



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:50 PM UTC

PDB ID : 2ZCH / pdb_00002zch
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) 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

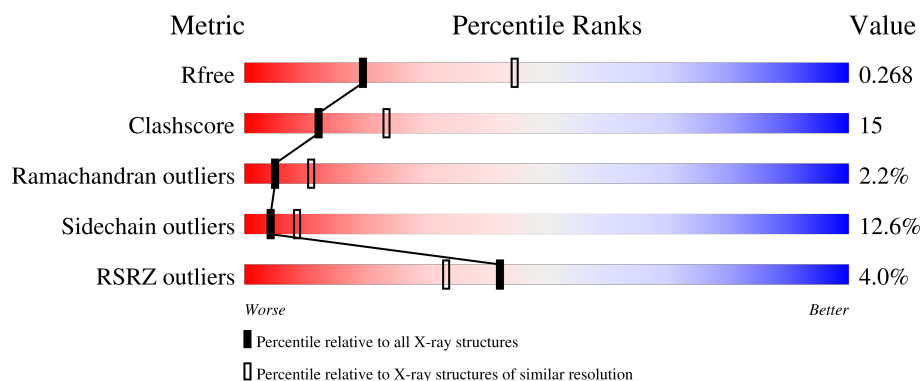
1 Overall quality at a glance

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}	180053	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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 $\leq 5\%$. 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	% 71% 25% ..
2	L	215	6% 66% 27% 7%
3	H	229	5% 64% 28% 6%

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			

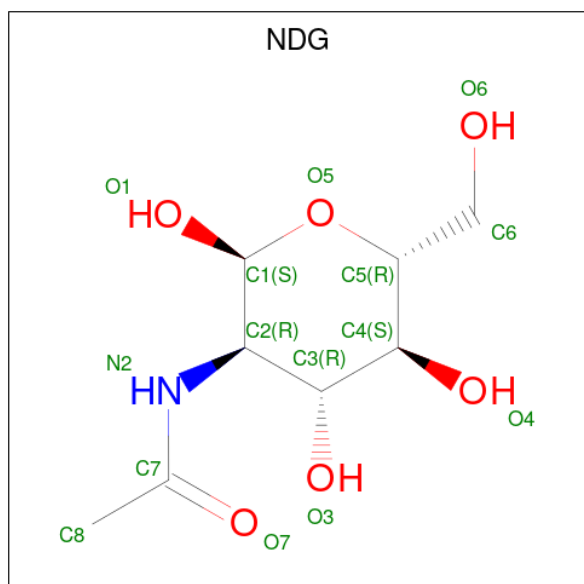
- Molecule 2 is a protein called monoclonal antibody 8G8F5 Fab.

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 2-acetamido-2-deoxy- α -D-glucopyranose (CCD ID: NDG) (formula: $C_8H_{15}NO_6$).

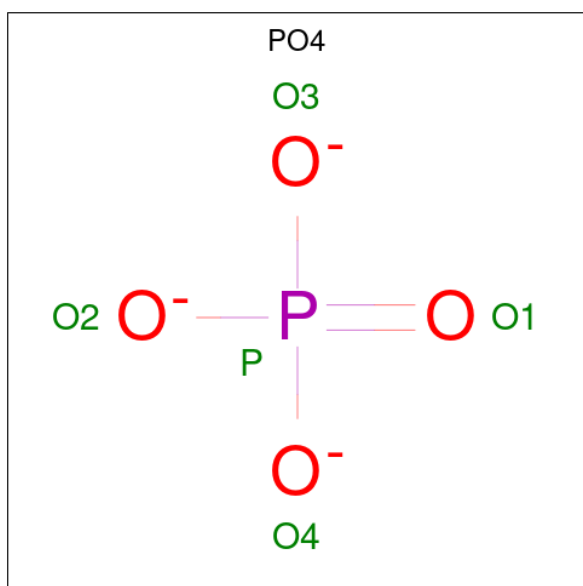


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	P	1	Total	C	N	O	0	0
			15	8	1	6		
4	P	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

