	All	505/536 (94%)	450 (89%)	55 (11%)	8	16

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	7	GLU
1	A	23	HIS
1	A	25	HIS
1	A	35	THR
1	A	37	PHE
1	A	40	HIS
1	A	45	THR
1	A	59	LEU
1	A	60	GLU
1	A	60(D)	ARG
1	A	72	GLN
1	A	74	VAL
1	A	76	LEU
1	A	84	GLU
1	A	90	LEU
1	A	94	ARG
1	A	116	ASP
1	A	133	ARG
1	A	143	GLU
1	A	144	THR
1	A	170(A)	TYR
1	A	179	THR
1	A	192	GLN
1	A	199	LEU
1	A	200	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	217	LEU
1	A	221(A)	ARG
1	B	8	PRO
1	B	36	ARG
1	B	78	PRO
1	B	82	GLU
1	B	91	GLU
1	B	101	LYS
1	B	133	ARG
1	B	155	LEU
1	B	165	ASN
1	B	168	CYS
1	B	182	CYS
1	B	189	ASP
1	B	191	CYS
1	B	204	LYS
1	B	229	VAL
1	B	230	ARG
1	B	235	VAL
2	C	39	LEU
2	C	45	VAL
2	C	46	GLU
2	C	55	LEU
2	C	66	TRP
2	C	81	LEU
2	C	96	LYS
2	C	99	GLU
2	C	103	SER
2	C	135	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	81	GLN
1	A	184(A)	HIS
1	A	192	GLN
1	B	30	GLN
1	B	40	HIS
1	B	71	HIS
1	B	81	GLN
1	B	165	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	169	ASN
1	B	192	GLN
2	C	126	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](#)

1 ligand is 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	0GJ	A	246	1	17,24,25	0.52	0	20,30,31	1.21	1 (5%)

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	0GJ	A	246	1	-	0/25/29/31	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	A	246	0GJ	C2-CA2-N2	-4.83	101.06	110.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.