



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:44 pm GMT

PDB ID : 2VUE  
Title : HUMAN SERUM ALBUMIN COMPLEXED WITH 4Z,15E-BILIRUBIN-IX-ALPHA  
Authors : Zunszain, P.A.; Ghuman, J.; Curry, S.  
Deposited on : 2008-05-24  
Resolution : 2.42 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.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

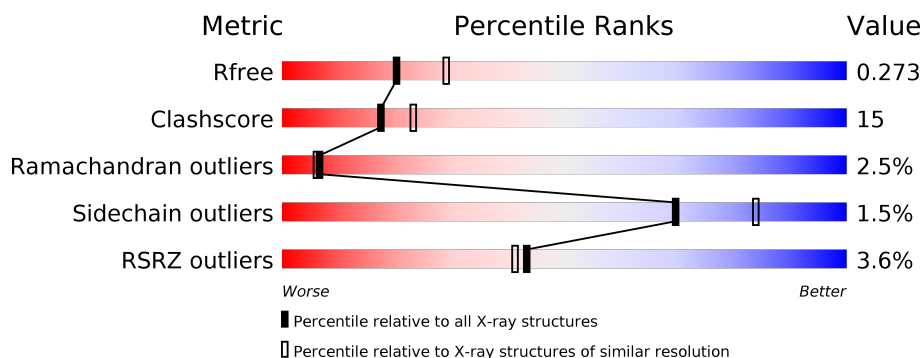
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.42 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	3709 (2.44-2.40)
Clashscore	112137	4241 (2.44-2.40)
Ramachandran outliers	110173	4178 (2.44-2.40)
Sidechain outliers	110143	4179 (2.44-2.40)
RSRZ outliers	101464	3740 (2.44-2.40)

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.

Mol	Chain	Length	Quality of chain
1	A	585	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>25%</div> <div>••</div> </div> </div>
1	B	585	<div> <div>4%</div> <div> <div></div> <div>62%</div> <div>32%</div> <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	BLA	A	2001	-	-	-	X

## 2 Entry composition [i](#)

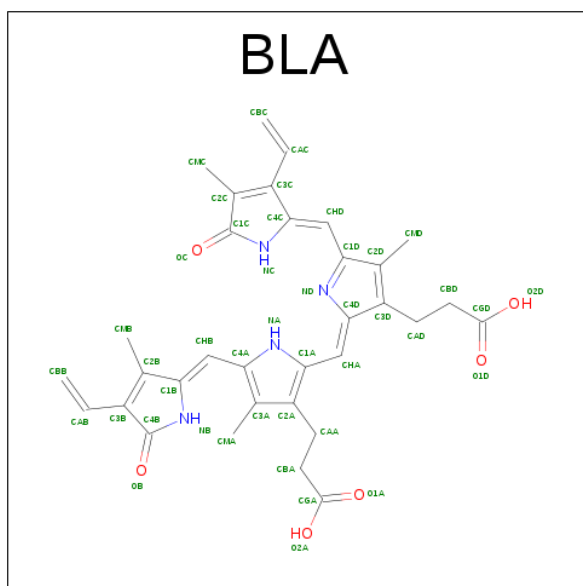
There are 3 unique types of molecules in this entry. The entry contains 8835 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SERUM ALBUMIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	565	Total	C	N	O	S	0	0	0
			4379	2768	732	839	40			
1	B	559	Total	C	N	O	S	0	0	0
			4355	2749	730	836	40			

- Molecule 2 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula:  $C_{33}H_{34}N_4O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			43	33	4	6		
2	B	1	Total	C	N	O	0	0
			43	33	4	6		

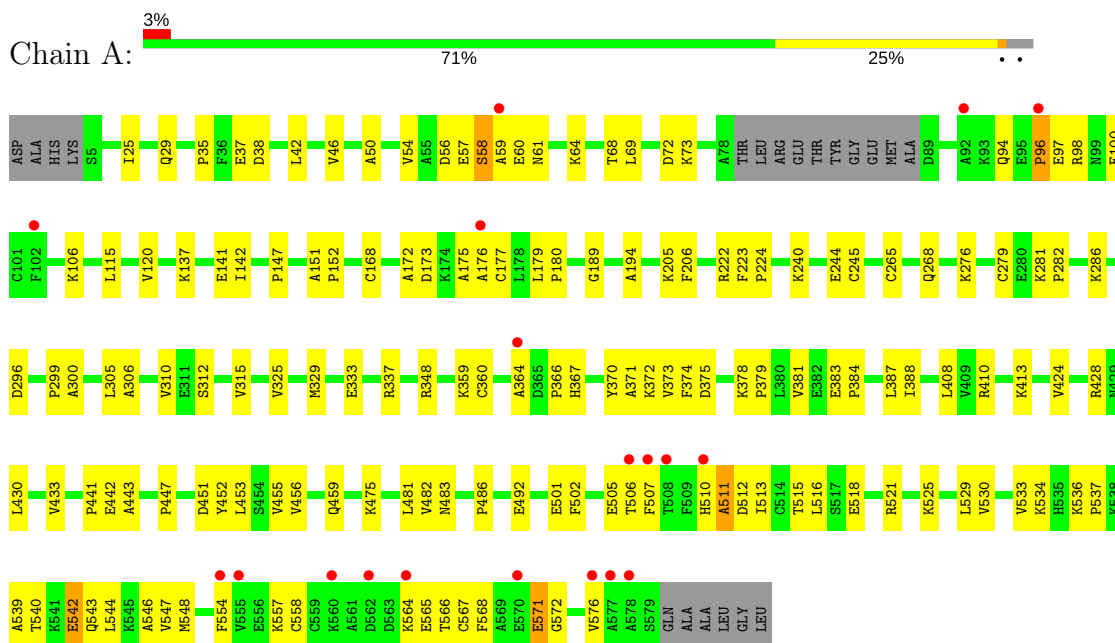
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total 8	O 8	0	0
3	B	7	Total 7	O 7	0	0

