



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:33 am BST

PDB ID : 4F5S  
Title : Crystal Structure of Bovine Serum Albumin  
Authors : Bujacz, A.; Bujacz, G.  
Deposited on : 2012-05-13  
Resolution : 2.47 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

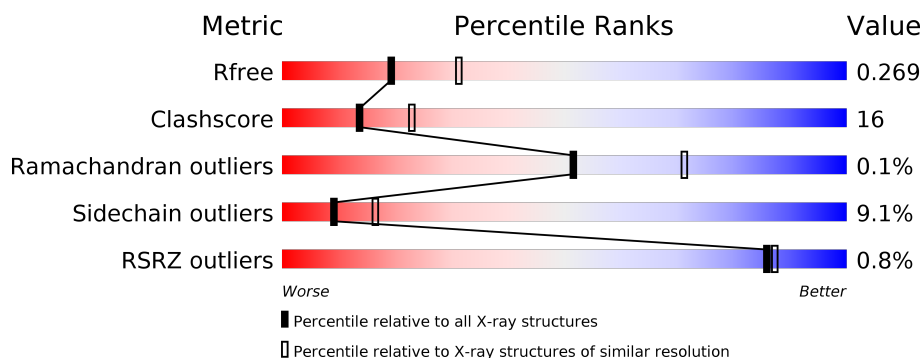
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.47 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))
$R_{free}$	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	583	<div> <div>%</div> <div> <div></div> <div>62%</div> <div>34%</div> <div>.</div> </div> </div>
1	B	583	<div> <div>%</div> <div> <div></div> <div>65%</div> <div>31%</div> <div>.</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9675 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.

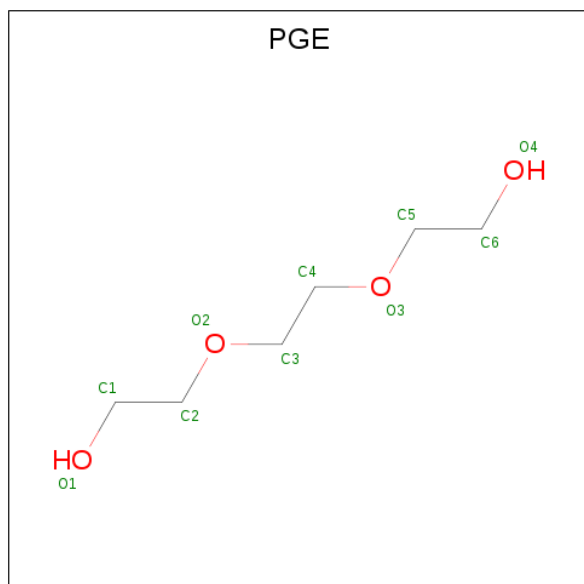
- Molecule 1 is a protein called Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	583	Total	C	N	O	S	0	3	0
			4672	2947	787	899	39			
1	B	583	Total	C	N	O	S	0	2	0
			4666	2943	784	900	39			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	190	THR	ALA	VARIANT	UNP P02769
B	190	THR	ALA	VARIANT	UNP P02769

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		

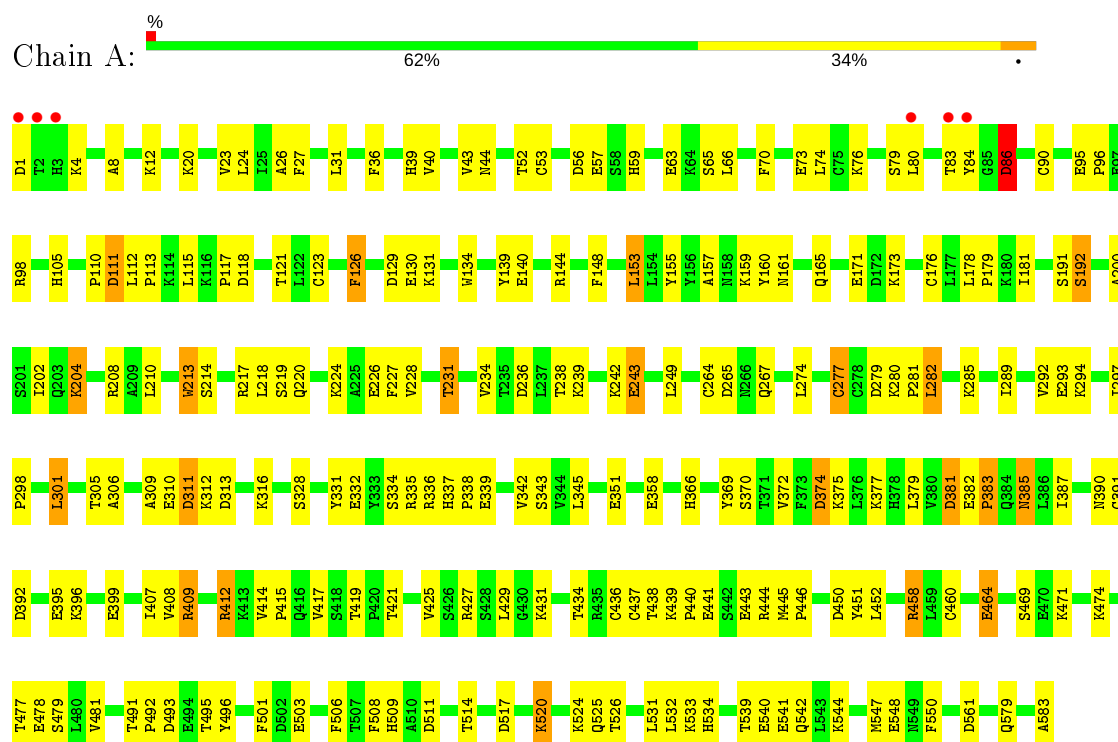
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	166	Total 166	O 166	0	0
3	B	161	Total 161	O 161	0	0

