Full wwPDB X-ray Structure Validation Report (i)

Mar 8, 2026 – 06:50 AM UTC

PDB ID	:	2ZCL / pdb_00002zcl
Title	:	Crystal structure of human prostate specific antigen complexed with an activating antibody
Authors	:	Menez, R.; Stura, E.; Jolivet-Reynaud, C.
Deposited on	:	2007-11-09
Resolution	:	3.25 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

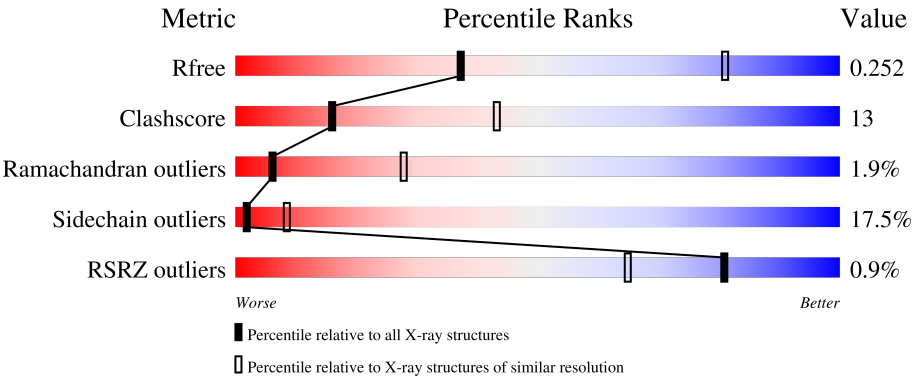
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	76% 20% .
2	L	218	% 53% 36% 10%
3	H	230	% 60% 30% 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5259 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
			Total	C	N	O	S			
1	P	237	1832	1162	323	333	14	0	0	0

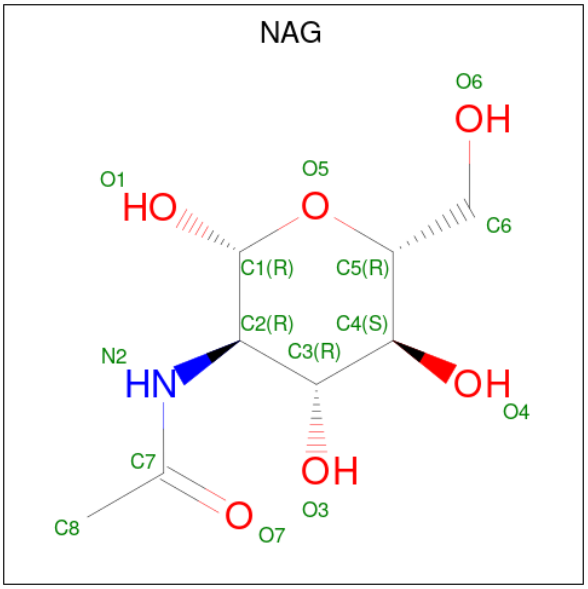
- Molecule 2 is a protein called monoclonal antibody 8G8F5 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	218	1671	1036	279	349	7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	230	1716	1077	280	348	11	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	P	1	Total	C	N	O	0	0
			14	8	1	5		
4	P	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

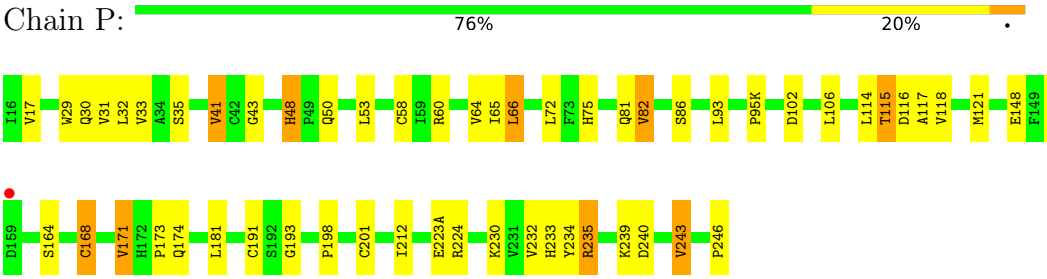
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	4	Total	O	0	0
			4	4		
5	L	6	Total	O	0	0
			6	6		
5	H	2	Total	O	0	0
			2	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

