



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:03 AM GMT

PDB ID : 2ZCH  
Title : Crystal structure of human prostate specific antigen complexed with an activating antibody  
Authors : Menez, R.; Stura, E.; Jolivet-Reynaud, C.  
Deposited on : 2007-11-08  
Resolution : 2.83 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

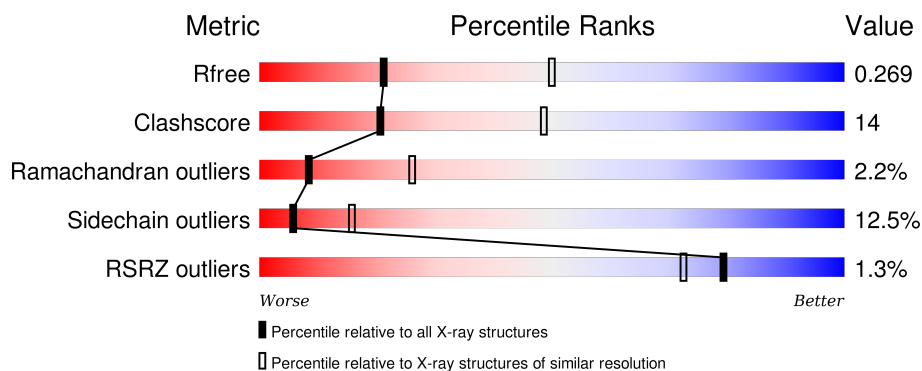
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.83 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3170 (2.88-2.80)
Clashscore	102246	3658 (2.88-2.80)
Ramachandran outliers	100387	3591 (2.88-2.80)
Sidechain outliers	100360	3594 (2.88-2.80)
RSRZ outliers	91569	3184 (2.88-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	P	237	<div> <div>74%</div> <div>22%</div> <div>• •</div> </div>
2	L	215	<div> <div>68%</div> <div>24%</div> <div>7%</div> <div>•</div> </div>
3	H	229	<div> <div>67%</div> <div>26%</div> <div>6%</div> <div>•</div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5290 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 Prostate-specific antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	237	Total	C	N	O	S	0	0	0
			1832	1162	323	333	14			

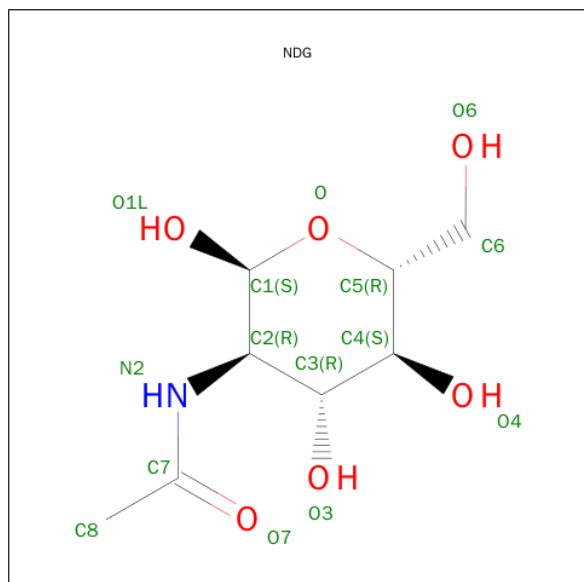
- Molecule 2 is a protein called monoclonal antibody 8G8F5 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	215	Total	C	N	O	S	0	0	0
			1648	1024	275	343	6			

- Molecule 3 is a protein called monoclonal antibody 8G8F5 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	229	Total	C	N	O	S	0	0	0
			1708	1071	279	347	11			