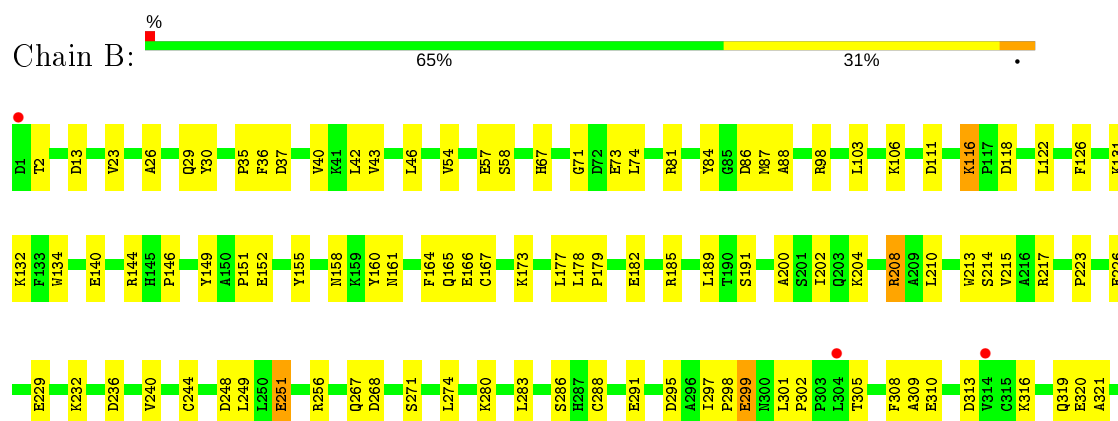
### 3 Residue-property plots

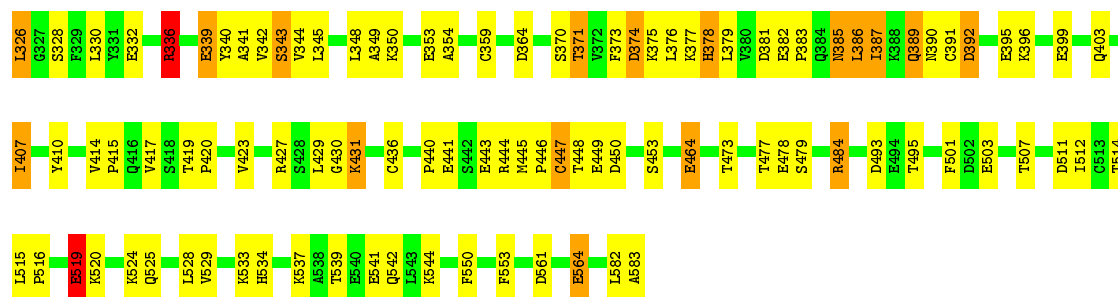
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	217.80Å 44.99Å 143.06Å 90.00° 114.13° 90.00°	Depositor
Resolution (Å)	40.00 – 2.47 37.22 – 2.47	Depositor EDS
% Data completeness (in resolution range)	94.6 (40.00-2.47) 94.7 (37.22-2.47)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.197 , 0.259 0.210 , 0.269	Depositor DCC
$R_{free}$ test set	1369 reflections (3.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.4	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 56.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9675	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	1.03	6/4776 (0.1%)	0.97	4/6446 (0.1%)
1	B	0.95	4/4767 (0.1%)	0.97	4/6435 (0.1%)
All	All	0.99	10/9543 (0.1%)	0.97	8/12881 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213	TRP	CB-CG	-6.00	1.39	1.50
1	B	251	GLU	CD-OE2	5.79	1.32	1.25
1	B	564	GLU	CB-CG	5.76	1.63	1.52
1	A	508	PHE	CD2-CE2	5.54	1.50	1.39
1	A	242	LYS	CD-CE	5.45	1.64	1.51
1	A	243	GLU	CD-OE2	-5.34	1.19	1.25
1	B	519	GLU	CG-CD	5.26	1.59	1.51
1	A	236	ASP	CB-CG	5.16	1.62	1.51
1	B	288	CYS	CB-SG	5.12	1.91	1.82
1	A	176	CYS	CB-SG	5.08	1.90	1.82