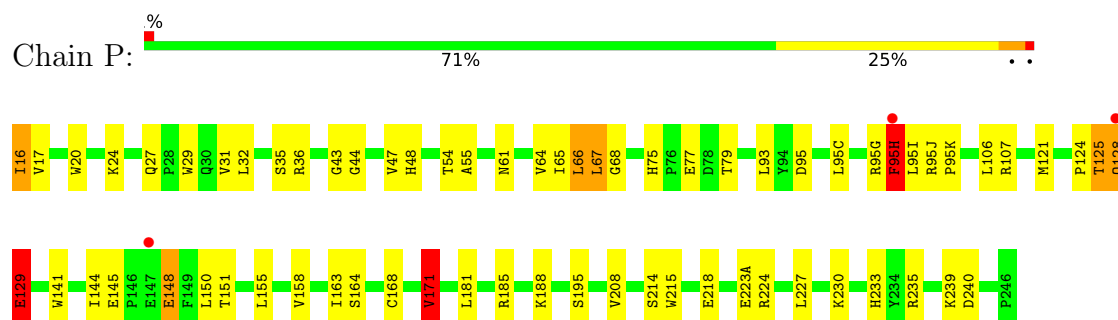
- Molecule 7 is water.

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		

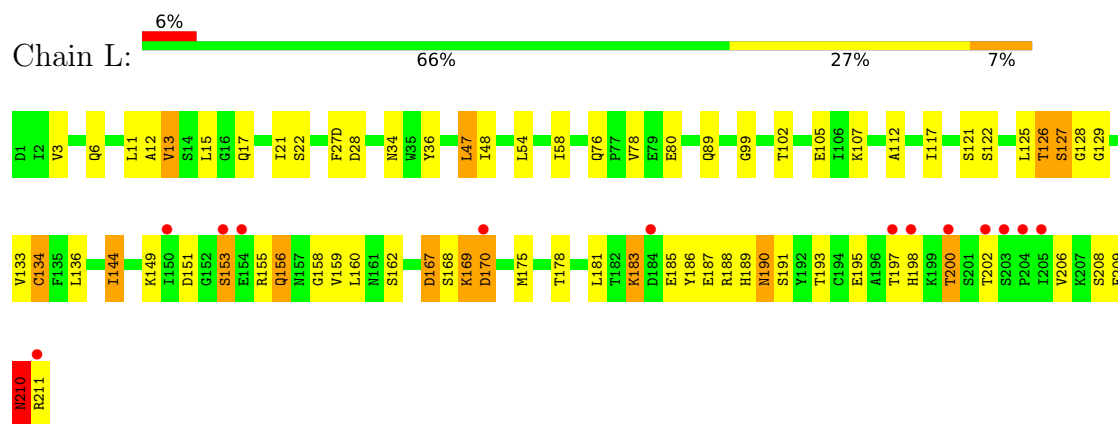
3 Residue-property plots [i](#)

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.

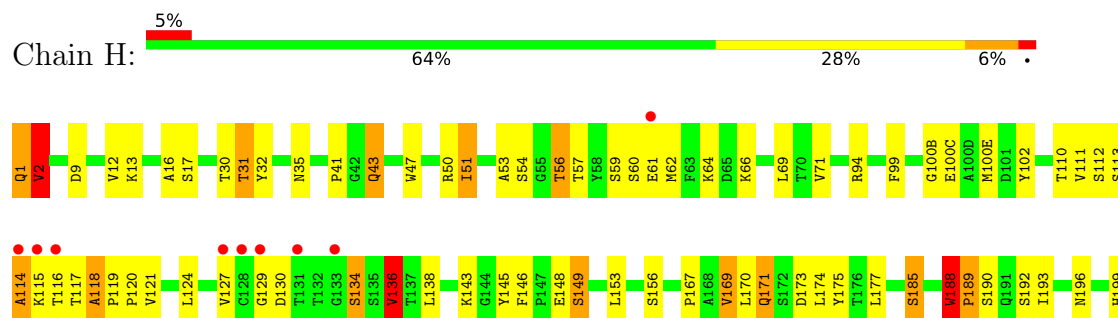
- Molecule 1: Prostate-specific antigen

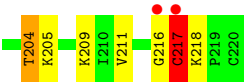


- Molecule 2: monoclonal antibody 8G8F5 Fab



- 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, α , β , γ	87.36Å 87.36Å 236.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.81 – 2.83 78.81 – 2.83	Depositor EDS
% Data completeness (in resolution range)	100.0 (78.81-2.83) 100.0 (78.81-2.83)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.203 , 0.270 0.209 , 0.268	Depositor DCC
R_{free} test set	1163 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5290	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CL, PO4, NDG