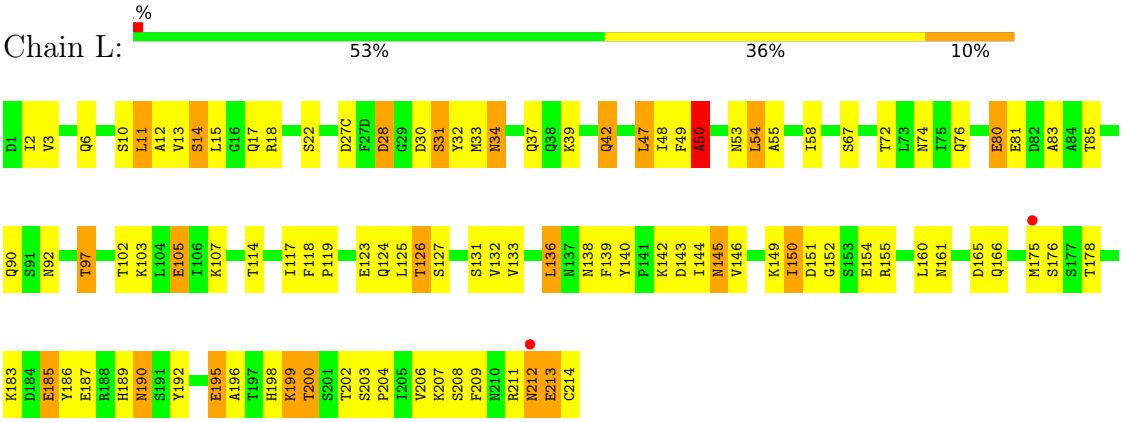
• Molecule 1: Prostate-specific antigen

Chain P:



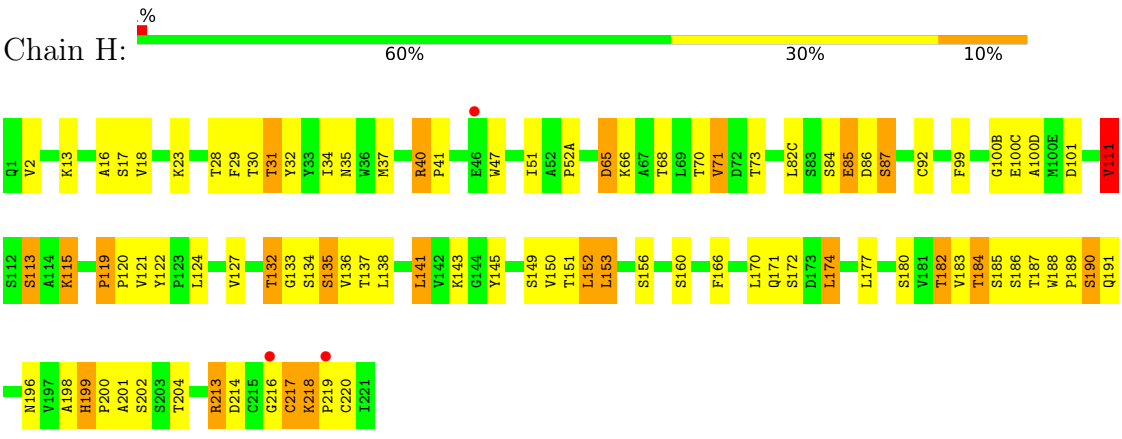
• Molecule 2: monoclonal antibody 8G8F5 Fab

Chain L:



• Molecule 3: monoclonal antibody 8G8F5 Fab

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	87.98Å 87.98Å 238.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.48 – 3.25 82.48 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (82.48-3.25) 99.8 (82.48-3.25)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	3.42 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.201 , 0.251 0.202 , 0.252	Depositor DCC
R_{free} test set	770 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	70.5	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 70.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5259	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NAG