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	479	SER	N-CA-CB	5.98	119.47	110.50
1	A	412	ARG	NE-CZ-NH1	-5.97	117.31	120.30
1	A	129	ASP	CB-CG-OD1	5.85	123.56	118.30
1	B	436	CYS	N-CA-C	5.79	126.64	111.00
1	B	336	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	4	LYS	N-CA-C	5.29	125.28	111.00
1	A	277	CYS	N-CA-CB	-5.18	101.27	110.60
1	B	42	LEU	CA-CB-CG	5.06	126.93	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	4672	0	4597	148	0
1	B	4666	0	4583	146	0
2	A	10	0	14	2	0
3	A	166	0	0	24	0
3	B	161	0	0	25	0
All	All	9675	0	9194	294	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 (294) 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:140:GLU:HG3	1:A:144:ARG:NH1	1.65	1.11
1:A:140:GLU:HG3	1:A:144:ARG:HH12	1.16	1.11
1:B:341:ALA:HB1	3:B:746:HOH:O	1.53	1.07
1:B:519:GLU:HG2	3:B:722:HOH:O	1.62	0.99
1:A:298:PRO:O	1:A:301:LEU:HD12	1.64	0.94
1:B:298:PRO:HG2	1:B:301:LEU:HD11	1.51	0.91
1:B:383:PRO:O	1:B:386:LEU:HD23	1.71	0.90
1:B:36:PHE:O	1:B:40:VAL:HG23	1.72	0.89
1:A:539:THR:OG1	1:A:542:GLN:HG3	1.73	0.89
1:B:503:GLU:HB3	3:B:749:HOH:O	1.73	0.87
1:B:84:TYR:HB3	1:B:87:MET:HG3	1.57	0.86
1:A:27:PHE:HB3	1:A:39:HIS:CD2	2.11	0.85
1:B:345:LEU:HA	1:B:348:LEU:HD12	1.60	0.83
1:A:298:PRO:O	1:A:301:LEU:CD1	2.27	0.83
1:A:493:ASP:HB2	3:A:864:HOH:O	1.80	0.82
1:A:436:CYS:O	1:A:444:ARG:HG2	1.81	0.80
1:A:391:CYS:O	1:A:395:GLU:HG2	1.82	0.80
1:B:215:VAL:HB	1:B:330:LEU:HD23	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:LYS:O	1:A:243:GLU:HG3	1.84	0.77
1:A:293:GLU:HG3	1:A:294:LYS:N	1.97	0.77
1:A:31:LEU:HD11	1:A:74:LEU:HD22	1.67	0.77
1:B:391:CYS:O	1:B:395:GLU:HG2	1.86	0.76
1:B:23:VAL:HG12	1:B:43:VAL:HG22	1.69	0.75
1:A:115:LEU:HD11	1:A:140:GLU:HG2	1.70	0.74
1:B:309:ALA:HB2	1:B:373:PHE:CE1	2.23	0.74
1:B:516:PRO:HD3	3:B:719:HOH:O	1.87	0.72
1:A:561:ASP:HB2	3:A:836:HOH:O	1.87	0.72
1:B:414:VAL:HG12	1:B:417:VAL:HG23	1.71	0.72
1:A:301:LEU:HB3	1:A:336:ARG:NH1	2.05	0.72
1:A:95:GLU:HA	1:A:95:GLU:OE2	1.90	0.71
1:B:158:ASN:ND2	1:B:283:LEU:HD12	2.05	0.71
1:B:297:ILE:HG13	3:B:754:HOH:O	1.90	0.71
1:A:210:LEU:O	1:A:213:TRP:HB3	1.90	0.71
1:A:86:ASP:OD2	1:A:105:HIS:NE2	2.23	0.71
1:A:39:HIS:CG	3:A:834:HOH:O	2.44	0.71
1:A:374:ASP:OD1	1:A:374:ASP:N	2.23	0.71
1:B:316:LYS:HG3	3:B:717:HOH:O	1.90	0.71
1:A:390:ASN:OD1	1:A:409:ARG:NH2	2.24	0.70
1:B:441:GLU:HA	1:B:444:ARG:HD3	1.73	0.70
1:A:293:GLU:HG3	1:A:294:LYS:H	1.57	0.70
1:B:427:ARG:HD2	1:B:525:GLN:OE1	1.91	0.70
1:A:23:VAL:HG12	1:A:43:VAL:HG22	1.74	0.69
1:B:46:LEU:HD21	1:B:73:GLU:HG3	1.74	0.69
1:B:271:SER:HA	1:B:295:ASP:OD2	1.91	0.69
1:A:579:GLN:O	1:A:583:ALA:HB3	1.91	0.68
1:A:451:TYR:HD2	3:A:812:HOH:O	1.75	0.68
1:A:20:LYS:NZ	1:A:44:ASN:OD1	2.26	0.68
1:A:218:LEU:HD12	1:A:234:VAL:HG23	1.75	0.67
1:A:445:MET:HB3	1:A:446:PRO:HD3	1.75	0.67
1:A:27:PHE:HB3	1:A:39:HIS:HD2	1.57	0.67
1:A:474:LYS:O	1:A:478:GLU:HB2	1.95	0.67
1:A:427:ARG:HD2	1:A:525:GLN:OE1	1.95	0.66
1:B:414:VAL:CG1	1:B:417:VAL:HG23	2.25	0.66
1:A:202:ILE:HD11	1:A:210:LEU:HD22	1.78	0.65
1:B:116:LYS:H	1:B:116:LYS:HD3	1.60	0.65
1:A:90:CYS:O	1:A:98:ARG:HG3	1.97	0.64
1:B:431:LYS:HD2	3:B:734:HOH:O	1.96	0.64
1:A:123:CYS:SG	1:A:173:LYS:HD2	2.38	0.64
1:A:471:LYS:NZ	1:A:491:THR:O	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:LYS:HD3	1:A:443:GLU:OE1	1.98	0.64
1:B:524:LYS:HG2	1:B:550:PHE:HE2	1.63	0.64
1:A:385:ASN:N	1:A:385:ASN:OD1	2.23	0.63