- Molecule 4 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

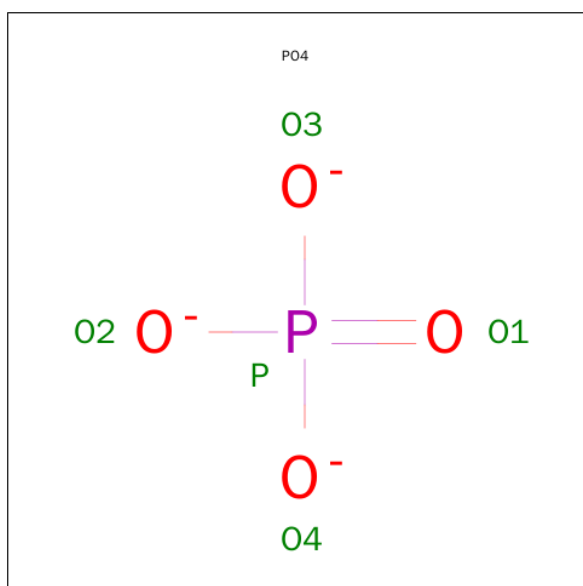


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	P	1	Total	C	N	O	0	0
			15	8	1	6		
4	P	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	1	Total	Cl	0	0
			1	1		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	O	P	0	0
			5	4	1		

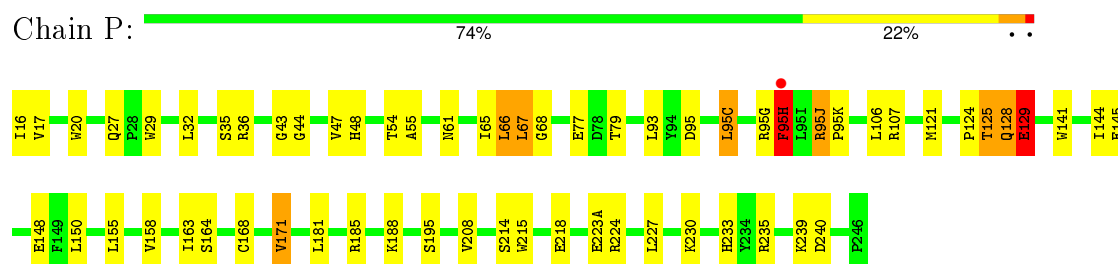
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	P	33	Total	O	0	0
			33	33		
7	L	20	Total	O	0	0
			20	20		
7	H	13	Total	O	0	0
			13	13		

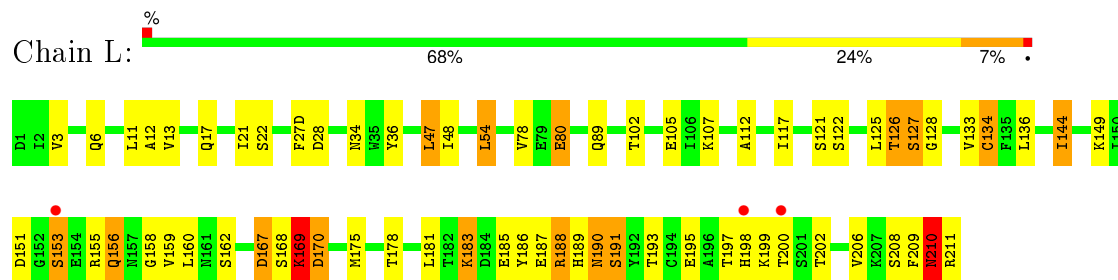
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

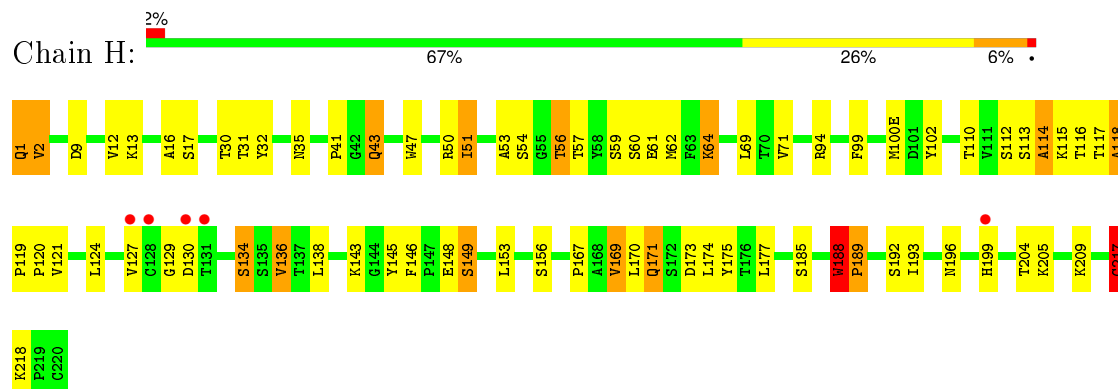
#### • Molecule 1: Prostate-specific antigen



