



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:43 PM GMT

PDB ID : 1YED
Title : STRUCTURE OF A CATALYTIC ANTIBODY IGG2A FAB FRAGMENT (D2.4)
Authors : Golinelli-Pimpaneau, B.; Knossow, M.
Deposited on : 1997-04-15
Resolution : 3.10 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) : **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

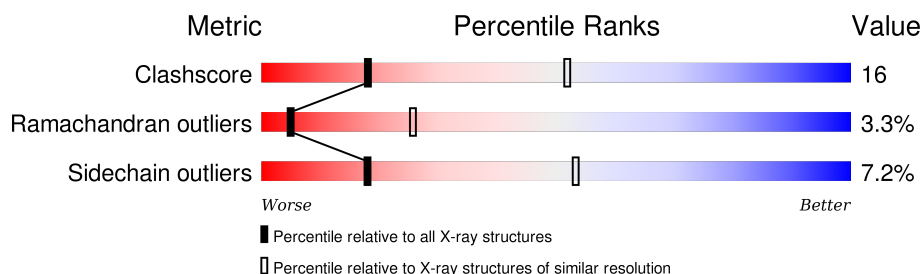
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	219	 63% 34% ..
1	L	219	 61% 36% ..
2	B	226	 68% 27% 5%
2	H	226	 68% 27% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6886 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 IGG1 FAB FRAGMENT (D.2.4).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	219	Total	C	N	O	S	0	0	0
			1693	1062	284	340	7			
1	A	219	Total	C	N	O	S	0	0	0
			1693	1062	284	340	7			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	2	ILE	VAL	CONFLICT	PIR S16112
L	7	SER	THR	CONFLICT	PIR S16112
L	10	THR	SER	CONFLICT	PIR S16112
L	12	SER	PRO	CONFLICT	PIR S16112
L	14	THR	SER	CONFLICT	PIR S16112
L	15	ILE	LEU	CONFLICT	PIR S16112
L	17	GLN	ASP	CONFLICT	PIR S16112
L	18	PRO	GLN	CONFLICT	PIR S16112
L	24	LYS	ARG	CONFLICT	PIR S16112
L	27B	LEU	VAL	CONFLICT	PIR S16112
L	27D	TYR	HIS	CONFLICT	PIR S16112
L	30	LYS	ASN	CONFLICT	PIR S16112
L	34	ASN	TYR	CONFLICT	PIR S16112
L	36	LEU	TYR	CONFLICT	PIR S16112
L	39	ARG	LYS	CONFLICT	PIR S16112
L	46	ARG	PRO	CONFLICT	PIR S16112
L	50	LEU	ARG	CONFLICT	PIR S16112
L	53	LYS	ASN	CONFLICT	PIR S16112
L	54	LEU	ARG	CONFLICT	PIR S16112
L	55	GLU	PHE	CONFLICT	PIR S16112
L	63	THR	SER	CONFLICT	PIR S16112
L	81	ALA	GLU	CONFLICT	PIR S16112
L	87	TYR	PHE	CONFLICT	PIR S16112
L	89	VAL	PHE	CONFLICT	PIR S16112
L	94	PHE	VAL	CONFLICT	PIR S16112

Continued on next page...