1:A:140:GLU:CG	1:A:144:ARG:HH12	2.02	0.63
1:A:228:VAL:HA	1:A:231:THR:OG1	1.99	0.63
1:B:35:PRO:HB2	3:B:759:HOH:O	1.97	0.63
1:B:414:VAL:HG12	1:B:414:VAL:O	1.97	0.63
1:A:496:TYR:N	3:A:848:HOH:O	2.31	0.63
1:A:451:TYR:CD2	3:A:812:HOH:O	2.49	0.62
1:A:503:GLU:CD	1:A:503:GLU:H	2.00	0.62
1:A:79:SER:O	1:A:83:THR:HB	1.98	0.62
1:B:132:LYS:HB2	3:B:707:HOH:O	1.99	0.62
1:B:81:ARG:HA	1:B:88:ALA:HB2	1.82	0.62
1:A:509:HIS:N	1:A:509:HIS:CD2	2.68	0.62
1:A:524:LYS:HG2	1:A:550:PHE:HE2	1.65	0.61
1:A:342:VAL:O	1:A:345:LEU:N	2.33	0.61
1:B:330:LEU:HD13	1:B:349:ALA:HB2	1.80	0.61
1:B:450:ASP:O	1:B:453:SER:HB3	2.00	0.61
1:A:544:LYS:O	1:A:548:GLU:HG3	1.99	0.61
1:A:381:ASP:N	1:A:381:ASP:OD1	2.32	0.61
1:A:382:GLU:HB3	1:A:383:PRO:HD3	1.83	0.60
1:B:106:LYS:HE2	1:B:146:PRO:O	2.02	0.60
1:B:134:TRP:HB2	1:B:161:ASN:HD21	1.66	0.60
1:B:30:TYR:HE1	1:B:103:LEU:HD23	1.66	0.60
1:B:200:ALA:O	1:B:204:LYS:HB2	2.01	0.60
1:B:106:LYS:HG2	1:B:146:PRO:HB2	1.84	0.59
1:A:126:PHE:O	1:A:130:GLU:HG3	2.03	0.59
1:A:495:THR:C	3:A:848:HOH:O	2.40	0.59
1:B:382:GLU:HB2	1:B:383:PRO:HD3	1.84	0.59
1:B:389:GLN:O	1:B:392:ASP:HB2	2.02	0.58
1:A:155:TYR:CE1	1:A:159:LYS:HE3	2.39	0.58
1:B:520:LYS:HD2	3:B:679:HOH:O	2.02	0.58
1:B:223:PRO:HG2	1:B:295:ASP:HB3	1.84	0.58
1:B:37:ASP:HB2	3:B:759:HOH:O	2.03	0.58
1:A:297:ILE:HG22	1:A:301:LEU:CD1	2.33	0.58
1:A:458:ARG:HG3	1:A:458:ARG:O	2.03	0.57
1:B:182:GLU:HG2	3:B:611:HOH:O	2.03	0.57
1:A:178:LEU:N	1:A:179:PRO:CD	2.67	0.57
1:B:415:PRO:O	1:B:533:LYS:HE2	2.04	0.57
1:B:374:ASP:N	1:B:374:ASP:OD1	2.37	0.57
1:A:309:ALA:O	1:A:369:TYR:HE2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:TYR:O	1:B:164:PHE:HD2	1.87	0.57
1:B:537:LYS:HD3	3:B:731:HOH:O	2.05	0.57
1:A:228:VAL:HG23	3:A:814:HOH:O	2.05	0.57
1:B:378:HIS:C	1:B:378:HIS:CD2	2.79	0.56
1:A:153:LEU:O	1:A:153:LEU:HD12	2.06	0.56
1:B:514:THR:O	1:B:514:THR:CG2	2.54	0.56
1:B:381:ASP:OD2	1:B:381:ASP:N	2.36	0.56
1:A:226:GLU:HG3	3:A:814:HOH:O	2.05	0.56
1:A:279:ASP:O	1:A:279:ASP:OD2	2.24	0.56
1:B:419:THR:HB	1:B:420:PRO:HD3	1.88	0.56
1:B:297:ILE:CG1	3:B:754:HOH:O	2.52	0.55
1:B:407:ILE:HG21	1:B:528:LEU:HG	1.88	0.55
1:B:514:THR:O	1:B:514:THR:HG22	2.06	0.55
1:A:409:ARG:NE	3:A:851:HOH:O	2.37	0.55
1:B:271:SER:HB3	1:B:274:LEU:HG	1.89	0.54
1:B:37:ASP:HA	1:B:40:VAL:HG23	1.89	0.54
1:B:484:ARG:HD2	1:B:484:ARG:C	2.27	0.54
1:A:220:GLN:HG2	1:A:338:PRO:HA	1.88	0.54
1:B:328:SER:O	1:B:332:GLU:HG2	2.08	0.54
1:A:39:HIS:CD2	3:A:834:HOH:O	2.61	0.54
1:A:95:GLU:OE2	1:A:96:PRO:HA	2.07	0.54
1:B:118:ASP:O	1:B:122:LEU:HG	2.08	0.54
1:A:399:GLU:OE1	1:A:434:THR:OG1	2.22	0.54
1:B:178:LEU:HB2	1:B:179:PRO:HD3	1.90	0.54
1:A:524:LYS:HG2	1:A:550:PHE:CE2	2.43	0.54
1:A:337:HIS:HA	1:A:339:GLU:OE1	2.08	0.54
1:A:372:VAL:O	1:A:375:LYS:HB2	2.08	0.53
1:B:309:ALA:HB2	1:B:373:PHE:HE1	1.73	0.53
1:B:342:VAL:O	1:B:343:SER:C	2.46	0.53
1:B:299:GLU:N	3:B:758:HOH:O	2.40	0.53
1:A:311:ASP:C	1:A:313:ASP:H	2.11	0.53
1:A:52:THR:HG23	3:A:724:HOH:O	2.09	0.53
1:B:313:ASP:HA	3:B:717:HOH:O	2.08	0.53
1:A:481:VAL:HG22	1:A:481:VAL:O	2.09	0.52
1:A:506:PHE:HB3	2:A:601:PGE:H6	1.90	0.52
1:B:344:VAL:O	1:B:348:LEU:HG	2.10	0.52
1:B:226:GLU:OE1	1:B:226:GLU:HA	2.09	0.52
1:A:148:PHE:CD2	1:A:192:SER:HB2	2.45	0.52
1:B:336:ARG:HB3	3:B:709:HOH:O	2.10	0.52
1:B:167:CYS:HB3	1:B:177:LEU:HD12	1.91	0.52
1:B:444:ARG:O	1:B:448:THR:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:582:LEU:O	1:B:583:ALA:C	2.48	0.51