#### • Molecule 2: monoclonal antibody 8G8F5 Fab



#### • Molecule 3: monoclonal antibody 8G8F5 Fab



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.36 Å 87.36 Å 236.33 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.81 – 2.83 78.78 – 2.83	Depositor EDS
% Data completeness (in resolution range)	100.0 (78.81-2.83) 100.0 (78.78-2.83)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.49 (at 2.81 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.203 , 0.270 0.209 , 0.269	Depositor DCC
$R_{free}$ test set	1163 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.7	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 52.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 22783 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5290	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, NDG, CL

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	P	0.85	0/1883	0.87	1/2564 (0.0%)
2	L	0.82	2/1684 (0.1%)	0.86	2/2288 (0.1%)
3	H	0.89	1/1749 (0.1%)	0.93	2/2387 (0.1%)
All	All	0.85	3/5316 (0.1%)	0.89	5/7239 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	H	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	80	GLU	CG-CD	5.50	1.60	1.51
2	L	80	GLU	CD-OE1	5.19	1.31	1.25
3	H	217	CYS	CB-SG	-5.14	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	H	188	TRP	C-N-CD	-10.83	96.78	120.60
1	P	95(H)	PHE	CB-CA-C	6.13	122.66	110.40
3	H	188	TRP	C-N-CA	6.12	147.69	122.00
2	L	54	LEU	CA-CB-CG	6.08	129.28	115.30
2	L	54	LEU	CB-CG-CD1	5.34	120.07	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	188	TRP	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	1832	0	1804	49	0
2	L	1648	0	1571	53	0
3	H	1708	0	1655	55	0
4	P	30	0	30	6	0
5	P	1	0	0	1	0
6	H	5	0	0	0	0
7	H	13	0	0	0	0
7	L	20	0	0	0	0
7	P	33	0	0	2	0
All	All	5290	0	5060	149	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 14.