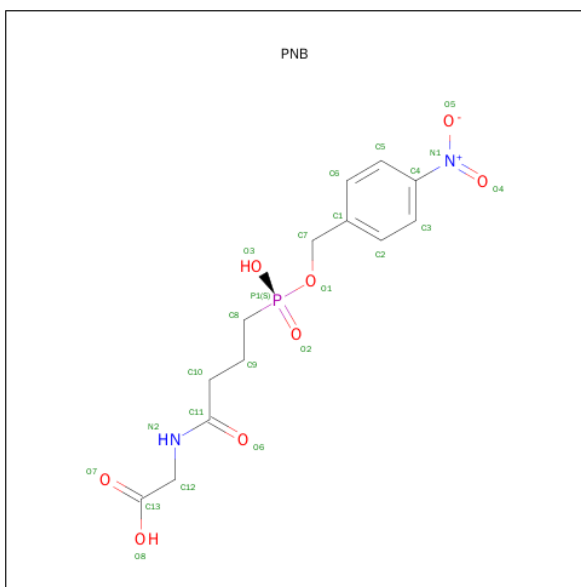
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	103	LYS	ARG	CONFLICT	PIR S16112
L	107	LEU	LYS	CONFLICT	PIR S16112
A	2	ILE	VAL	CONFLICT	PIR S16112
A	7	SER	THR	CONFLICT	PIR S16112
A	10	THR	SER	CONFLICT	PIR S16112
A	12	SER	PRO	CONFLICT	PIR S16112
A	14	THR	SER	CONFLICT	PIR S16112
A	15	ILE	LEU	CONFLICT	PIR S16112
A	17	GLN	ASP	CONFLICT	PIR S16112
A	18	PRO	GLN	CONFLICT	PIR S16112
A	24	LYS	ARG	CONFLICT	PIR S16112
A	27B	LEU	VAL	CONFLICT	PIR S16112
A	27D	TYR	HIS	CONFLICT	PIR S16112
A	30	LYS	ASN	CONFLICT	PIR S16112
A	34	ASN	TYR	CONFLICT	PIR S16112
A	36	LEU	TYR	CONFLICT	PIR S16112
A	39	ARG	LYS	CONFLICT	PIR S16112
A	46	ARG	PRO	CONFLICT	PIR S16112
A	50	LEU	ARG	CONFLICT	PIR S16112
A	53	LYS	ASN	CONFLICT	PIR S16112
A	54	LEU	ARG	CONFLICT	PIR S16112
A	55	GLU	PHE	CONFLICT	PIR S16112
A	63	THR	SER	CONFLICT	PIR S16112
A	81	ALA	GLU	CONFLICT	PIR S16112
A	87	TYR	PHE	CONFLICT	PIR S16112
A	89	VAL	PHE	CONFLICT	PIR S16112
A	94	PHE	VAL	CONFLICT	PIR S16112
A	103	LYS	ARG	CONFLICT	PIR S16112
A	107	LEU	LYS	CONFLICT	PIR S16112

- Molecule 2 is a protein called IGG1 FAB FRAGMENT (D.2.4).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	226	Total	C	N	O	S	0	0	0
			1724	1097	283	336	8			
2	B	226	Total	C	N	O	S	0	0	0
			1724	1097	283	336	8			

- Molecule 3 is 4-NITRO-BENZYLPHOSPHONOBUTANOYL-GLYCINE (three-letter code: PNB) (formula: C₁₃H₁₇N₂O₈P).




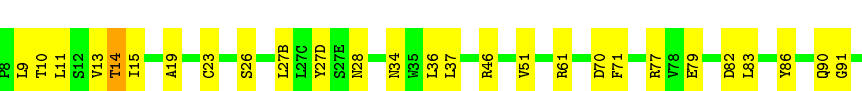
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	L	1	Total	C	N	O	P	0	0
			24	13	2	8	1		
3	A	1	Total	C	N	O	P	0	0
			24	13	2	8	1		


- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	1	Total	O	0	0
			1	1		
4	H	1	Total	O	0	0
			1	1		
4	L	1	Total	O	0	0
			1	1		

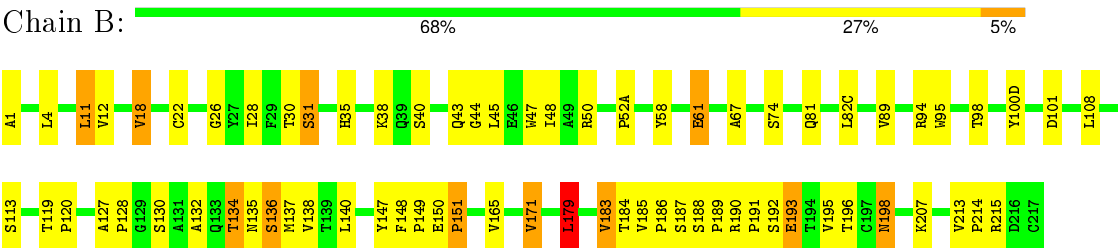
Note EDS was not executed.

- Chain L:
-
- 61% 36%
- ..