1:B:319:GLN:HA	1:B:319:GLN:NE2	2.26	0.51
1:B:321:ALA:HA	3:B:753:HOH:O	2.11	0.51
1:B:71:GLY:HA2	1:B:74:LEU:HD12	1.92	0.51
1:A:285:LYS:O	1:A:289:ILE:HG13	2.10	0.51
1:A:531:LEU:HD22	2:A:601:PGE:H4	1.91	0.51
1:B:248:ASP:HB3	1:B:251:GLU:CG	2.41	0.51
1:A:112:LEU:HB2	3:A:711:HOH:O	2.11	0.51
1:A:218:LEU:HD12	1:A:234:VAL:CG2	2.40	0.51
1:A:202:ILE:CD1	1:A:210:LEU:HD22	2.41	0.50
1:B:373:PHE:HA	1:B:376:LEU:HB2	1.93	0.50
1:B:445:MET:N	1:B:446:PRO:HD2	2.27	0.50
1:B:515:LEU:N	3:B:679:HOH:O	2.43	0.50
1:A:208:ARG:HB2	3:A:773:HOH:O	2.12	0.50
1:A:477:THR:HG22	3:A:776:HOH:O	2.11	0.50
1:B:151:PRO:HB2	1:B:256:ARG:HH11	1.74	0.50
1:A:511:ASP:O	1:A:514:THR:N	2.42	0.50
1:B:126:PHE:HZ	1:B:165:GLN:CG	2.25	0.50
1:A:280:LYS:HB3	1:A:281:PRO:CD	2.42	0.50
1:A:73:GLU:OE1	1:A:76:LYS:NZ	2.45	0.50
1:B:158:ASN:HD21	1:B:283:LEU:HD12	1.76	0.50
1:A:382:GLU:HB3	1:A:383:PRO:CD	2.42	0.50
1:B:29:GLN:HG2	1:B:146:PRO:HA	1.94	0.50
1:B:67:HIS:NE2	1:B:248:ASP:OD1	2.40	0.50
1:B:111:ASP:OD1	1:B:111:ASP:O	2.30	0.49
1:B:537:LYS:HB2	3:B:755:HOH:O	2.12	0.49
1:A:26:ALA:HB2	1:A:249:LEU:HD12	1.94	0.49
1:A:412:ARG:HB3	1:A:492:PRO:HB3	1.94	0.49
1:A:56:ASP:OD2	1:A:59:HIS:HB2	2.13	0.49
1:B:140:GLU:OE1	1:B:144:ARG:NH1	2.35	0.49
1:B:232:LYS:HG3	3:B:624:HOH:O	2.13	0.49
1:A:115:LEU:O	1:A:117:PRO:HD3	2.13	0.49
1:B:407:ILE:CG2	1:B:528:LEU:HG	2.43	0.49
1:A:421:THR:O	1:A:425:VAL:HG23	2.13	0.49
1:B:501:PHE:HB2	1:B:534:HIS:CE1	2.48	0.48
1:B:213:TRP:HZ2	1:B:217:ARG:HH11	1.62	0.48
1:A:409:ARG:HD2	3:A:847:HOH:O	2.13	0.48
1:B:544:LYS:HG3	3:B:643:HOH:O	2.13	0.48
1:A:126:PHE:CE1	1:A:130:GLU:HG2	2.49	0.48
1:B:26:ALA:HB2	1:B:249:LEU:HD12	1.96	0.48
1:A:282:LEU:HG	3:A:859:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:LYS:HG2	1:B:116:LYS:O	2.14	0.48
1:A:63:GLU:OE2	1:A:63:GLU:N	2.42	0.48
1:A:419:THR:HG21	1:A:526:THR:HG23	1.96	0.48
1:B:213:TRP:HZ2	1:B:217:ARG:NH1	2.11	0.48
1:B:473:THR:O	1:B:477:THR:HG23	2.13	0.48
1:B:202:ILE:HD11	1:B:210:LEU:HD22	1.96	0.47
1:A:267:GLN:HG2	1:A:274:LEU:HB2	1.96	0.47
1:B:529:VAL:O	1:B:533:LYS:HG3	2.15	0.47
1:B:134:TRP:HB2	1:B:161:ASN:ND2	2.29	0.47
1:A:210:LEU:HD23	1:A:238:THR:HG23	1.97	0.47
1:B:151:PRO:HB2	1:B:256:ARG:NH1	2.30	0.47
1:A:306:ALA:HA	1:A:310:GLU:OE1	2.16	0.46
1:A:520:LYS:HE3	3:A:747:HOH:O	2.14	0.46
1:A:309:ALA:O	1:A:369:TYR:CE2	2.68	0.46
1:B:185:ARG:CZ	1:B:189:LEU:HD11	2.46	0.46
1:B:429:LEU:HA	1:B:429:LEU:HD23	1.60	0.46
1:A:407:ILE:CD1	1:A:525:GLN:HB3	2.45	0.46
1:B:248:ASP:HB3	1:B:251:GLU:CD	2.36	0.46
1:B:440:PRO:HB2	1:B:443:GLU:OE2	2.15	0.46
1:A:351:GLU:OE2	1:A:375:LYS:NZ	2.39	0.46
1:B:447:CYS:SG	1:B:447:CYS:O	2.67	0.46
1:B:493:ASP:OD2	1:B:495:THR:OG1	2.33	0.45
1:B:449:GLU:HA	1:B:449:GLU:OE2	2.16	0.45
1:B:302:PRO:O	1:B:336:ARG:NH1	2.49	0.45
1:A:217:ARG:NH1	3:A:804:HOH:O	2.49	0.45
1:B:223:PRO:HD2	1:B:295:ASP:CB	2.47	0.45
1:B:582:LEU:HA	1:B:582:LEU:HD23	1.72	0.45
1:A:8:ALA:O	1:A:12:LYS:HE3	2.16	0.45
1:A:228:VAL:CA	1:A:231:THR:OG1	2.64	0.45
1:B:414:VAL:HG12	1:B:417:VAL:CG2	2.44	0.45
1:A:409:ARG:CD	3:A:847:HOH:O	2.65	0.44
1:B:308:PHE:HE2	1:B:332:GLU:HG3	1.83	0.44
1:A:399:GLU:OE2	1:A:431:LYS:HG2	2.18	0.44
1:B:399:GLU:O	1:B:403:GLN:HG3	2.17	0.44
1:A:293:GLU:CG	1:A:294:LYS:N	2.76	0.44
1:B:423:VAL:HG12	1:B:427:ARG:HD3	1.99	0.44
1:A:110:PRO:O	1:A:111:ASP:HB3	2.16	0.44
1:A:280:LYS:HB3	1:A:281:PRO:HD2	1.99	0.44
1:A:80:LEU:O	1:A:84:TYR:N	2.47	0.44