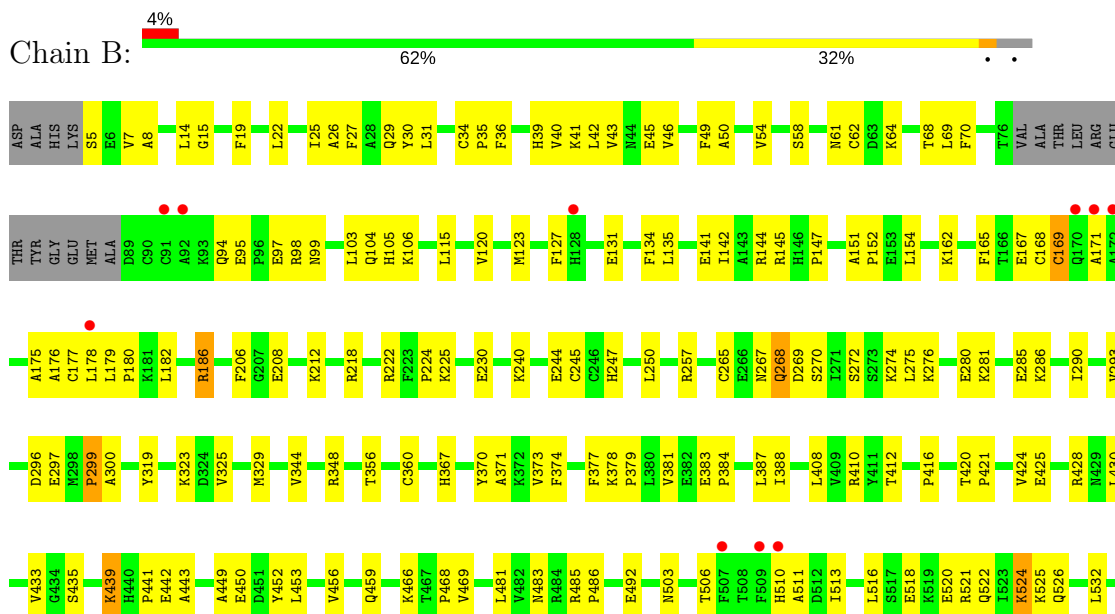
### 3 Residue-property plots

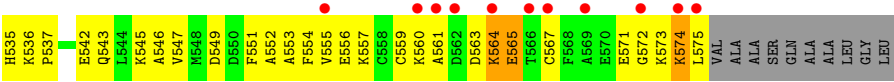
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: SERUM ALBUMIN



#### • Molecule 1: SERUM ALBUMIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.09Å 55.54Å 119.83Å 81.22° 90.70° 65.42°	Depositor
Resolution (Å)	35.07 – 2.42 35.07 – 2.42	Depositor EDS
% Data completeness (in resolution range)	94.9 (35.07-2.42) 90.0 (35.07-2.42)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.42Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.218 , 0.273 0.218 , 0.273	Depositor DCC
$R_{free}$ test set	2297 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.1	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 53.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8835	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.00% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.45	0/4465	0.63	1/6047 (0.0%)
1	B	0.44	0/4437	0.59	0/6001
All	All	0.45	0/8902	0.61	1/12048 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	PRO	CA-N-CD	-8.64	99.41	111.50

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4379	0	4183	107	0
1	B	4355	0	4184	150	0
2	A	43	0	34	10	0
2	B	43	0	34	15	0
3	A	8	0	0	1	0
3	B	7	0	0	0	0
All	All	8835	0	8435	266	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 15.