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	1.04	1/1883 (0.1%)	1.10	7/2564 (0.3%)
2	L	0.94	0/1707	1.05	3/2319 (0.1%)
3	H	1.06	2/1757 (0.1%)	1.11	8/2398 (0.3%)
All	All	1.01	3/5347 (0.1%)	1.09	18/7281 (0.2%)

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
2	L	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	53	LEU	CA-C	-5.49	1.46	1.52
3	H	111	VAL	CA-CB	5.25	1.60	1.53
3	H	132	THR	CA-CB	5.10	1.61	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	43	GLY	N-CA-C	-6.72	101.96	112.58
3	H	101	ASP	N-CA-C	6.35	119.19	111.82
3	H	220	CYS	N-CA-C	6.23	119.11	108.02
1	P	193	GLY	N-CA-C	-6.21	107.09	114.48
2	L	50	ALA	N-CA-C	-5.75	98.56	110.80
3	H	113	SER	N-CA-C	5.64	117.23	111.14
2	L	83	ALA	N-CA-C	-5.57	101.12	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	75	HIS	CA-C-N	5.55	125.83	119.83
1	P	75	HIS	C-N-CA	5.55	125.83	119.83
1	P	58	CYS	CB-CA-C	-5.53	101.24	110.81
3	H	119	PRO	N-CA-C	5.53	117.45	110.70
1	P	116	ASP	N-CA-C	-5.52	106.55	113.28
1	P	240	ASP	N-CA-C	-5.48	105.22	111.14
3	H	199	HIS	CA-C-N	5.16	124.82	119.56
3	H	199	HIS	C-N-CA	5.16	124.82	119.56
3	H	216	GLY	N-CA-C	-5.16	106.60	112.79
3	H	71	VAL	N-CA-C	5.04	115.91	108.45
2	L	139	PHE	N-CA-C	5.02	116.87	108.99

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	50	ALA	Peptide

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	P	1832	0	1804	29	0
2	L	1671	0	1588	62	0
3	H	1716	0	1666	53	0
4	P	28	0	26	0	0
5	H	2	0	0	0	0
5	L	6	0	0	0	0
5	P	4	0	0	0	0
All	All	5259	0	5084	136	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 13.