1:B:13:ASP:HB3	3:B:667:HOH:O	2.17	0.44
1:B:208:ARG:HG2	3:B:691:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ILE:HG22	1:A:301:LEU:HD13	1.99	0.44
1:B:57:GLU:OE2	1:B:57:GLU:HA	2.17	0.43
1:A:264:CYS:SG	1:A:285:LYS:HD2	2.58	0.43
1:A:219:SER:HB2	1:A:334:SER:HB2	2.00	0.43
1:B:371:THR:O	1:B:373:PHE:N	2.51	0.43
1:B:385:ASN:ND2	1:B:385:ASN:N	2.66	0.43
1:A:161:ASN:ND2	3:A:769:HOH:O	2.50	0.43
1:A:452:LEU:HA	1:A:452:LEU:HD23	1.68	0.43
1:B:386:LEU:HG	1:B:387:ILE:N	2.32	0.43
1:B:389:GLN:HG3	1:B:390:ASN:N	2.34	0.43
1:A:227:PHE:O	1:A:231:THR:OG1	2.27	0.43
1:A:157:ALA:O	1:A:160:TYR:HB3	2.18	0.43
1:A:36:PHE:O	1:A:40:VAL:HG23	2.18	0.43
1:A:412:ARG:HH11	1:A:412:ARG:HD2	1.68	0.43
1:B:326:LEU:HD21	1:B:353:GLU:HB2	2.01	0.43
1:A:53:CYS:O	1:A:57:GLU:HG3	2.19	0.43
1:B:236:ASP:O	1:B:240:VAL:HG23	2.19	0.43
1:B:515:LEU:HA	1:B:516:PRO:HD2	1.88	0.43
1:A:112:LEU:HA	1:A:112:LEU:HD23	1.77	0.42
1:A:213:TRP:HE3	1:A:214:SER:HG	1.63	0.42
1:A:342:VAL:O	1:A:343:SER:C	2.55	0.42
1:A:392:ASP:O	1:A:396:LYS:HB2	2.19	0.42
1:A:414:VAL:N	1:A:415:PRO:HD3	2.34	0.42
1:A:417:VAL:O	1:A:533:LYS:NZ	2.47	0.42
1:B:353:GLU:HG2	1:B:354:ALA:N	2.34	0.42
1:B:541:GLU:CD	1:B:541:GLU:H	2.23	0.42
1:A:547:MET:CE	3:A:862:HOH:O	2.67	0.42
1:B:126:PHE:HZ	1:B:165:GLN:HG2	1.85	0.42
1:B:339:GLU:HG2	1:B:340:TYR:N	2.34	0.42
1:B:403:GLN:HG2	1:B:430:GLY:HA3	2.01	0.42
1:B:126:PHE:HZ	1:B:165:GLN:HG3	1.85	0.42
1:B:223:PRO:HB2	1:B:297:ILE:HA	2.01	0.42
1:B:414:VAL:CG1	1:B:417:VAL:CG2	2.95	0.42
1:B:539:THR:OG1	1:B:542:GLN:HG3	2.19	0.42
1:A:366:HIS:O	1:A:370:SER:HB3	2.20	0.42
1:B:377:LYS:O	1:B:381:ASP:OD2	2.37	0.42
1:B:511:ASP:OD2	1:B:512:ILE:N	2.53	0.42
1:A:153:LEU:HD13	1:A:153:LEU:HA	1.81	0.42
1:A:408:VAL:CG1	1:A:412:ARG:NH1	2.83	0.41
1:B:519:GLU:CG	3:B:722:HOH:O	2.42	0.41
1:A:131:LYS:O	1:A:134:TRP:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:VAL:O	1:A:429:LEU:HG	2.20	0.41
1:A:66:LEU:O	1:A:70:PHE:HD2	2.03	0.41
1:B:305:THR:HB	1:B:310:GLU:HG3	2.01	0.41
1:A:460:CYS:O	1:A:464:GLU:N	2.42	0.41
1:B:223:PRO:HB2	1:B:298:PRO:HD2	2.02	0.41
1:A:328:SER:O	1:A:332:GLU:HG2	2.20	0.41
1:A:331:TYR:OH	1:A:335:ARG:CZ	2.69	0.41
1:A:495:THR:CA	3:A:848:HOH:O	2.68	0.41
1:B:431:LYS:HB3	1:B:431:LYS:HE2	1.82	0.41
1:A:298:PRO:O	1:A:301:LEU:HD11	2.15	0.41
1:A:274:LEU:O	1:A:277:CYS:HB2	2.21	0.41
1:A:24:LEU:HB2	1:A:43:VAL:HG21	2.01	0.41
1:B:464:GLU:O	1:B:464:GLU:OE2	2.38	0.41
1:A:387:ILE:HD11	1:A:445:MET:HG2	2.03	0.41
1:B:330:LEU:CD1	1:B:349:ALA:HB2	2.46	0.41
1:A:112:LEU:HA	1:A:113:PRO:HD2	1.90	0.41
1:A:171:GLU:N	1:A:171:GLU:OE2	2.42	0.41
1:A:200:ALA:O	1:A:204:LYS:HB2	2.21	0.41
1:B:152:GLU:O	1:B:155:TYR:HB3	2.21	0.41
1:A:579:GLN:OE1	3:A:806:HOH:O	2.22	0.40
1:A:159:LYS:HA	1:A:159:LYS:HD3	1.81	0.40
1:B:267:GLN:CG	1:B:274:LEU:HB2	2.51	0.40
1:B:378:HIS:O	1:B:382:GLU:HG3	2.21	0.40
1:B:377:LYS:HD3	1:B:377:LYS:HA	1.77	0.40
1:A:437:CYS:HA	1:A:444:ARG:HD3	2.03	0.40
1:A:501:PHE:HB2	1:A:534:HIS:CE1	2.56	0.40
1:B:173:LYS:HB2	1:B:173:LYS:HE2	1.86	0.40
1:B:213:TRP:CZ2	1:B:217:ARG:HD2	2.57	0.40
1:B:223:PRO:CG	1:B:295:ASP:HB3	2.51	0.40
1:B:131:LYS:HA	1:B:131:LYS:HD2	1.80	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	584/583 (100%)	545 (93%)	38 (6%)	1 (0%)	47	66
1	B	583/583 (100%)	532 (91%)	51 (9%)	0	100	100
All	All	1167/1166 (100%)	1077 (92%)	89 (8%)	1 (0%)	51	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	ASP