All (149) 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)
3:H:117:THR:O	3:H:118:ALA:HB3	1.75	0.85
3:H:35:ASN:HD22	3:H:47:TRP:HE1	1.22	0.85
3:H:13:LYS:NZ	3:H:113:SER:O	2.09	0.85
3:H:136:VAL:HG23	3:H:185:SER:HA	1.60	0.82
3:H:120:PRO:HD2	3:H:143:LYS:O	1.82	0.80
2:L:126:THR:HG22	2:L:126:THR:O	1.85	0.77
3:H:51:ILE:HG12	3:H:57:THR:CG2	2.17	0.75
1:P:48:HIS:NE2	5:P:2001:CL:CL	2.57	0.74
3:H:188:TRP:CE3	3:H:189:PRO:HD3	2.22	0.74
3:H:156:SER:H	3:H:196:ASN:HD21	1.36	0.73
2:L:112:ALA:HB2	2:L:200:THR:HG21	1.71	0.72
3:H:35:ASN:ND2	3:H:47:TRP:HE1	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:117:THR:O	3:H:118:ALA:CB	2.37	0.70
2:L:149:LYS:HB2	2:L:153:SER:O	1.91	0.70
1:P:215:TRP:CZ2	1:P:227:LEU:HD13	2.25	0.70
2:L:183:LYS:O	2:L:187:GLU:HG2	1.90	0.70
3:H:51:ILE:HG12	3:H:57:THR:HG22	1.72	0.70
1:P:61:ASN:CG	4:P:401:NDG:H6C1	2.12	0.69
3:H:136:VAL:CG2	3:H:185:SER:HA	2.22	0.69
1:P:61:ASN:ND2	4:P:401:NDG:H6C1	2.08	0.67
3:H:31:THR:HG22	3:H:32:TYR:CD2	2.29	0.67
3:H:31:THR:HG22	3:H:32:TYR:CE2	2.30	0.67
3:H:54:SER:OG	3:H:56:THR:HG23	1.95	0.66
2:L:190:ASN:O	2:L:210:ASN:O	2.14	0.65
2:L:209:PHE:HB2	3:H:127:VAL:HG21	1.78	0.64
2:L:198:HIS:HD2	2:L:200:THR:HB	1.62	0.63
2:L:13:VAL:HG11	2:L:78:VAL:HG21	1.79	0.63
1:P:233:HIS:HD2	3:H:99:PHE:H	1.46	0.61
2:L:193:THR:HB	2:L:208:SER:OG	2.03	0.59
1:P:144:ILE:O	1:P:144:ILE:HG22	2.02	0.59
2:L:133:VAL:HG12	2:L:178:THR:HG23	1.85	0.59
2:L:210:ASN:HD22	2:L:210:ASN:H	1.50	0.58
2:L:125:LEU:C	2:L:127:SER:H	2.04	0.58
3:H:134:SER:O	3:H:185:SER:HB2	2.04	0.57
2:L:159:VAL:O	2:L:160:LEU:HD12	2.04	0.57
1:P:145:GLU:HB2	1:P:148:GLU:O	2.04	0.57
2:L:128:GLY:O	2:L:183:LYS:HB2	2.04	0.57
3:H:188:TRP:CD2	3:H:189:PRO:HD3	2.40	0.57
1:P:32:LEU:HB3	1:P:66:LEU:CD2	2.34	0.57
1:P:32:LEU:HB3	1:P:66:LEU:HD21	1.87	0.57
1:P:171:VAL:HG21	1:P:223(A):GLU:O	2.05	0.56
1:P:239:LYS:HE2	1:P:240:ASP:OD1	2.06	0.55
2:L:126:THR:CG2	2:L:126:THR:O	2.55	0.55
3:H:113:SER:O	3:H:114:ALA:O	2.25	0.55
2:L:155:ARG:HE	2:L:158:GLY:H	1.55	0.55
3:H:12:VAL:HG22	3:H:16:ALA:HB3	1.89	0.55
1:P:171:VAL:HG22	1:P:224:ARG:HE	1.72	0.54
2:L:12:ALA:HA	2:L:105:GLU:O	2.07	0.54
3:H:127:VAL:HG22	3:H:129:GLY:H	1.72	0.54
1:P:27:GLN:NE2	7:P:2005:HOH:O	2.40	0.54
3:H:153:LEU:HD13	3:H:156:SER:HA	1.91	0.53