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	1.09	0/1883	1.14	9/2564 (0.4%)
2	L	0.99	1/1684 (0.1%)	1.07	2/2288 (0.1%)
3	H	1.11	2/1749 (0.1%)	1.29	7/2387 (0.3%)
All	All	1.07	3/5316 (0.1%)	1.17	18/7239 (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
3	H	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	111	VAL	CA-CB	6.29	1.61	1.53
2	L	129	GLY	N-CA	5.38	1.49	1.44
3	H	2	VAL	CA-CB	5.29	1.60	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	188	TRP	CA-C-N	22.28	147.69	119.84
3	H	188	TRP	C-N-CA	22.28	147.69	119.84
1	P	75	HIS	CA-C-N	10.24	130.31	119.76
1	P	75	HIS	C-N-CA	10.24	130.31	119.76
3	H	188	TRP	C-N-CD	-6.88	96.78	125.00
3	H	185	SER	N-CA-C	6.53	119.22	111.71
1	P	95(H)	PHE	CB-CA-C	6.15	122.66	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	24	LYS	CA-C-N	-5.88	113.31	123.25
1	P	24	LYS	C-N-CA	-5.88	113.31	123.25
3	H	136	VAL	CB-CA-C	-5.78	102.01	110.62
1	P	151	THR	N-CA-C	5.70	116.83	109.65
3	H	112	SER	N-CA-C	5.46	117.14	108.79
2	L	58	ILE	CA-C-O	5.36	122.67	119.19
1	P	148	GLU	N-CA-C	-5.27	99.57	110.80
1	P	95(I)	LEU	N-CA-C	5.10	116.87	110.24
1	P	171	VAL	N-CA-CB	-5.08	105.71	112.26
2	L	99	GLY	N-CA-C	-5.04	104.74	112.85
3	H	66	LYS	N-CA-C	5.02	116.56	111.14