- Chain A: 
- 
- | Residue | Category |
|---------|----------|
| D1 | Green |
| E104 | Green |
| E105 | Green |
| V3 | Green |
| I106 | Green |
| L107 | Green |
| R111 | Green |
| A112 | Green |
| S7 | Green |
| P8 | Green |
| L9 | Green |
| T10 | Green |
| L11 | Green |
| S12 | Green |
| V13 | Green |
| T14 | Green |
| I15 | Green |
| A19 | Green |
| C23 | Green |
| S26 | Green |
| L27B | Green |
| Y27C | Green |
| Y27D | Green |
| S27E | Green |
| I28 | Green |
| N34 | Green |
| G35 | Green |
| L36 | Green |
| L37 | Green |
| R46 | Green |
| V51 | Green |
| R61 | Green |
| D70 | Green |
| F71 | Green |
| R77 | Green |
| Y78 | Green |
| E79 | Green |
| D82 | Green |
| L83 | Green |
| Y86 | Green |
| Q90 | Green |
| G91 | Green |
| F94 | Orange |
| P95 | Orange |
| Y96 | Green |
| G101 | Green |
| T102 | Green |
| E103 | Green |
| L104 | Green |
| E105 | Green |
| V118 | Green |
| S119 | Green |
| G137 | Green |
| F138 | Green |
| L139 | Green |
| M140 | Green |
| N141 | Green |
| K145 | Green |
| W151 | Green |
| K152 | Green |
| I153 | Green |
| D154 | Green |
| E157 | Green |
| R158 | Green |
| Q159 | Green |
| M160 | Green |
| G161 | Green |
| V162 | Green |
| L163 | Green |
| M164 | Green |
| S165 | Green |
| Q169 | Green |
| K172 | Red |
| D173 | Red |
| S174 | Orange |
| S177 | Green |
| M178 | Green |
| L182 | Green |
| T183 | Green |
| L184 | Red |
| D187 | Green |
| R191 | Green |
| T196 | Green |
| G197 | Green |
| E198 | Green |
| A199 | Green |
| T200 | Green |
| S204 | Green |
| T205 | Green |
| S206 | Green |
| P207 | Green |

- Chain H: 

- 
- WORLD WIDE
PDB
PROTEIN DATA BANK



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	99.25Å 104.79Å 223.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-3.10)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.84	Depositor
R, R_{free}	0.215 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6886	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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: PNB

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	0.39	0/1730	0.76	3/2348 (0.1%)
1	L	0.40	0/1730	0.76	3/2348 (0.1%)
2	B	0.40	0/1772	0.73	1/2419 (0.0%)
2	H	0.41	0/1772	0.73	1/2419 (0.0%)
All	All	0.40	0/7004	0.74	8/9534 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	LYS	N-CA-C	-7.75	90.07	111.00
1	L	172	LYS	N-CA-C	-7.73	90.14	111.00
1	A	161	GLY	N-CA-C	5.69	127.33	113.10
1	L	161	GLY	N-CA-C	5.50	126.85	113.10
1	A	184	LEU	CA-CB-CG	5.33	127.55	115.30
1	L	184	LEU	CA-CB-CG	5.32	127.54	115.30
2	H	179	LEU	CA-CB-CG	5.24	127.36	115.30
2	B	179	LEU	CA-CB-CG	5.07	126.96	115.30

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	1693	0	1655	54	0
1	L	1693	0	1655	57	0
2	B	1724	0	1694	52	0
2	H	1724	0	1694	55	0
3	A	24	0	15	3	0
3	L	24	0	15	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	H	1	0	0	2	0
4	L	1	0	0	0	0
All	All	6886	0	6728	213	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 16.