All (266) 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:B:2001:BLA:CMA	2:B:2001:BLA:HMB3	1.87	1.05
1:B:123:MET:HA	2:B:2001:BLA:HBB2	1.45	0.98
2:B:2001:BLA:HMD1	2:B:2001:BLA:HBD2	1.48	0.94
2:B:2001:BLA:HMB3	2:B:2001:BLA:HMA2	1.51	0.90
1:B:410:ARG:HH22	1:B:492:GLU:HA	1.41	0.86
1:B:123:MET:HA	2:B:2001:BLA:CBB	2.07	0.85
1:B:433:VAL:HG22	1:B:452:TYR:HD2	1.43	0.83
1:B:120:VAL:HG21	1:B:175:ALA:CB	2.11	0.81
1:B:433:VAL:HG22	1:B:452:TYR:CD2	2.16	0.80
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.64	0.79
1:A:424:VAL:O	1:A:428:ARG:HG3	1.84	0.77
1:B:152:PRO:HB2	1:B:257:ARG:HH11	1.48	0.77
1:A:433:VAL:HG22	1:A:452:TYR:CD2	2.20	0.77
1:B:120:VAL:HG21	1:B:175:ALA:HB1	1.67	0.76
1:A:224:PRO:HB2	1:A:299:PRO:HD3	1.70	0.74
1:A:240:LYS:O	1:A:244:GLU:HG3	1.88	0.74
1:B:134:PHE:HE1	2:B:2001:BLA:HAB	1.54	0.73
1:B:39:HIS:O	1:B:43:VAL:HG23	1.87	0.73
1:B:134:PHE:CE1	2:B:2001:BLA:HAB	2.23	0.73
1:A:25:ILE:O	1:A:29:GLN:HG2	1.89	0.72
1:B:36:PHE:O	1:B:40:VAL:HG23	1.90	0.71
1:A:430:LEU:O	1:A:433:VAL:HG23	1.91	0.71
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.72	0.70
1:A:359:LYS:HG3	1:A:360:CYS:N	2.06	0.70
1:B:290:ILE:O	1:B:293:VAL:HG12	1.91	0.70
1:B:274:LYS:HE3	1:B:296:ASP:HA	1.74	0.70
1:A:502:PHE:HE1	1:A:506:THR:HG21	1.56	0.70
1:B:378:LYS:HB2	1:B:379:PRO:HD3	1.74	0.69
2:B:2001:BLA:HMD1	2:B:2001:BLA:CBD	2.22	0.69
1:B:441:PRO:O	1:B:443:ALA:N	2.25	0.69
1:B:424:VAL:O	1:B:428:ARG:HG3	1.93	0.69
1:A:115:LEU:HD21	2:A:2001:BLA:C3A	2.23	0.68
1:A:306:ALA:HA	1:A:310:VAL:HG22	1.74	0.68
1:A:513:ILE:HG13	1:A:516:LEU:HD12	1.74	0.68
1:B:521:ARG:HG2	1:B:525:LYS:NZ	2.09	0.68
1:A:142:ILE:HG23	2:A:2001:BLA:HBC1	1.77	0.67
1:A:281:LYS:HB2	1:A:282:PRO:HD2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ILE:O	1:B:29:GLN:HG3	1.94	0.66
1:B:106:LYS:HD3	1:B:147:PRO:HB2	1.76	0.66
1:B:115:LEU:HD13	1:B:145:ARG:NH2	2.10	0.66
1:B:179:LEU:HB2	1:B:180:PRO:HD3	1.76	0.65
1:A:115:LEU:HD21	2:A:2001:BLA:C4A	2.26	0.65
1:A:115:LEU:CD2	2:A:2001:BLA:C4A	2.75	0.65
1:A:94:GLN:O	1:A:98:ARG:CB	2.45	0.64
1:A:543:GLN:O	1:A:547:VAL:HG23	1.97	0.64
1:A:433:VAL:HG22	1:A:452:TYR:HD2	1.62	0.64
1:A:373:VAL:HG13	1:A:374:PHE:HD1	1.62	0.63
1:A:281:LYS:HB2	1:A:282:PRO:CD	2.28	0.63
1:B:572:GLY:O	1:B:575:LEU:HD13	1.98	0.63
1:A:37:GLU:N	1:A:37:GLU:OE1	2.24	0.63
1:A:433:VAL:HG21	1:A:453:LEU:HD21	1.80	0.63
1:B:410:ARG:NH2	1:B:492:GLU:HA	2.11	0.63
1:B:115:LEU:HD22	1:B:145:ARG:NH1	2.13	0.62
1:B:120:VAL:HG21	1:B:175:ALA:HB2	1.80	0.62
1:B:520:GLU:O	1:B:524:LYS:HG2	1.99	0.62
1:A:35:PRO:HD2	1:A:38:ASP:OD2	2.00	0.62
1:A:115:LEU:HD23	2:A:2001:BLA:C1A	2.29	0.62
1:B:68:THR:HA	1:B:98:ARG:NH2	2.15	0.62
1:A:483:ASN:C	1:A:486:PRO:HD2	2.21	0.61
1:B:532:LEU:HD11	1:B:547:VAL:HG11	1.81	0.61
2:B:2001:BLA:HMB3	2:B:2001:BLA:HMA1	1.78	0.61
1:B:68:THR:HA	1:B:98:ARG:HH21	1.66	0.61
1:A:408:LEU:HD21	1:A:424:VAL:HA	1.84	0.60
1:B:556:GLU:O	1:B:560:LYS:HG2	2.02	0.60
1:B:387:LEU:HD23	1:B:388:ILE:HD13	1.83	0.60
1:B:384:PRO:O	1:B:388:ILE:HG12	2.02	0.59