All (136) 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:L:90:GLN:HG3	2:L:97:THR:HG22	1.55	0.88
1:P:233:HIS:HD2	3:H:99:PHE:H	1.22	0.81
3:H:40:ARG:HH21	3:H:85:GLU:HA	1.48	0.79
3:H:156:SER:H	3:H:196:ASN:HD21	1.33	0.77
1:P:235:ARG:HH21	2:L:28:ASP:HB3	1.49	0.77
3:H:153:LEU:HB3	3:H:196:ASN:HD22	1.54	0.72
1:P:171:VAL:HG11	1:P:223(A):GLU:O	1.91	0.69
2:L:34:ASN:ND2	2:L:49:PHE:O	2.25	0.69
2:L:39:LYS:HB2	2:L:42:GLN:NE2	2.08	0.69
1:P:233:HIS:HD2	3:H:99:PHE:N	1.92	0.67
3:H:199:HIS:HB3	3:H:204:THR:HB	1.78	0.66
1:P:30:GLN:NE2	1:P:198:PRO:HD2	2.10	0.65
3:H:119:PRO:HB3	3:H:145:TYR:HB3	1.77	0.65
2:L:33:MET:O	2:L:50:ALA:O	2.15	0.65
3:H:16:ALA:O	3:H:82(C):LEU:HD12	1.97	0.65
2:L:133:VAL:HG21	3:H:124:LEU:HD13	1.78	0.64
3:H:35:ASN:HD22	3:H:47:TRP:HE1	1.43	0.64
2:L:124:GLN:HE22	2:L:131:SER:HB2	1.62	0.64
2:L:125:LEU:C	2:L:127:SER:H	2.05	0.63
2:L:198:HIS:CD2	2:L:200:THR:HB	2.34	0.62
2:L:195:GLU:HB2	2:L:206:VAL:HG22	1.81	0.61
2:L:144:ILE:HG22	2:L:198:HIS:ND1	2.17	0.60
1:P:233:HIS:CD2	3:H:99:PHE:H	2.13	0.59
2:L:85:THR:HA	2:L:102:THR:O	2.01	0.59
3:H:218:LYS:HB3	3:H:218:LYS:NZ	2.18	0.59
3:H:31:THR:HG23	3:H:32:TYR:CE2	2.37	0.59
3:H:218:LYS:HB3	3:H:218:LYS:HZ3	1.68	0.59
1:P:32:LEU:HD23	1:P:33:VAL:N	2.18	0.58
2:L:183:LYS:O	2:L:187:GLU:HG2	2.04	0.57
2:L:190:ASN:ND2	2:L:212:ASN:OD1	2.37	0.57
3:H:17:SER:OG	3:H:18:VAL:N	2.34	0.57
2:L:90:GLN:CG	2:L:97:THR:HG22	2.34	0.56
1:P:243:VAL:O	1:P:246:PRO:HD3	2.06	0.56
2:L:32:TYR:HB2	2:L:92:ASN:HB2	1.87	0.56
2:L:80:GLU:CD	2:L:80:GLU:H	2.13	0.56
3:H:217:CYS:C	3:H:218:LYS:HZ3	2.13	0.55
1:P:35:SER:HB2	1:P:60:ARG:HG3	1.89	0.55
2:L:146:VAL:HG12	2:L:196:ALA:HB2	1.89	0.55
2:L:192:TYR:O	2:L:208:SER:HB2	2.07	0.54
2:L:39:LYS:HB2	2:L:42:GLN:HE21	1.70	0.54
3:H:171:GLN:CG	3:H:172:SER:N	2.70	0.54
3:H:171:GLN:CG	3:H:172:SER:H	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:137:THR:HA	3:H:182:THR:HA	1.90	0.53
2:L:212:ASN:O	2:L:214:CYS:N	2.43	0.52
2:L:123:GLU:OE1	2:L:123:GLU:N	2.32	0.52
1:P:115:THR:HB	1:P:117:ALA:H	1.75	0.51
3:H:199:HIS:CE1	3:H:201:ALA:HB3	2.45	0.51
1:P:29:TRP:CE2	1:P:121:MET:HE2	2.45	0.51
2:L:151:ASP:OD1	2:L:190:ASN:HB3	2.11	0.51
2:L:175:MET:HA	3:H:166:PHE:HE1	1.75	0.51
3:H:100(B):GLY:O	3:H:100(C):GLU:C	2.54	0.51
2:L:12:ALA:HA	2:L:105:GLU:O	2.12	0.50
2:L:133:VAL:HG12	2:L:178:THR:HG23	1.93	0.50
1:P:81:GLN:NE2	1:P:118:VAL:HG21	2.26	0.50
3:H:156:SER:H	3:H:196:ASN:ND2	2.06	0.50
3:H:84:SER:O	3:H:86:ASP:N	2.45	0.50
3:H:171:GLN:HG2	3:H:172:SER:H	1.76	0.49
2:L:18:ARG:HH11	2:L:74:ASN:HD21	1.61	0.49
1:P:32:LEU:HD23	1:P:32:LEU:C	2.38	0.49
3:H:31:THR:HG23	3:H:32:TYR:CD2	2.48	0.49
3:H:134:SER:O	3:H:135:SER:C	2.57	0.48
3:H:30:THR:HA	3:H:52(A):PRO:HB2	1.96	0.48
3:H:187:THR:HA	3:H:191:GLN:NE2	2.29	0.48
3:H:141:LEU:HD12	3:H:143:LYS:HB2	1.96	0.48
2:L:37:GLN:HB2	2:L:47:LEU:HD21	1.95	0.47
1:P:168:CYS:HA	1:P:171:VAL:HG23	1.95	0.47
2:L:149:LYS:HA	2:L:154:GLU:HA	1.96	0.47
1:P:66:LEU:HD22	1:P:66:LEU:N	2.29	0.47
1:P:33:VAL:O	1:P:41:VAL:HG13	2.14	0.47
2:L:211:ARG:O	2:L:213:GLU:N	2.47	0.47