All (213) 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:163:LEU:HD21	2:B:171:VAL:HG11	1.25	1.15
2:B:134:THR:HB	2:B:138:VAL:HA	1.25	1.15
2:H:134:THR:HB	2:H:138:VAL:HA	1.25	1.11
1:L:160:ASN:HB2	1:L:184:LEU:HD12	1.34	1.08
1:L:163:LEU:HD21	2:H:171:VAL:HG11	1.29	1.06
1:A:160:ASN:HB2	1:A:184:LEU:HD12	1.35	1.06
2:B:12:VAL:HG21	2:B:82(C):LEU:HD13	1.59	0.84
2:H:12:VAL:HG21	2:H:82(C):LEU:HD13	1.59	0.81
1:L:153:ILE:HD11	1:L:182:LEU:HD21	1.65	0.76
1:A:153:ILE:HD11	1:A:182:LEU:HD21	1.70	0.73
1:A:153:ILE:HD12	1:A:159:GLN:HB3	1.69	0.73
1:L:159:GLN:O	1:L:182:LEU:HD11	1.90	0.72
1:A:159:GLN:O	1:A:182:LEU:HD11	1.90	0.71
1:L:198:GLU:HG2	1:L:209:VAL:HG22	1.72	0.71
1:L:91:GLY:O	3:L:551:PNB:H101	1.89	0.71
1:A:198:GLU:HG2	1:A:209:VAL:HG22	1.74	0.70
1:L:153:ILE:HD12	1:L:159:GLN:HB3	1.73	0.70
2:H:134:THR:CB	2:H:138:VAL:HA	2.15	0.69
2:H:18:VAL:HG22	2:H:82(C):LEU:HD11	1.76	0.68
2:B:18:VAL:HG22	2:B:82(C):LEU:HD11	1.77	0.67
2:B:40:SER:HB3	2:B:43:GLN:HB2	1.77	0.67
2:H:40:SER:HB3	2:H:43:GLN:HB2	1.77	0.67
2:H:165:VAL:HG22	2:H:183:VAL:CG2	2.24	0.66
2:B:134:THR:CB	2:B:138:VAL:HA	2.15	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLY:O	3:A:552:PNB:H101	1.95	0.65
2:B:165:VAL:HG22	2:B:183:VAL:HG23	1.78	0.65
1:L:196:THR:HG22	1:L:211:SER:HB3	1.79	0.65
1:A:196:THR:HG22	1:A:211:SER:HB3	1.79	0.64
2:H:165:VAL:HG22	2:H:183:VAL:HG23	1.78	0.64
2:B:28:ILE:HG23	2:B:31:SER:HB2	1.79	0.64
2:B:165:VAL:HG22	2:B:183:VAL:CG2	2.28	0.64
1:L:159:GLN:OE1	1:L:159:GLN:HA	1.98	0.63
1:A:159:GLN:OE1	1:A:159:GLN:HA	1.96	0.63
2:H:28:ILE:HG23	2:H:31:SER:HB2	1.81	0.63
2:H:137:MET:HE1	2:H:186:PRO:HB3	1.81	0.63
2:H:35:HIS:HD2	2:H:47:TRP:HE1	1.46	0.62
2:B:188:SER:HB2	2:B:189:PRO:HD3	1.82	0.61
2:B:35:HIS:HD2	2:B:47:TRP:HE1	1.49	0.61
1:L:36:LEU:HD23	1:L:46:ARG:HA	1.83	0.60
1:L:94:PHE:HB3	1:L:95:PRO:HD3	1.82	0.60
2:B:213:VAL:HG13	2:B:214:PRO:HD2	1.82	0.59
2:B:192:SER:O	2:B:193:GLU:HB2	2.01	0.59
1:A:172:LYS:O	1:A:173:ASP:HB3	2.02	0.59
1:L:163:LEU:HD21	2:H:171:VAL:CG1	2.20	0.59
2:H:192:SER:O	2:H:193:GLU:HB2	2.01	0.58
1:L:172:LYS:O	1:L:173:ASP:HB3	2.03	0.58
2:B:134:THR:O	2:B:138:VAL:HG12	2.02	0.58
2:H:213:VAL:HG13	2:H:214:PRO:HD2	1.85	0.58
2:B:140:LEU:HD13	2:B:195:VAL:HG11	1.86	0.57
2:B:137:MET:HB3	2:B:184:THR:CG2	2.35	0.57
1:A:86:TYR:O	1:A:101:GLY:HA2	2.04	0.57
1:A:83:LEU:HG	1:A:106:ILE:HG12	1.86	0.57
2:H:188:SER:HB2	2:H:189:PRO:HD3	1.86	0.57
2:B:190:ARG:HB3	2:B:191:PRO:HD3	1.86	0.57
2:B:137:MET:HE1	2:B:186:PRO:HB3	1.87	0.56
2:B:67:ALA:HA	2:B:81:GLN:O	2.05	0.56
1:A:10:THR:HG22	1:A:103:LYS:HB3	1.86	0.56
1:L:86:TYR:O	1:L:101:GLY:HA2	2.05	0.56
1:A:36:LEU:HD23	1:A:46:ARG:HA	1.86	0.56
1:L:83:LEU:HG	1:L:106:ILE:HG12	1.88	0.56
2:H:134:THR:O	2:H:138:VAL:HG12	2.06	0.56
2:H:137:MET:HB3	2:H:184:THR:CG2	2.36	0.56
1:L:4:MET:HE3	1:L:23:CYS:SG	2.46	0.56
1:L:160:ASN:CB	1:L:184:LEU:HD12	2.23	0.55
2:H:190:ARG:HB3	2:H:191:PRO:HD3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:THR:HG22	1:A:211:SER:CB	2.36	0.55
1:A:2:ILE:HG21	1:A:90:GLN:HG2	1.88	0.55
1:A:94:PHE:HB3	1:A:95:PRO:HD3	1.89	0.55
2:B:186:PRO:O	2:B:189:PRO:HD2	2.06	0.55
1:A:214:ARG:O	1:A:220:ASN:HB3	2.06	0.54
2:B:38:LYS:HE2	2:B:40:SER:HB2	1.89	0.54
1:L:196:THR:HG22	1:L:211:SER:CB	2.37	0.54