1:A:557:LYS:HG3	1:A:558:CYS:N	2.18	0.59
1:B:15:GLY:O	1:B:19:PHE:HB2	2.03	0.59
1:A:42:LEU:O	1:A:46:VAL:HG23	2.03	0.59
1:B:208:GLU:OE2	1:B:212:LYS:NZ	2.35	0.59
1:B:388:ILE:HD12	1:B:449:ALA:CB	2.33	0.59
1:A:106:LYS:HD3	1:A:147:PRO:HB2	1.85	0.59
1:A:364:ALA:O	1:A:366:PRO:HD3	2.02	0.59
1:A:179:LEU:HB2	1:A:180:PRO:HD3	1.85	0.59
1:B:441:PRO:C	1:B:443:ALA:H	2.06	0.58
1:B:115:LEU:HD13	1:B:145:ARG:HH22	1.66	0.58
1:B:26:ALA:HB2	1:B:250:LEU:HD12	1.85	0.58
1:A:378:LYS:HB3	1:A:379:PRO:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ALA:C	1:B:177:CYS:H	2.07	0.58
1:B:123:MET:HE1	1:B:165:PHE:HZ	1.69	0.58
1:A:50:ALA:O	1:A:54:VAL:HG23	2.04	0.57
1:A:189:GLY:HA3	2:A:2001:BLA:HAC	1.85	0.57
1:B:564:LYS:N	1:B:564:LYS:HD2	2.20	0.57
1:A:502:PHE:CE1	1:A:506:THR:HG21	2.39	0.57
1:B:545:LYS:HD3	1:B:545:LYS:O	2.05	0.57
1:B:240:LYS:O	1:B:244:GLU:HG3	2.05	0.56
1:A:413:LYS:HE2	1:A:537:PRO:O	2.06	0.55
1:A:306:ALA:CA	1:A:310:VAL:HG22	2.37	0.55
2:B:2001:BLA:ND	2:B:2001:BLA:HAA1	2.22	0.55
1:B:281:LYS:HD2	1:B:285:GLU:OE1	2.05	0.55
1:A:265:CYS:O	1:A:268:GLN:HG3	2.07	0.55
1:B:25:ILE:HD13	1:B:154:LEU:HD23	1.88	0.55
1:A:325:VAL:HG12	1:A:329:MET:CE	2.37	0.55
1:B:388:ILE:HD12	1:B:449:ALA:HB1	1.87	0.55
1:B:50:ALA:O	1:B:54:VAL:HG23	2.07	0.55
1:A:265:CYS:SG	1:A:286:LYS:HD2	2.48	0.54
1:B:319:TYR:CE1	1:B:323:LYS:HB2	2.42	0.54
1:B:435:SER:O	1:B:439:LYS:HE2	2.07	0.54
1:A:483:ASN:O	1:A:486:PRO:HD2	2.07	0.54
1:B:275:LEU:HD22	1:B:290:ILE:HG22	1.90	0.54
1:B:561:ALA:HB3	1:B:563:ASP:OD1	2.08	0.54
1:B:521:ARG:NH1	1:B:521:ARG:HB2	2.23	0.53
1:A:433:VAL:HG22	1:A:452:TYR:CE2	2.43	0.53
1:B:206:PHE:CD2	1:B:481:LEU:HD22	2.42	0.53
1:B:574:LYS:C	1:B:575:LEU:HD12	2.28	0.53
1:B:535:HIS:C	1:B:537:PRO:HD3	2.29	0.53
1:B:485:ARG:HB3	1:B:486:PRO:HD3	1.91	0.53
2:A:2001:BLA:HAA1	2:A:2001:BLA:ND	2.24	0.53
1:A:512:ASP:O	1:A:515:THR:HG22	2.09	0.52
1:A:530:VAL:O	1:A:534:LYS:HG3	2.08	0.52
1:B:513:ILE:HG13	1:B:516:LEU:HD12	1.90	0.52
1:B:521:ARG:HG2	1:B:525:LYS:HZ2	1.73	0.52
1:A:572:GLY:O	1:A:576:VAL:HG23	2.10	0.51
1:B:168:CYS:SG	1:B:177:CYS:C	2.88	0.51
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.93	0.51
1:A:557:LYS:HE3	1:A:571:GLU:HG2	1.93	0.51
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.93	0.51
1:A:372:LYS:O	1:A:375:ASP:HB2	2.11	0.51
1:B:265:CYS:SG	1:B:286:LYS:HD2	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:PHE:O	1:B:381:VAL:HG23	2.11	0.51
1:B:127:PHE:O	1:B:131:GLU:HB3	2.11	0.51
1:B:123:MET:CE	1:B:165:PHE:HZ	2.23	0.50
1:B:218:ARG:HH21	1:B:222:ARG:HH21	1.57	0.50
1:A:173:ASP:HB3	1:A:176:ALA:HB3	1.94	0.50
1:A:61:ASN:OD1	1:A:64:LYS:HE3	2.10	0.50
1:B:141:GLU:HA	1:B:141:GLU:OE2	2.11	0.50
1:B:42:LEU:O	1:B:46:VAL:HG23	2.11	0.50
1:B:433:VAL:HG21	1:B:453:LEU:HD21	1.94	0.50
1:B:49:PHE:CE2	1:B:69:LEU:HD21	2.46	0.50
1:A:115:LEU:HG	2:A:2001:BLA:NA	2.26	0.50
1:A:168:CYS:SG	1:A:177:CYS:C	2.90	0.50
1:B:123:MET:HG2	2:B:2001:BLA:CBB	2.42	0.50
1:A:367:HIS:O	1:A:371:ALA:HB2	2.12	0.49