1:P:125:THR:HG22	1:P:128:GLN:HB2	1.90	0.53
2:L:210:ASN:O	2:L:211:ARG:CB	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:61:ASN:ND2	4:P:401:NDG:C6	2.71	0.53
1:P:128:GLN:O	1:P:129:GLU:CB	2.57	0.53
2:L:168:SER:O	2:L:169:LYS:HB3	2.09	0.53
2:L:198:HIS:CD2	2:L:200:THR:HB	2.43	0.52
1:P:233:HIS:HD2	3:H:99:PHE:N	2.07	0.52
1:P:43:GLY:O	1:P:54:THR:HG22	2.09	0.52
1:P:29:TRP:CE2	1:P:121:MET:CE	2.93	0.51
1:P:239:LYS:HD3	2:L:27(D):PHE:CE2	2.46	0.51
2:L:34:ASN:HD22	2:L:89:GLN:HE22	1.58	0.51
1:P:235:ARG:NH1	2:L:28:ASP:OD2	2.44	0.51
2:L:11:LEU:HD21	2:L:13:VAL:HG23	1.91	0.50
1:P:29:TRP:CE2	1:P:121:MET:HE3	2.46	0.50
1:P:67:LEU:N	1:P:67:LEU:HD23	2.27	0.50
1:P:185:ARG:HG3	1:P:188:LYS:HG3	1.94	0.50
1:P:68:GLY:O	1:P:79:THR:HG23	2.12	0.50
3:H:1:GLN:OE1	3:H:1:GLN:N	2.39	0.50
3:H:148:GLU:HG2	3:H:175:TYR:CE2	2.46	0.50
2:L:112:ALA:CB	2:L:200:THR:HG21	2.39	0.50
2:L:11:LEU:CD2	2:L:13:VAL:HG23	2.42	0.50
2:L:160:LEU:HD21	3:H:171:GLN:HB3	1.94	0.49
1:P:77:GLU:C	1:P:79:THR:H	2.16	0.49
1:P:128:GLN:O	1:P:129:GLU:HB3	2.12	0.49
2:L:210:ASN:O	2:L:211:ARG:HB3	2.13	0.48
3:H:61:GLU:HG3	3:H:62:MET:N	2.28	0.48
2:L:21:ILE:HD12	2:L:102:THR:HG21	1.96	0.48
3:H:2:VAL:CG2	3:H:102:TYR:CD2	2.97	0.48
3:H:1:GLN:CD	3:H:1:GLN:H3	2.16	0.48
3:H:148:GLU:O	3:H:149:SER:CB	2.61	0.48
3:H:2:VAL:HG21	3:H:102:TYR:CD2	2.49	0.48
3:H:192:SER:HB2	3:H:209:LYS:HE3	1.97	0.47
3:H:1:GLN:CD	3:H:1:GLN:N	2.67	0.47
2:L:195:GLU:HB2	2:L:206:VAL:HG12	1.96	0.47
2:L:160:LEU:HD23	3:H:169:VAL:CG1	2.44	0.47
1:P:107:ARG:HD3	7:P:2027:HOH:O	2.14	0.47
3:H:170:LEU:HD13	3:H:175:TYR:CE1	2.49	0.47
1:P:61:ASN:OD1	4:P:401:NDG:O	2.33	0.47
1:P:47:VAL:O	1:P:48:HIS:CD2	2.68	0.47
1:P:230:LYS:HD2	1:P:233:HIS:CE1	2.49	0.47
3:H:51:ILE:HG12	3:H:57:THR:HG23	1.93	0.46
2:L:144:ILE:HD12	2:L:175:MET:CE	2.45	0.46
2:L:36:TYR:HE2	2:L:89:GLN:HE21	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:136:LEU:N	2:L:136:LEU:HD12	2.31	0.46
1:P:29:TRP:CZ2	1:P:121:MET:CE	2.99	0.46
3:H:153:LEU:HB2	3:H:196:ASN:HD22	1.81	0.46
2:L:117:ILE:HD12	2:L:134:CYS:CB	2.46	0.46
3:H:59:SER:HB2	3:H:64:LYS:HE3	1.97	0.45
3:H:188:TRP:CD1	3:H:193:ILE:HD12	2.51	0.45
2:L:47:LEU:HB3	2:L:48:ILE:HD12	1.98	0.45
1:P:16:ILE:HG21	1:P:158:VAL:HB	1.98	0.45
2:L:187:GLU:OE2	2:L:211:ARG:NH2	2.49	0.45