1:A:119:SER:O	1:A:137:CYS:HA	2.06	0.54
2:H:67:ALA:HA	2:H:81:GLN:O	2.07	0.54
1:L:119:SER:O	1:L:137:CYS:HA	2.07	0.54
2:H:186:PRO:O	2:H:189:PRO:HD2	2.07	0.53
2:H:140:LEU:HD13	2:H:195:VAL:HG11	1.89	0.53
1:L:214:ARG:O	1:L:220:ASN:HB3	2.08	0.53
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.90	0.53
1:A:160:ASN:CB	1:A:184:LEU:HD12	2.24	0.53
2:H:38:LYS:HE2	2:H:40:SER:HB2	1.91	0.53
1:A:83:LEU:HD21	1:A:169:GLN:OE1	2.09	0.53
1:L:10:THR:HG22	1:L:103:LYS:HB3	1.91	0.53
1:L:83:LEU:HD21	1:L:169:GLN:OE1	2.10	0.52
1:A:4:MET:HE3	1:A:23:CYS:SG	2.49	0.52
1:A:152:LYS:HB2	1:A:196:THR:OG1	2.10	0.52
2:B:4:LEU:HD23	2:B:22:CYS:SG	2.50	0.52
1:L:111:ARG:HG2	1:L:112:ALA:N	2.25	0.52
1:L:118:VAL:HG13	1:L:137:CYS:SG	2.50	0.51
1:A:140:ASN:HB2	1:A:177:SER:OG	2.11	0.51
1:L:198:GLU:HG2	1:L:209:VAL:CG2	2.40	0.51
2:B:38:LYS:HB2	2:B:48:ILE:HD11	1.93	0.51
2:H:35:HIS:HE1	4:H:218:HOH:O	1.94	0.51
2:H:11:LEU:HG	2:H:149:PRO:HG3	1.92	0.51
2:H:30:THR:HA	2:H:52(A):PRO:HB2	1.93	0.51
1:L:152:LYS:HB2	1:L:196:THR:OG1	2.11	0.50
2:B:11:LEU:HG	2:B:149:PRO:HG3	1.93	0.50
2:H:12:VAL:CG2	2:H:82(C):LEU:HD13	2.37	0.50
2:H:35:HIS:CE1	4:H:218:HOH:O	2.63	0.50
1:L:96:TYR:CG	3:L:551:PNB:H71	2.45	0.50
1:A:118:VAL:HG13	1:A:137:CYS:SG	2.52	0.50
1:L:13:VAL:HG21	1:L:19:ALA:HB2	1.92	0.50
2:B:196:THR:HG22	2:B:198:ASN:ND2	2.26	0.50
1:L:2:ILE:HG21	1:L:90:GLN:HG2	1.93	0.49
2:B:127:ALA:O	2:B:215:ARG:NH1	2.46	0.49
2:H:4:LEU:HD23	2:H:22:CYS:SG	2.52	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:VAL:HG21	1:A:19:ALA:HB2	1.95	0.49
1:A:173:ASP:CG	1:A:174:SER:H	2.16	0.49
2:H:147:TYR:OH	2:H:179:LEU:HD23	2.12	0.49
1:A:96:TYR:CG	3:A:552:PNB:H71	2.48	0.49
1:A:196:THR:HA	1:A:211:SER:HB3	1.95	0.48
1:L:173:ASP:CG	1:L:174:SER:H	2.17	0.48
1:L:27(D):TYR:HB3	1:L:28:ASN:OD1	2.13	0.48
1:A:94:PHE:O	1:A:96:TYR:N	2.46	0.48
1:A:160:ASN:OD1	1:A:184:LEU:HG	2.13	0.48
1:A:27(D):TYR:HB3	1:A:28:ASN:OD1	2.12	0.48
1:L:94:PHE:O	1:L:96:TYR:N	2.47	0.48
1:L:11:LEU:CD1	1:L:13:VAL:HG23	2.43	0.48
2:H:94:ARG:O	2:H:101:ASP:HA	2.13	0.48
1:A:163:LEU:C	1:A:163:LEU:HD23	2.34	0.48
2:B:12:VAL:HG11	2:B:18:VAL:HG13	1.95	0.48
2:H:215:ARG:HH11	2:H:215:ARG:CG	2.27	0.48
1:L:140:ASN:HB2	1:L:177:SER:OG	2.13	0.47
2:B:215:ARG:HH11	2:B:215:ARG:CG	2.27	0.47
2:B:30:THR:HA	2:B:52(A):PRO:HB2	1.96	0.47
1:L:4:MET:CE	1:L:23:CYS:SG	3.02	0.47
2:B:147:TYR:OH	2:B:179:LEU:HD23	2.15	0.47
2:B:12:VAL:CG2	2:B:82(C):LEU:HD13	2.38	0.47
1:A:1:ASP:O	1:A:2:ILE:HB	2.14	0.47
2:B:94:ARG:O	2:B:101:ASP:HA	2.14	0.47
2:H:150:GLU:OE1	2:H:151:PRO:HA	2.15	0.47
1:A:11:LEU:CD1	1:A:13:VAL:HG23	2.45	0.47
1:A:165:SER:O	1:A:178:MET:HA	2.14	0.47
1:L:96:TYR:CD1	3:L:551:PNB:H71	2.50	0.46
1:A:111:ARG:HG2	1:A:112:ALA:N	2.29	0.46
1:L:61:ARG:NH2	1:L:82:ASP:OD2	2.49	0.46
2:H:12:VAL:HG11	2:H:18:VAL:HG13	1.97	0.46
1:L:196:THR:HA	1:L:211:SER:HB3	1.97	0.46
1:A:14:THR:HA	1:A:107:LEU:HB3	1.98	0.46
2:B:213:VAL:CG1	2:B:214:PRO:HD2	2.45	0.46
1:L:144:PRO:CD	1:L:202:LYS:HE2	2.45	0.46
2:H:6:GLN:HE21	2:H:104:GLY:HA3	1.79	0.46
2:B:50:ARG:HG2	2:B:58:TYR:HB2	1.98	0.46
1:A:4:MET:CE	1:A:23:CYS:SG	3.04	0.46
2:B:150:GLU:OE1	2:B:151:PRO:HA	2.16	0.46
2:B:190:ARG:O	2:B:190:ARG:HD2	2.16	0.46