1:B:483:ASN:C	1:B:486:PRO:HD2	2.32	0.49
1:B:103:LEU:C	1:B:105:HIS:H	2.14	0.49
1:A:564:LYS:C	1:A:566:THR:H	2.14	0.49
1:A:305:LEU:HD21	1:A:333:GLU:HB3	1.94	0.49
1:B:186:ARG:HG2	2:B:2001:BLA:CHD	2.42	0.49
1:B:168:CYS:SG	1:B:177:CYS:O	2.70	0.49
1:B:536:LYS:N	1:B:537:PRO:HD3	2.28	0.49
1:A:554:PHE:HZ	1:A:568:PHE:HA	1.77	0.49
1:B:224:PRO:HD2	1:B:296:ASP:HB3	1.94	0.49
1:A:373:VAL:HG13	1:A:374:PHE:CD1	2.47	0.49
1:A:518:GLU:HA	1:A:521:ARG:NH1	2.28	0.48
1:B:178:LEU:HG	1:B:182:LEU:CD1	2.43	0.48
1:B:30:TYR:O	1:B:31:LEU:HG	2.13	0.48
1:B:430:LEU:O	1:B:433:VAL:HG23	2.13	0.48
1:B:573:LYS:C	1:B:575:LEU:H	2.16	0.48
1:A:222:ARG:HG2	1:A:223:PHE:CE1	2.49	0.48
1:A:69:LEU:O	1:A:73:LYS:HG2	2.14	0.48
1:A:410:ARG:NH2	1:A:492:GLU:O	2.46	0.48
1:B:218:ARG:NH2	1:B:222:ARG:HH21	2.12	0.48
1:B:511:ALA:C	1:B:513:ILE:H	2.17	0.48
1:B:567:CYS:HA	1:B:571:GLU:HG2	1.96	0.48
1:B:5:SER:N	1:B:62:CYS:O	2.46	0.48
1:B:319:TYR:O	1:B:323:LYS:HB3	2.14	0.48
1:A:97:GLU:HA	1:A:100:GLU:HG2	1.96	0.48
1:A:279:CYS:HA	1:A:286:LYS:HD3	1.96	0.47
1:A:325:VAL:HG12	1:A:329:MET:HE3	1.96	0.47
1:B:441:PRO:C	1:B:443:ALA:N	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:LYS:CE	1:B:296:ASP:HA	2.41	0.47
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.97	0.47
1:B:142:ILE:HG23	2:B:2001:BLA:HBC1	1.96	0.47
1:B:152:PRO:CB	1:B:257:ARG:HH11	2.22	0.47
1:A:115:LEU:CD2	2:A:2001:BLA:C3A	2.91	0.47
1:B:175:ALA:O	1:B:177:CYS:N	2.41	0.47
2:B:2001:BLA:HMB3	2:B:2001:BLA:C3A	2.43	0.47
1:B:483:ASN:O	1:B:486:PRO:HD2	2.15	0.47
1:B:543:GLN:O	1:B:546:ALA:HB3	2.14	0.47
1:A:333:GLU:OE1	1:A:337:ARG:NH2	2.47	0.47
1:A:567:CYS:HA	1:A:571:GLU:H	1.79	0.47
1:A:115:LEU:HG	2:A:2001:BLA:C4A	2.45	0.47
1:A:433:VAL:HG21	1:A:453:LEU:CD2	2.45	0.46
1:B:466:LYS:O	1:B:468:PRO:HD3	2.16	0.46
1:A:384:PRO:O	1:A:388:ILE:HD13	2.15	0.46
1:B:152:PRO:HB2	1:B:257:ARG:NH1	2.25	0.46
1:A:37:GLU:CD	1:A:37:GLU:H	2.14	0.46
1:A:387:LEU:HD23	1:A:388:ILE:HD12	1.97	0.46
1:B:94:GLN:O	1:B:97:GLU:HB2	2.15	0.46
1:A:525:LYS:O	1:A:548:MET:HE1	2.16	0.46
1:B:135:LEU:HD11	1:B:162:LYS:HB2	1.97	0.46
1:B:178:LEU:HG	1:B:182:LEU:HD11	1.98	0.46
1:B:367:HIS:O	1:B:371:ALA:HB2	2.15	0.46
1:B:410:ARG:HH22	1:B:492:GLU:CA	2.22	0.46
1:B:516:LEU:O	1:B:521:ARG:NH2	2.49	0.45
1:B:412:THR:O	1:B:416:PRO:HG3	2.16	0.45
1:B:225:LYS:NZ	1:B:297:GLU:HB3	2.32	0.45
1:B:513:ILE:HG12	1:B:513:ILE:O	2.17	0.45
1:A:536:LYS:CB	1:A:539:ALA:HB2	2.47	0.45
2:B:2001:BLA:CMA	2:B:2001:BLA:CMB	2.77	0.45
1:B:356:THR:O	1:B:360:CYS:HB2	2.16	0.45
1:A:501:GLU:HA	1:A:501:GLU:OE1	2.17	0.45
1:B:165:PHE:O	1:B:167:GLU:N	2.50	0.45
1:A:502:PHE:CE2	1:A:576:VAL:HG11	2.51	0.45
1:B:165:PHE:C	1:B:167:GLU:N	2.69	0.45
1:B:433:VAL:HG21	1:B:453:LEU:CD2	2.46	0.45
1:B:456:VAL:O	1:B:459:GLN:HB2	2.17	0.45
1:A:370:TYR:CD1	1:A:370:TYR:C	2.91	0.44
1:B:560:LYS:O	1:B:560:LYS:HG3	2.17	0.44
1:B:27:PHE:HE1	1:B:70:PHE:CD2	2.35	0.44
1:B:41:LYS:HG2	1:B:45:GLU:OE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:GLU:OE2	1:B:99:ASN:HB2	2.17	0.44