1:P:32:LEU:HB2	1:P:141:TRP:CZ3	2.50	0.45
1:P:215:TRP:CE2	1:P:227:LEU:HD13	2.52	0.44
2:L:155:ARG:HD2	2:L:156:GLN:H	1.81	0.44
3:H:30:THR:HB	3:H:53:ALA:HB2	1.99	0.44
3:H:153:LEU:CB	3:H:196:ASN:HD22	2.31	0.44
4:P:401:NDG:H8C1	4:P:403:NDG:C8	2.47	0.44
2:L:186:TYR:O	2:L:188:ARG:O	2.36	0.44
1:P:95:ASP:O	1:P:95(C):LEU:HB2	2.18	0.44
3:H:69:LEU:HD23	3:H:69:LEU:N	2.31	0.44
3:H:119:PRO:HB3	3:H:145:TYR:HB3	2.00	0.43
1:P:95(J):ARG:HB2	1:P:95(K):PRO:CD	2.47	0.43
2:L:167:ASP:OD1	2:L:169:LYS:N	2.51	0.43
1:P:27:GLN:NE2	1:P:29:TRP:CZ2	2.86	0.43
2:L:117:ILE:HD12	2:L:134:CYS:HB3	2.00	0.43
1:P:124:PRO:O	1:P:235:ARG:HD2	2.18	0.43
2:L:136:LEU:HD22	2:L:175:MET:HE3	2.01	0.43
2:L:6:GLN:HA	2:L:22:SER:O	2.19	0.43
3:H:199:HIS:HB3	3:H:204:THR:HB	2.01	0.43
1:P:54:THR:HB	1:P:55:ALA:H	1.70	0.43
2:L:162:SER:OG	3:H:167:PRO:HG2	2.18	0.43
3:H:51:ILE:CG1	3:H:57:THR:HG22	2.46	0.42
2:L:151:ASP:HA	2:L:191:SER:HB3	2.01	0.42
2:L:168:SER:O	2:L:169:LYS:CB	2.67	0.42
1:P:95(J):ARG:HB2	1:P:95(K):PRO:HD2	2.01	0.42
1:P:77:GLU:HB3	1:P:79:THR:HG22	2.01	0.42
3:H:156:SER:N	3:H:196:ASN:HD21	2.11	0.42
1:P:66:LEU:HD13	1:P:66:LEU:N	2.34	0.42
3:H:51:ILE:HD12	3:H:71:VAL:HG13	2.02	0.42
1:P:65:ILE:HG22	1:P:67:LEU:HD21	2.01	0.42
2:L:21:ILE:CD1	2:L:102:THR:HG21	2.50	0.42
2:L:133:VAL:HG21	3:H:124:LEU:HD13	2.01	0.41
2:L:34:ASN:HD22	2:L:89:GLN:NE2	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:61:ASN:OD1	4:P:401:NDG:H6C1	2.21	0.41
3:H:94:ARG:O	3:H:100(E):MET:HA	2.21	0.41
1:P:95(G):ARG:O	1:P:95(H):PHE:HB3	2.20	0.41
3:H:41:PRO:O	3:H:43:GLN:NE2	2.49	0.41
1:P:171:VAL:HG22	1:P:224:ARG:NE	2.35	0.41
2:L:11:LEU:HD23	2:L:12:ALA:N	2.35	0.41
2:L:187:GLU:OE2	2:L:187:GLU:HA	2.21	0.41
2:L:155:ARG:HE	2:L:158:GLY:N	2.17	0.41
3:H:146:PHE:HB2	3:H:174:LEU:HD22	2.01	0.41
2:L:125:LEU:C	2:L:127:SER:N	2.72	0.40
3:H:113:SER:O	3:H:114:ALA:C	2.59	0.40
1:P:44:GLY:HA2	1:P:54:THR:HG22	2.04	0.40
3:H:170:LEU:HD12	3:H:174:LEU:O	2.21	0.40
1:P:20:TRP:CZ3	1:P:158:VAL:HA	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	P	235/237 (99%)	216 (92%)	17 (7%)	2 (1%)	21	52
2	L	213/215 (99%)	189 (89%)	17 (8%)	7 (3%)	5	15
3	H	227/229 (99%)	198 (87%)	23 (10%)	6 (3%)	7	21
All	All	675/681 (99%)	603 (89%)	57 (8%)	15 (2%)	8	26