### 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	524/521 (101%)	478 (91%)	46 (9%)	10	18
1	B	523/521 (100%)	473 (90%)	50 (10%)	8	15
All	All	1047/1042 (100%)	951 (91%)	96 (9%)	9	16

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	65[A]	SER
1	A	65[B]	SER
1	A	86	ASP
1	A	111	ASP
1	A	118	ASP
1	A	121	THR
1	A	126	PHE
1	A	139	TYR
1	A	153	LEU
1	A	165	GLN
1	A	181	ILE

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Mol	Chain	Res	Type
1	A	191	SER
1	A	192	SER
1	A	204	LYS
1	A	224	LYS
1	A	231	THR
1	A	265	ASP
1	A	282	LEU
1	A	292	VAL
1	A	301	LEU
1	A	305	THR
1	A	311	ASP
1	A	312	LYS
1	A	316	LYS
1	A	358	GLU
1	A	374	ASP
1	A	377	LYS
1	A	379	LEU
1	A	381	ASP
1	A	383	PRO
1	A	385	ASN
1	A	409	ARG
1	A	438	THR
1	A	440	PRO
1	A	441	GLU
1	A	450	ASP
1	A	458	ARG
1	A	464	GLU
1	A	469	SER
1	A	479	SER
1	A	517	ASP
1	A	520	LYS
1	A	532	LEU
1	A	540	GLU
1	A	541	GLU
1	B	2	THR
1	B	54	VAL
1	B	58	SER
1	B	86	ASP
1	B	98	ARG
1	B	116	LYS
1	B	149	TYR
1	B	166	GLU