1:B:25:ILE:CD1	1:B:154:LEU:HD23	2.47	0.44
1:B:151:ALA:CB	1:B:152:PRO:HD3	2.43	0.44
1:B:230:GLU:HA	1:B:230:GLU:OE1	2.17	0.44
1:A:456:VAL:O	1:A:459:GLN:HB3	2.18	0.43
1:B:522:GLN:O	1:B:526:GLN:HG3	2.18	0.43
1:A:506:THR:HG23	1:A:507:PHE:N	2.33	0.43
1:B:549:ASP:O	1:B:552:ALA:HB3	2.18	0.43
1:B:344:VAL:O	1:B:348:ARG:HB2	2.18	0.43
1:A:348:ARG:HG3	1:A:482:VAL:HG12	1.99	0.43
1:A:56:ASP:C	1:A:58:SER:H	2.22	0.43
1:B:420:THR:N	1:B:421:PRO:CD	2.82	0.43
1:A:518:GLU:HA	1:A:521:ARG:HH11	1.84	0.43
1:A:557:LYS:NZ	1:A:571:GLU:HG2	2.34	0.43
1:B:7:VAL:HG13	1:B:8:ALA:N	2.34	0.43
1:B:165:PHE:HD1	1:B:169:CYS:SG	2.42	0.43
1:B:565:GLU:HG3	1:B:565:GLU:O	2.19	0.43
1:A:120:VAL:HG21	1:A:175:ALA:HA	2.00	0.42
1:B:410:ARG:NH2	1:B:492:GLU:OE1	2.51	0.42
1:A:205:LYS:NZ	3:A:2002:HOH:O	2.52	0.42
1:A:447:PRO:O	1:A:451:ASP:HB2	2.19	0.42
1:A:206:PHE:CD2	1:A:481:LEU:HD22	2.54	0.42
1:A:511:ALA:HB3	1:A:565:GLU:OE2	2.19	0.42
1:B:545:LYS:NZ	1:B:549:ASP:HB2	2.35	0.42
1:A:513:ILE:HA	1:A:516:LEU:HD12	2.02	0.42
1:B:175:ALA:C	1:B:177:CYS:N	2.72	0.42
1:A:68:THR:HG22	1:A:72:ASP:OD2	2.18	0.42
1:B:34:CYS:HA	1:B:35:PRO:HD3	1.83	0.42
1:B:553:ALA:HB1	1:B:557:LYS:HD2	2.02	0.42
1:A:475:LYS:HB3	1:A:475:LYS:HE3	1.91	0.42
1:B:267:ASN:O	1:B:270:SER:HB3	2.20	0.42
1:B:551:PHE:O	1:B:555:VAL:HG23	2.19	0.42
1:A:381:VAL:O	1:A:384:PRO:HD2	2.20	0.42
1:A:348:ARG:HG3	1:A:482:VAL:CG1	2.50	0.42
1:A:542:GLU:OE1	1:A:542:GLU:N	2.52	0.42
1:B:268:GLN:O	1:B:270:SER:N	2.52	0.42
1:B:408:LEU:HD21	1:B:424:VAL:HA	2.02	0.42
1:A:441:PRO:O	1:A:443:ALA:N	2.53	0.42
1:B:518:GLU:HA	1:B:521:ARG:NH1	2.34	0.42
1:B:272:SER:HB3	1:B:275:LEU:HG	2.01	0.41
1:B:276:LYS:O	1:B:280:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:LEU:O	1:A:533:VAL:HG23	2.20	0.41
1:A:61:ASN:HB3	1:A:64:LYS:HG3	2.02	0.41
1:B:373:VAL:HG13	1:B:374:PHE:HD1	1.85	0.41
1:A:279:CYS:HA	1:A:286:LYS:CD	2.49	0.41
1:A:544:LEU:C	1:A:546:ALA:H	2.23	0.41
1:A:525:LYS:HG2	1:A:548:MET:HE3	2.03	0.41
1:A:137:LYS:O	1:A:141:GLU:HG2	2.21	0.41
1:A:168:CYS:SG	1:A:177:CYS:O	2.79	0.41
1:B:325:VAL:HG12	1:B:329:MET:CE	2.51	0.41
1:A:540:THR:OG1	1:A:543:GLN:HG2	2.21	0.41
1:B:103:LEU:HD11	1:B:247:HIS:O	2.21	0.41
1:B:555:VAL:O	1:B:559:CYS:SG	2.78	0.41
1:B:14:LEU:HD13	1:B:22:LEU:HD12	2.02	0.41
1:B:503:ASN:O	1:B:506:THR:HB	2.21	0.41
1:A:510:HIS:C	1:A:512:ASP:H	2.25	0.40
1:B:513:ILE:HA	1:B:516:LEU:HD12	2.03	0.40
1:B:141:GLU:OE2	1:B:144:ARG:HD3	2.20	0.40
1:B:208:GLU:CD	1:B:212:LYS:NZ	2.75	0.40
1:B:370:TYR:C	1:B:370:TYR:CD1	2.95	0.40
1:B:567:CYS:HA	1:B:571:GLU:CG	2.51	0.40
1:B:123:MET:HE1	1:B:165:PHE:CZ	2.52	0.40
1:B:374:PHE:O	1:B:377:PHE:HB2	2.21	0.40
1:B:378:LYS:CB	1:B:379:PRO:HD3	2.45	0.40
1:A:194:ALA:HB1	1:A:455:VAL:CG1	2.52	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	561/585 (96%)	500 (89%)	48 (9%)	13 (2%)	<b>7</b> <b>7</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	555/585 (95%)	495 (89%)	45 (8%)	15 (3%)	6	5
All	All	1116/1170 (95%)	995 (89%)	93 (8%)	28 (2%)	6	6