2:H:135:ASN:O	2:H:136:SER:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:137:MET:HB3	2:H:184:THR:HG23	1.97	0.45
2:H:50:ARG:HG2	2:H:58:TYR:HB2	1.98	0.45
1:A:182:LEU:HG	1:A:184:LEU:HD13	1.98	0.45
1:A:96:TYR:CD1	3:A:552:PNB:H71	2.51	0.45
1:L:160:ASN:OD1	1:L:184:LEU:HG	2.17	0.45
1:A:198:GLU:HG2	1:A:209:VAL:CG2	2.43	0.45
1:L:2:ILE:N	1:L:2:ILE:HD12	2.31	0.45
1:L:14:THR:HA	1:L:107:LEU:HB3	1.98	0.45
2:B:188:SER:HB2	2:B:189:PRO:CD	2.47	0.45
1:L:1:ASP:O	1:L:2:ILE:HB	2.17	0.44
2:B:137:MET:HB3	2:B:184:THR:HG23	1.99	0.44
1:A:2:ILE:N	1:A:2:ILE:HD12	2.33	0.44
2:B:135:ASN:O	2:B:136:SER:HB2	2.17	0.44
1:L:188:GLU:O	1:L:192:HIS:HD2	2.00	0.44
1:L:35:TRP:CZ3	1:L:88:CYS:HB3	2.53	0.44
1:L:165:SER:O	1:L:178:MET:HA	2.17	0.44
1:A:61:ARG:NH2	1:A:82:ASP:OD2	2.51	0.44
2:H:1:ALA:O	2:H:26:GLY:HA3	2.18	0.44
2:H:61:GLU:HG2	2:H:61:GLU:H	1.64	0.43
2:H:98:THR:HG21	2:H:100(D):TYR:HB3	2.01	0.43
1:L:163:LEU:C	1:L:163:LEU:HD23	2.39	0.43
1:A:118:VAL:HG22	1:A:139:LEU:HG	2.00	0.43
1:L:118:VAL:HG22	1:L:139:LEU:HG	2.01	0.43
1:A:151:TRP:CD1	1:A:162:VAL:HG21	2.53	0.43
2:H:127:ALA:O	2:H:215:ARG:NH1	2.52	0.43
2:B:1:ALA:O	2:B:26:GLY:HA3	2.18	0.43
2:B:61:GLU:HG2	2:B:61:GLU:H	1.62	0.43
2:B:119:THR:HA	2:B:120:PRO:HD3	1.87	0.43
2:H:96:GLY:HA3	2:H:100(F):ALA:O	2.19	0.43
2:H:196:THR:HG22	2:H:198:ASN:ND2	2.34	0.42
2:H:138:VAL:HG22	2:H:185:VAL:O	2.19	0.42
2:H:140:LEU:CD1	2:H:195:VAL:HG11	2.48	0.42
2:H:130:SER:C	2:H:132:ALA:H	2.23	0.42
2:B:89:VAL:HG22	2:B:108:LEU:HD23	2.00	0.42
1:L:158:ARG:O	1:L:159:GLN:HB2	2.19	0.42
1:L:46:ARG:HD3	2:H:95:TRP:CH2	2.55	0.42
1:A:103:LYS:HZ2	1:A:105:GLU:HG2	1.85	0.42
1:A:27(B):LEU:HD12	1:A:71:PHE:CE2	2.54	0.42
2:B:148:PHE:HA	2:B:149:PRO:HA	1.87	0.42
1:L:13:VAL:HG11	1:L:78:VAL:HG21	2.02	0.42
2:B:215:ARG:NH1	2:B:215:ARG:CG	2.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:182:LEU:HG	1:L:184:LEU:CD1	2.50	0.41
1:A:158:ARG:O	1:A:159:GLN:HB2	2.19	0.41
1:A:182:LEU:HG	1:A:184:LEU:CD1	2.51	0.41
1:L:182:LEU:HG	1:L:184:LEU:HD13	2.02	0.41
1:L:21:ILE:HD12	1:L:21:ILE:N	2.35	0.41
1:L:187:ASP:O	1:L:191:ARG:HG3	2.21	0.41
1:L:189:TYR:HA	1:L:195:TYR:OH	2.20	0.41
2:B:130:SER:C	2:B:132:ALA:H	2.22	0.41
1:A:77:ARG:HH12	1:A:79:GLU:CG	2.34	0.41
1:A:46:ARG:HD3	2:B:95:TRP:CH2	2.56	0.41
2:H:215:ARG:NH1	2:H:215:ARG:CG	2.83	0.41
2:H:57:THR:HG1	2:H:59:TYR:HE1	1.68	0.41
2:H:192:SER:O	2:H:193:GLU:CB	2.68	0.40
2:B:190:ARG:CB	2:B:191:PRO:HD3	2.49	0.40
2:B:215:ARG:HH11	2:B:215:ARG:HG3	1.85	0.40
1:A:187:ASP:HB3	1:A:191:ARG:HH21	1.85	0.40
2:H:6:GLN:HE21	2:H:104:GLY:C	2.24	0.40
2:B:28:ILE:O	2:B:28:ILE:HG23	2.22	0.40
2:B:138:VAL:HG22	2:B:185:VAL:O	2.22	0.40
2:H:213:VAL:CG1	2:H:214:PRO:HD2	2.50	0.40
2:H:215:ARG:HH11	2:H:215:ARG:HG3	1.85	0.40
2:H:188:SER:HB2	2:H:189:PRO:CD	2.51	0.40
1:A:187:ASP:O	1:A:191:ARG:HG3	2.22	0.40
2:B:98:THR:HG21	2:B:100(D):TYR:HB3	2.03	0.40
1:L:121:PHE:HA	1:L:122:PRO:HD3	1.90	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	217/219 (99%)	188 (87%)	19 (9%)	10 (5%)	3 17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	217/219 (99%)	187 (86%)	21 (10%)	9 (4%)	3	20
2	B	224/226 (99%)	197 (88%)	22 (10%)	5 (2%)	8	36
2	H	224/226 (99%)	199 (89%)	20 (9%)	5 (2%)	8	36
All	All	882/890 (99%)	771 (87%)	82 (9%)	29 (3%)	5	26