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Mol	Chain	Res	Type
1	B	191	SER
1	B	208	ARG
1	B	214	SER
1	B	229	GLU
1	B	244	CYS
1	B	268	ASP
1	B	280	LYS
1	B	286	SER
1	B	291	GLU
1	B	299	GLU
1	B	320	GLU
1	B	326	LEU
1	B	336	ARG
1	B	339	GLU
1	B	343	SER
1	B	350	LYS
1	B	359	CYS
1	B	364	ASP
1	B	370	SER
1	B	371	THR
1	B	374	ASP
1	B	375	LYS
1	B	378	HIS
1	B	379	LEU
1	B	385	ASN
1	B	386	LEU
1	B	387	ILE
1	B	389	GLN
1	B	392	ASP
1	B	396	LYS
1	B	407	ILE
1	B	410	TYR
1	B	431	LYS
1	B	447	CYS
1	B	464	GLU
1	B	478	GLU
1	B	484	ARG
1	B	507	THR
1	B	519	GLU
1	B	553	PHE
1	B	561	ASP
1	B	564	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	319	GLN
1	A	337	HIS
1	A	509	HIS
1	B	267	GLN
1	B	319	GLN
1	B	337	HIS
1	B	378	HIS
1	B	385	ASN
1	B	549	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	$\# Z  > 2$
2	PGE	A	601	-	9,9,9	0.54	0	8,8,8	0.45	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	PGE	A	601	-	-	4/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	PGE	O2-C3-C4-O3
2	A	601	PGE	O1-C1-C2-O2
2	A	601	PGE	C3-C4-O3-C5
2	A	601	PGE	O3-C5-C6-O4

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	PGE	2	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](#)

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	583/583 (100%)	-0.19	6 (1%) 82 84	47, 68, 96, 118	0
1	B	583/583 (100%)	-0.11	3 (0%) 91 91	50, 74, 107, 127	0
All	All	1166/1166 (100%)	-0.15	9 (0%) 86 87	47, 71, 102, 127	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	ASP	5.5
1	A	2	THR	5.2
1	A	1	ASP	4.2
1	A	3	HIS	3.3
1	B	304	LEU	3.2
1	A	84	TYR	2.4
1	A	83	THR	2.2
1	A	80	LEU	2.1
1	B	314	VAL	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. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PGE	A	601	10/10	0.90	0.24	61,65,66,69	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.