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	ALA
1	A	276	LYS
1	A	300	ALA
1	B	61	ASN
1	B	64	LYS
1	B	268	GLN
1	B	300	ALA
1	B	442	GLU
1	B	510	HIS
1	B	565	GLU
1	A	59	ALA
1	A	511	ALA
1	A	60	GLU
1	A	96	PRO
1	A	312	SER
1	A	315	VAL
1	A	442	GLU
1	A	505	GLU
1	B	104	GLN
1	B	171	ALA
1	B	176	ALA
1	B	269	ASP
1	A	57	GLU
1	A	58	SER
1	B	169	CYS
1	B	554	PHE
1	B	574	LYS
1	B	299	PRO

### 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	467/511 (91%)	464 (99%)	3 (1%)	89	95
1	B	466/511 (91%)	455 (98%)	11 (2%)	54	73
All	All	933/1022 (91%)	919 (98%)	14 (2%)	70	84

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

Mol	Chain	Res	Type
1	A	245	CYS
1	A	542	GLU
1	A	571	GLU
1	B	58	SER
1	B	186	ARG
1	B	245	CYS
1	B	299	PRO
1	B	425	GLU
1	B	439	LYS
1	B	450	GLU
1	B	469	VAL
1	B	524	LYS
1	B	542	GLU
1	B	564	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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

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	$\# Z  > 2$
2	BLA	A	2001	-	36,46,46	2.53	7 (19%)	46,67,67	1.61	10 (21%)
2	BLA	B	2001	-	36,46,46	2.43	7 (19%)	46,67,67	1.64	11 (23%)