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	95(H)	PHE
2	L	169	LYS
3	H	149	SER

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Mol	Chain	Res	Type
3	H	189	PRO
2	L	126	THR
2	L	170	ASP
2	L	210	ASN
3	H	114	ALA
2	L	153	SER
2	L	156	GLN
3	H	217	CYS
1	P	129	GLU
2	L	189	HIS
3	H	116	THR
3	H	118	ALA

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	205/205 (100%)	181 (88%)	24 (12%)	7	18
2	L	186/186 (100%)	162 (87%)	24 (13%)	5	14
3	H	195/195 (100%)	170 (87%)	25 (13%)	5	15
All	All	586/586 (100%)	513 (88%)	73 (12%)	6	16

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	17	VAL
1	P	35	SER
1	P	36	ARG
1	P	66	LEU
1	P	67	LEU
1	P	93	LEU
1	P	95(C)	LEU
1	P	95(H)	PHE
1	P	95(J)	ARG
1	P	106	LEU

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Mol	Chain	Res	Type
1	P	125	THR
1	P	128	GLN
1	P	129	GLU
1	P	150	LEU
1	P	155	LEU
1	P	163	ILE
1	P	164	SER
1	P	168	CYS
1	P	171	VAL
1	P	181	LEU
1	P	195	SER
1	P	208	VAL
1	P	214	SER
1	P	218	GLU
2	L	3	VAL
2	L	17	GLN
2	L	47	LEU
2	L	54	LEU
2	L	80	GLU
2	L	107	LYS
2	L	121	SER
2	L	122	SER
2	L	127	SER
2	L	134	CYS
2	L	144	ILE
2	L	167	ASP
2	L	169	LYS
2	L	170	ASP
2	L	181	LEU
2	L	183	LYS
2	L	185	GLU
2	L	188	ARG
2	L	190	ASN
2	L	191	SER
2	L	197	THR
2	L	199	LYS
2	L	202	THR
2	L	210	ASN
3	H	1	GLN
3	H	2	VAL
3	H	9	ASP
3	H	17	SER

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Mol	Chain	Res	Type
3	H	43	GLN
3	H	50	ARG
3	H	51	ILE
3	H	56	THR
3	H	60	SER
3	H	64	LYS
3	H	110	THR
3	H	112	SER
3	H	115	LYS
3	H	121	VAL
3	H	130	ASP
3	H	134	SER
3	H	136	VAL
3	H	138	LEU
3	H	169	VAL
3	H	171	GLN
3	H	173	ASP
3	H	177	LEU
3	H	205	LYS
3	H	217	CYS
3	H	218	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	27	GLN
1	P	30	GLN
1	P	50	GLN
1	P	95(F)	ASN
1	P	128	GLN
1	P	233	HIS
2	L	17	GLN
2	L	37	GLN
2	L	53	ASN
2	L	76	GLN
2	L	89	GLN
2	L	161	ASN
2	L	198	HIS
2	L	210	ASN
3	H	3	GLN
3	H	35	ASN
3	H	81	GLN

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Mol	Chain	Res	Type
3	H	100	ASN
3	H	196	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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	$\# Z  > 2$
6	PO4	H	1001	-	4,4,4	0.58	0	6,6,6	0.30	0
4	NDG	P	401	-	15,15,15	1.08	1 (6%)	17,21,21	1.95	5 (29%)
4	NDG	P	403	-	15,15,15	0.98	1 (6%)	17,21,21	1.33	3 (17%)

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
6	PO4	H	1001	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NDG	P	401	-	-	0/6/26/26	0/1/1/1
4	NDG	P	403	-	-	0/6/26/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	403	NDG	C2-N2	2.35	1.49	1.45
4	P	401	NDG	O1L-C1	3.39	1.51	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	401	NDG	C1-O-C5	-4.35	105.43	113.47
4	P	401	NDG	O7-C7-C8	-2.53	117.42	122.06
4	P	403	NDG	O7-C7-C8	-2.18	118.06	122.06
4	P	403	NDG	O-C5-C6	2.02	111.45	106.36
4	P	401	NDG	C3-C2-N2	2.39	115.61	110.66
4	P	403	NDG	C3-C2-N2	2.63	116.11	110.66
4	P	401	NDG	C3-C4-C5	2.69	114.89	110.20
4	P	401	NDG	C4-C3-C2	3.57	115.38	110.43

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
4	P	401	NDG	6	0
4	P	403	NDG	1	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	P	237/237 (100%)	-0.13	1 (0%)	93 90	23, 34, 53, 63	0
2	L	215/215 (100%)	0.09	3 (1%)	78 71	25, 42, 76, 82	0
3	H	229/229 (100%)	-0.01	5 (2%)	65 56	26, 39, 64, 82	0
All	All	681/681 (100%)	-0.02	9 (1%)	79 72	23, 38, 70, 82	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	200	THR	3.1
3	H	131	THR	2.7
3	H	127	VAL	2.7
3	H	128	CYS	2.5
2	L	153	SER	2.3
2	L	198	HIS	2.3
3	H	199	HIS	2.2
3	H	130	ASP	2.2
1	P	95(H)	PHE	2.2

### 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
6	PO4	H	1001	5/5	0.98	0.19	0.66	13,13,15,15	5
5	CL	P	2001	1/1	0.90	0.10	-5.46	64,64,64,64	0
4	NDG	P	401	15/15	0.78	0.22	-	94,96,98,98	0
4	NDG	P	403	15/15	0.80	0.24	-	107,109,110,110	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.