3:H:141:LEU:CD1	3:H:143:LYS:HB2	2.45	0.47
2:L:160:LEU:C	2:L:161:ASN:HD22	2.23	0.47
3:H:41:PRO:HD2	3:H:87:SER:O	2.15	0.47
3:H:156:SER:N	3:H:196:ASN:HD21	2.08	0.47
3:H:170:LEU:HD12	3:H:174:LEU:C	2.40	0.47
2:L:54:LEU:HD11	2:L:58:ILE:O	2.14	0.47
3:H:188:TRP:CD1	3:H:189:PRO:HA	2.50	0.46
1:P:32:LEU:HD12	1:P:72:LEU:HD21	1.98	0.46
2:L:125:LEU:C	2:L:127:SER:N	2.74	0.46
2:L:195:GLU:CB	2:L:206:VAL:HG22	2.45	0.46
3:H:51:ILE:HD13	3:H:71:VAL:HG13	1.97	0.46
2:L:150:ILE:O	2:L:151:ASP:HB2	2.16	0.46
1:P:48:HIS:C	1:P:48:HIS:CD2	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:185:GLU:O	2:L:186:TYR:C	2.57	0.46
1:P:60:ARG:HD3	1:P:60:ARG:HA	1.79	0.45
2:L:34:ASN:HD22	2:L:49:PHE:HA	1.81	0.45
2:L:136:LEU:HD13	2:L:175:MET:HG3	1.97	0.45
1:P:65:ILE:O	1:P:82:VAL:HA	2.16	0.45
2:L:149:LYS:HD2	2:L:152:GLY:O	2.17	0.45
2:L:107:LYS:HA	2:L:140:TYR:OH	2.17	0.45
2:L:34:ASN:ND2	3:H:100(D):ALA:HB2	2.32	0.44
2:L:212:ASN:O	2:L:213:GLU:C	2.60	0.44
2:L:6:GLN:HA	2:L:22:SER:O	2.17	0.44
3:H:35:ASN:O	3:H:92:CYS:HA	2.18	0.44
1:P:95(K):PRO:HB3	1:P:173:PRO:HB2	1.99	0.44
2:L:145:ASN:HD22	2:L:146:VAL:H	1.65	0.44
3:H:133:GLY:O	3:H:185:SER:HB3	2.17	0.44
2:L:11:LEU:HD22	2:L:12:ALA:N	2.33	0.44
1:P:235:ARG:NH2	2:L:28:ASP:HB3	2.23	0.44
3:H:218:LYS:NZ	3:H:218:LYS:CB	2.79	0.44
3:H:151:THR:HB	3:H:198:ALA:HB3	1.98	0.44
2:L:53:ASN:HD22	2:L:53:ASN:HA	1.61	0.43
2:L:27(C):ASP:OD2	2:L:31:SER:OG	2.34	0.43
2:L:199:LYS:HD3	2:L:199:LYS:C	2.42	0.43
1:P:48:HIS:CD2	1:P:50:GLN:H	2.36	0.43
2:L:14:SER:O	2:L:17:GLN:HB2	2.18	0.43
2:L:203:SER:O	2:L:204:PRO:C	2.61	0.43
3:H:151:THR:O	3:H:198:ALA:N	2.45	0.43
2:L:119:PRO:HB3	2:L:209:PHE:CZ	2.54	0.43
3:H:199:HIS:HA	3:H:200:PRO:HD2	1.88	0.43
2:L:124:GLN:HE22	2:L:131:SER:CB	2.29	0.43
2:L:206:VAL:O	2:L:207:LYS:HG3	2.20	0.42
2:L:18:ARG:NH1	2:L:74:ASN:HD21	2.16	0.42
3:H:40:ARG:HH11	3:H:40:ARG:HB3	1.84	0.42
3:H:119:PRO:HD2	3:H:204:THR:HG21	2.01	0.42
3:H:152:LEU:C	3:H:152:LEU:CD1	2.93	0.42
1:P:29:TRP:CD2	1:P:121:MET:HE2	2.54	0.42
3:H:183:VAL:HG12	3:H:184:THR:N	2.35	0.42
2:L:55:ALA:HB3	2:L:58:ILE:HG13	2.02	0.42
2:L:118:PHE:HB2	2:L:133:VAL:CG2	2.49	0.42
3:H:28:THR:O	3:H:29:PHE:C	2.62	0.41
1:P:235:ARG:HH11	1:P:235:ARG:HG3	1.85	0.41
3:H:115:LYS:HE2	3:H:115:LYS:H	1.84	0.41
1:P:171:VAL:HG11	1:P:224:ARG:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:187:GLU:HA	2:L:187:GLU:OE1	2.19	0.41
3:H:120:PRO:HB2	3:H:122:TYR:CZ	2.55	0.41
1:P:48:HIS:HD2	1:P:50:GLN:H	1.69	0.41
3:H:213:ARG:H	3:H:213:ARG:HG2	1.79	0.41
3:H:82(C):LEU:HB3	3:H:111:VAL:HG21	2.02	0.41
1:P:171:VAL:O	1:P:224:ARG:NH1	2.54	0.41
1:P:234:TYR:O	1:P:235:ARG:C	2.64	0.41
2:L:189:HIS:HB2	2:L:192:TYR:OH	2.21	0.41
3:H:65:ASP:OD2	3:H:65:ASP:N	2.53	0.40
2:L:90:GLN:CD	2:L:90:GLN:C	2.90	0.40
2:L:2:ILE:O	2:L:97:THR:HG21	2.21	0.40
2:L:165:ASP:O	2:L:166:GLN:C	2.64	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%)	213 (91%)	21 (9%)	1 (0%)	30 59
2	L	216/218 (99%)	190 (88%)	20 (9%)	6 (3%)	4 20
3	H	228/230 (99%)	194 (85%)	28 (12%)	6 (3%)	4 21
All	All	679/685 (99%)	597 (88%)	69 (10%)	13 (2%)	6 28