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	BLA	A	2001	-	-	1/22/74/74	0/4/4/4
2	BLA	B	2001	-	-	1/22/74/74	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	BLA	CAB-C3B	-2.50	1.40	1.47
2	A	2001	BLA	CAB-C3B	-2.47	1.40	1.47
2	A	2001	BLA	CMD-C2D	2.07	1.55	1.50
2	B	2001	BLA	CMD-C2D	2.13	1.55	1.50
2	B	2001	BLA	C1B-C2B	3.16	1.50	1.45
2	A	2001	BLA	CBC-CAC	3.21	1.46	1.30
2	B	2001	BLA	CBC-CAC	3.25	1.46	1.30
2	A	2001	BLA	C1B-C2B	3.29	1.51	1.45
2	A	2001	BLA	CHB-C1B	3.82	1.42	1.34
2	B	2001	BLA	CHB-C1B	3.93	1.42	1.34
2	A	2001	BLA	C3C-C4C	4.11	1.52	1.45
2	B	2001	BLA	C3C-C4C	4.60	1.53	1.45
2	B	2001	BLA	CHA-C4D	10.63	1.44	1.35
2	A	2001	BLA	CHA-C4D	11.59	1.45	1.35

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	BLA	CHA-C4D-ND	-4.49	121.98	128.79
2	A	2001	BLA	CHA-C4D-ND	-4.35	122.20	128.79
2	B	2001	BLA	C1B-NB-C4B	-4.30	104.98	110.70
2	A	2001	BLA	C1B-NB-C4B	-4.26	105.03	110.70
2	A	2001	BLA	CHB-C1B-NB	-2.95	120.22	130.29
2	B	2001	BLA	C1A-CHA-C4D	-2.87	125.29	128.77
2	B	2001	BLA	C4C-NC-C1C	-2.84	106.92	110.70
2	B	2001	BLA	CHB-C1B-NB	-2.83	120.64	130.29
2	A	2001	BLA	C4C-NC-C1C	-2.62	107.21	110.70
2	B	2001	BLA	C4B-C3B-C2B	-2.56	104.61	108.08
2	A	2001	BLA	C4B-C3B-C2B	-2.52	104.67	108.08
2	B	2001	BLA	OB-C4B-C3B	-2.13	124.84	129.77
2	A	2001	BLA	OB-C4B-C3B	-2.09	124.93	129.77
2	B	2001	BLA	CMB-C2B-C1B	2.02	126.81	124.17
2	B	2001	BLA	C2C-C1C-NC	2.03	111.98	106.44
2	A	2001	BLA	C2C-C1C-NC	2.03	111.99	106.44
2	A	2001	BLA	CMB-C2B-C1B	2.17	127.00	124.17
2	B	2001	BLA	CAA-CBA-CGA	2.47	116.89	112.66
2	A	2001	BLA	CAA-CBA-CGA	2.61	117.12	112.66
2	B	2001	BLA	C2B-C1B-NB	2.63	110.95	107.04
2	A	2001	BLA	C2B-C1B-NB	2.64	110.98	107.04

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	BLA	C4A-CHB-C1B-NB
2	B	2001	BLA	C4A-CHB-C1B-NB

There are no ring outliers.

2 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	BLA	10	0
2	B	2001	BLA	15	0

## 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

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	565/585 (96%)	-0.03	19 (3%)	46 43	38, 72, 136, 156	0
1	B	559/585 (95%)	-0.06	21 (3%)	41 39	40, 76, 139, 164	0
All	All	1124/1170 (96%)	-0.04	40 (3%)	43 41	38, 73, 138, 164	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	561	ALA	5.1
1	A	554	PHE	4.4
1	A	577	ALA	4.3
1	A	508	THR	4.2
1	B	562	ASP	4.1
1	A	555	VAL	4.1
1	A	92	ALA	4.0
1	A	578	ALA	3.8
1	A	570	GLU	3.8
1	B	171	ALA	3.7
1	A	510	HIS	3.7
1	A	562	ASP	3.7
1	B	555	VAL	3.7
1	B	564	LYS	3.6
1	B	575	LEU	3.5
1	B	509	PHE	3.2
1	A	506	THR	3.0
1	A	560	LYS	3.0
1	A	507	PHE	3.0
1	B	566	THR	3.0
1	B	574	LYS	2.8
1	B	172	ALA	2.8
1	A	96	PRO	2.7
1	A	176	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	560	LYS	2.6
1	B	567	CYS	2.6
1	A	59	ALA	2.5
1	B	92	ALA	2.5
1	B	507	PHE	2.5
1	B	569	ALA	2.5
1	B	572	GLY	2.5
1	A	564	LYS	2.5
1	B	178	LEU	2.5
1	B	128	HIS	2.3
1	A	102	PHE	2.2
1	A	576	VAL	2.2
1	B	170	GLN	2.2
1	B	510	HIS	2.1
1	A	364	ALA	2.1
1	B	91	CYS	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 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	BLA	A	2001	43/43	0.89	0.31	3.15	87,110,120,120	0
2	BLA	B	2001	43/43	0.90	0.21	1.73	83,106,120,121	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.