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	157	GLU
1	L	161	GLY
1	A	157	GLU
1	A	161	GLY
2	H	136	SER
2	B	136	SER
1	L	2	ILE
1	L	172	LYS
1	A	2	ILE
1	A	172	LYS
2	H	44	GLY
2	H	45	LEU
2	H	193	GLU
2	B	44	GLY
2	B	45	LEU
2	B	193	GLU
1	L	204	SER
1	A	204	SER
1	L	145	LYS
1	A	145	LYS
1	L	207	PRO
1	A	141	ASN
1	A	207	PRO
1	L	94	PHE
1	A	94	PHE
2	H	128	PRO
2	B	128	PRO
1	L	51	VAL
1	A	51	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	195/195 (100%)	181 (93%)	14 (7%)	18	53
1	L	195/195 (100%)	181 (93%)	14 (7%)	18	53
2	B	195/195 (100%)	181 (93%)	14 (7%)	18	53
2	H	195/195 (100%)	181 (93%)	14 (7%)	18	53
All	All	780/780 (100%)	724 (93%)	56 (7%)	18	53

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	SER
1	L	9	LEU
1	L	14	THR
1	L	15	ILE
1	L	26	SER
1	L	34	ASN
1	L	37	LEU
1	L	70	ASP
1	L	104	LEU
1	L	154	ASP
1	L	174	SER
1	L	184	LEU
1	L	200	THR
1	L	206	SER
1	A	7	SER
1	A	9	LEU
1	A	14	THR
1	A	15	ILE
1	A	26	SER
1	A	34	ASN
1	A	37	LEU
1	A	70	ASP
1	A	104	LEU
1	A	154	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	174	SER
1	A	184	LEU
1	A	200	THR
1	A	206	SER
2	H	11	LEU
2	H	18	VAL
2	H	31	SER
2	H	61	GLU
2	H	74	SER
2	H	113	SER
2	H	134	THR
2	H	171	VAL
2	H	179	LEU
2	H	183	VAL
2	H	187	SER
2	H	188	SER
2	H	198	ASN
2	H	207	LYS
2	B	11	LEU
2	B	18	VAL
2	B	31	SER
2	B	61	GLU
2	B	74	SER
2	B	113	SER
2	B	134	THR
2	B	151	PRO
2	B	171	VAL
2	B	179	LEU
2	B	183	VAL
2	B	187	SER
2	B	198	ASN
2	B	207	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	127	GLN
1	L	201	HIS
1	L	220	ASN
1	A	201	HIS
1	A	220	ASN
2	H	6	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	35	HIS
2	B	6	GLN
2	B	35	HIS