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	212	ASN
2	L	213	GLU
3	H	149	SER
1	P	102	ASP
2	L	126	THR

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Mol	Chain	Res	Type
3	H	85	GLU
3	H	135	SER
2	L	138	ASN
2	L	199	LYS
3	H	190	SER
3	H	217	CYS
2	L	50	ALA
3	H	219	PRO

5.3.2 Protein sidechains (i)

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%)	177 (86%)	28 (14%)	3 16
2	L	189/189 (100%)	151 (80%)	38 (20%)	1 5
3	H	196/196 (100%)	159 (81%)	37 (19%)	1 6
All	All	590/590 (100%)	487 (82%)	103 (18%)	2 8

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	17	VAL
1	P	31	VAL
1	P	41	VAL
1	P	48	HIS
1	P	64	VAL
1	P	66	LEU
1	P	82	VAL
1	P	86	SER
1	P	93	LEU
1	P	106	LEU
1	P	114	LEU
1	P	115	THR
1	P	148	GLU
1	P	150	LEU

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Mol	Chain	Res	Type
1	P	155	LEU
1	P	164	SER
1	P	168	CYS
1	P	171	VAL
1	P	174	GLN
1	P	181	LEU
1	P	191	CYS
1	P	201	CYS
1	P	212	ILE
1	P	230	LYS
1	P	232	VAL
1	P	235	ARG
1	P	239	LYS
1	P	243	VAL
2	L	3	VAL
2	L	10	SER
2	L	11	LEU
2	L	13	VAL
2	L	14	SER
2	L	15	LEU
2	L	28	ASP
2	L	30	ASP
2	L	31	SER
2	L	34	ASN
2	L	42	GLN
2	L	47	LEU
2	L	48	ILE
2	L	54	LEU
2	L	67	SER
2	L	72	THR
2	L	76	GLN
2	L	80	GLU
2	L	81	GLU
2	L	97	THR
2	L	103	LYS
2	L	105	GLU
2	L	114	THR
2	L	117	ILE
2	L	126	THR
2	L	132	VAL
2	L	136	LEU
2	L	142	LYS