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](#)

2 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	PNB	A	552	-	19,24,24	3.36	5 (26%)	25,32,32	1.48	5 (20%)
3	PNB	L	551	-	19,24,24	2.69	5 (26%)	25,32,32	1.53	5 (20%)

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	PNB	A	552	-	-	0/20/22/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PNB	L	551	-	-	0/20/22/22	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	552	PNB	P1-C8	-9.66	1.72	1.80
3	L	551	PNB	P1-C8	-5.98	1.75	1.80
3	A	552	PNB	C12-N2	-5.52	1.35	1.46
3	L	551	PNB	C12-N2	-5.16	1.35	1.46
3	A	552	PNB	P1-O3	-4.21	1.46	1.56
3	A	552	PNB	P1-O2	-3.47	1.42	1.51
3	L	551	PNB	P1-O3	-2.79	1.49	1.56
3	L	551	PNB	P1-O2	-2.68	1.44	1.51
3	A	552	PNB	P1-O1	7.14	1.65	1.57
3	L	551	PNB	P1-O1	7.17	1.65	1.57

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	552	PNB	O1-P1-O2	-2.73	106.72	113.98
3	L	551	PNB	O1-P1-O2	-2.70	106.81	113.98
3	A	552	PNB	O6-C11-C10	-2.25	118.10	121.98
3	L	551	PNB	O6-C11-C10	-2.02	118.49	121.98
3	L	551	PNB	C13-C12-N2	2.02	116.95	111.74
3	A	552	PNB	C10-C11-N2	2.70	121.15	116.46
3	L	551	PNB	C10-C11-N2	2.80	121.32	116.46
3	A	552	PNB	O3-P1-C8	2.94	111.69	105.41
3	L	551	PNB	O3-P1-C8	2.99	111.80	105.41
3	A	552	PNB	O1-C7-C1	3.10	114.42	109.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	552	PNB	3	0
3	L	551	PNB	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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