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Mol	Chain	Res	Type
2	L	143	ASP
2	L	145	ASN
2	L	150	ILE
2	L	155	ARG
2	L	176	SER
2	L	185	GLU
2	L	190	ASN
2	L	195	GLU
2	L	200	THR
2	L	202	THR
3	H	2	VAL
3	H	13	LYS
3	H	23	LYS
3	H	31	THR
3	H	34	ILE
3	H	37	MET
3	H	40	ARG
3	H	65	ASP
3	H	66	LYS
3	H	68	THR
3	H	70	THR
3	H	73	THR
3	H	87	SER
3	H	111	VAL
3	H	113	SER
3	H	115	LYS
3	H	121	VAL
3	H	127	VAL
3	H	132	THR
3	H	136	VAL
3	H	138	LEU
3	H	141	LEU
3	H	150	VAL
3	H	152	LEU
3	H	153	LEU
3	H	160	SER
3	H	174	LEU
3	H	177	LEU
3	H	180	SER
3	H	182	THR
3	H	184	THR
3	H	186	SER

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Mol	Chain	Res	Type
3	H	190	SER
3	H	202	SER
3	H	213	ARG
3	H	214	ASP
3	H	218	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	27	GLN
1	P	30	GLN
1	P	48	HIS
1	P	50	GLN
1	P	81	GLN
1	P	91	HIS
1	P	165	ASN
1	P	210	GLN
1	P	233	HIS
2	L	34	ASN
2	L	53	ASN
2	L	74	ASN
2	L	89	GLN
2	L	124	GLN
2	L	145	ASN
2	L	156	GLN
2	L	157	ASN
2	L	161	ASN
2	L	190	ASN
2	L	212	ASN
3	H	35	ASN
3	H	43	GLN
3	H	164	HIS
3	H	191	GLN
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 (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides 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	$\#\|Z\| > 2$
4	NAG	P	401	-	14,14,15	0.68	0	17,19,21	1.91	4 (23%)
4	NAG	P	403	-	14,14,15	0.95	0	17,19,21	1.69	5 (29%)

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
4	NAG	P	401	-	-	3/6/23/26	0/1/1/1
4	NAG	P	403	-	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	401	NAG	C1-O5-C5	4.86	118.70	112.19
4	P	403	NAG	O3-C3-C2	3.70	117.09	109.40
4	P	401	NAG	O5-C5-C4	3.28	118.81	110.83
4	P	403	NAG	C1-O5-C5	2.95	116.14	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	401	NAG	O3-C3-C2	2.66	114.93	109.40
4	P	403	NAG	O7-C7-C8	-2.64	117.35	122.05
4	P	401	NAG	C3-C4-C5	2.61	114.96	110.23
4	P	403	NAG	O3-C3-C4	-2.51	104.46	110.38
4	P	403	NAG	C8-C7-N2	2.16	119.69	116.12

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	401	NAG	C8-C7-N2-C2
4	P	401	NAG	O7-C7-N2-C2
4	P	403	NAG	O5-C5-C6-O6
4	P	403	NAG	C4-C5-C6-O6
4	P	401	NAG	C4-C5-C6-O6
4	P	403	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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

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, 95th 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^2)	Q<0.9
1	P	237/237 (100%)	-0.20	1 (0%)	88	78	45, 59, 75, 85	0
2	L	218/218 (100%)	0.08	2 (0%)	81	65	49, 71, 100, 100	0
3	H	230/230 (100%)	0.05	3 (1%)	75	56	44, 70, 97, 100	0
All	All	685/685 (100%)	-0.03	6 (0%)	81	65	44, 66, 100, 100	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	212	ASN	3.6
1	P	159	ASP	2.6
3	H	46	GLU	2.3
3	H	219	PRO	2.3
2	L	175	MET	2.2
3	H	216	GLY	2.1

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

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, 95th 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(Å^2)	Q<0.9
4	NAG	P	403	14/15	0.52	0.16	99,100,100,100	0
4	NAG	P	401	14/15	0.79	0.12	97,98,99,100	0

6.5 Other polymers (i)

There are no such residues in this entry.