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	52	0
2	L	1648	0	1571	55	0
3	H	1708	0	1655	60	0
4	P	30	0	24	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	5054	159	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 (159) 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: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:117:THR:O	3:H:118:ALA:HB3	1.75	0.83
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:61:ASN:CG	4:P:401:NDG:H6C1	2.12	0.74
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
1:P:215:TRP:CZ2	1:P:227:LEU:HD13	2.25	0.70
2:L:149:LYS:HB2	2:L:153:SER:O	1.91	0.70
3:H:117:THR:O	3:H:118:ALA:CB	2.37	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
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:125:LEU:C	2:L:127:SER:H	2.04	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
2:L:133:VAL:HG12	2:L:178:THR:HG23	1.85	0.59
1:P:144:ILE:O	1:P:144:ILE:HG22	2.02	0.59
2:L:210:ASN:HD22	2:L:210:ASN:H	1.50	0.58
3:H:134:SER:O	3:H:185:SER:HB2	2.04	0.57
1:P:145:GLU:HB2	1:P:148:GLU:O	2.04	0.57
2:L:159:VAL:O	2:L:160:LEU:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:126:THR:O	2:L:126:THR:CG2	2.55	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
3:H:113:SER:O	3:H:114:ALA:O	2.25	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
1:P:27:GLN:NE2	7:P:2005:HOH:O	2.40	0.54
3:H:127:VAL:HG22	3:H:129:GLY:H	1.72	0.54
1:P:77:GLU:C	1:P:79:THR:H	2.16	0.54
1:P:125:THR:HG22	1:P:128:GLN:HB2	1.90	0.53
3:H:153:LEU:HD13	3:H:156:SER:HA	1.91	0.53
1:P:61:ASN:ND2	4:P:401:NDG:C6	2.71	0.53
2:L:210:ASN:O	2:L:211:ARG:CB	2.56	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
3:H:1:GLN:H3	3:H:1:GLN:CD	2.16	0.52
3:H:1:GLN:CD	3:H:1:GLN:N	2.67	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:67:LEU:HD23	1:P:67:LEU:N	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:N	3:H:1:GLN:OE1	2.39	0.50
3:H:148:GLU:HG2	3:H:175:TYR:CE2	2.46	0.50
2:L:11:LEU:CD2	2:L:13:VAL:HG23	2.42	0.50
2:L:112:ALA:CB	2:L:200:THR:HG21	2.39	0.50
2:L:160:LEU:HD21	3:H:171:GLN:HB3	1.94	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:2:VAL:HG21	3:H:102:TYR:CD2	2.49	0.48
3:H:148:GLU:O	3:H:149:SER:CB	2.61	0.48
3:H:192:SER:HB2	3:H:209:LYS:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:125:LEU:C	2:L:127:SER:N	2.72	0.47
2:L:195:GLU:HB2	2:L:206:VAL:HG12	1.96	0.47
1:P:107:ARG:HD3	7:P:2027:HOH:O	2.14	0.47
2:L:160:LEU:HD23	3:H:169:VAL:CG1	2.44	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:O5	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:136:LEU:HD22	2:L:175:MET:HE3	1.97	0.46
2:L:36:TYR:HE2	2:L:89:GLN:HE21	1.64	0.46
2:L:136:LEU:HD12	2:L:136:LEU:N	2.31	0.46
3:H:35:ASN:HD22	3:H:47:TRP:NE1	2.01	0.46
1:P:29:TRP:CZ2	1:P:121:MET:CE	2.99	0.46
3:H:216:GLY:C	3:H:217:CYS:SG	2.99	0.46
2:L:117:ILE:HD12	2:L:134:CYS:CB	2.46	0.46
3:H:153:LEU:HB2	3:H:196:ASN:HD22	1.81	0.46
3:H:59:SER:HB2	3:H:64:LYS:HE3	1.97	0.45
1:P:29:TRP:CD2	1:P:121:MET:HE2	2.51	0.45
2:L:47:LEU:HB3	2:L:48:ILE:HD12	1.98	0.45
3:H:188:TRP:CD1	3:H:193:ILE:HD12	2.51	0.45
1:P:16:ILE:HG21	1:P:158:VAL:HB	1.98	0.45
3:H:113:SER:O	3:H:114:ALA:C	2.59	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
3:H:189:PRO:O	3:H:190:SER:C	2.60	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
1:P:66:LEU:C	1:P:67:LEU:HD23	2.43	0.44
1:P:95:ASP:O	1:P:95(C):LEU:HB2	2.18	0.44
2:L:186:TYR:O	2:L:188:ARG:O	2.36	0.44
3:H:69:LEU:HD23	3:H:69:LEU:N	2.31	0.44
1:P:95(J):ARG:HB2	1:P:95(K):PRO:CD	2.47	0.43
3:H:119:PRO:HB3	3:H:145:TYR:HB3	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:124:PRO:O	1:P:235:ARG:HD2	2.18	0.43
2:L:6:GLN:HA	2:L:22:SER:O	2.19	0.43
1:P:29:TRP:CE2	1:P:121:MET:HE3	2.54	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
3:H:192:SER:C	3:H:193:ILE:HG13	2.42	0.42
2:L:167:ASP:OD1	2:L:167:ASP:C	2.62	0.42
1:P:95(J):ARG:HB2	1:P:95(K):PRO:HD2	2.01	0.42
2:L:168:SER:O	2:L:169:LYS:CB	2.67	0.42
1:P:77:GLU:HB3	1:P:79:THR:HG22	2.01	0.42
1:P:66:LEU:HD13	1:P:66:LEU:N	2.34	0.42
3:H:156:SER:N	3:H:196:ASN:HD21	2.11	0.42
1:P:65:ILE:HG22	1:P:67:LEU:HD21	2.01	0.42
3:H:51:ILE:HD12	3:H:71:VAL:HG13	2.02	0.42
2:L:21:ILE:CD1	2:L:102:THR:HG21	2.50	0.42
1:P:29:TRP:CE3	1:P:121:MET:HE2	2.55	0.41
2:L:34:ASN:HD22	2:L:89:GLN:NE2	2.17	0.41
2:L:133:VAL:HG21	3:H:124:LEU:HD13	2.01	0.41
3:H:100(B):GLY:O	3:H:100(C):GLU:C	2.62	0.41
1:P:61:ASN:OD1	4:P:401:NDG:H6C1	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
3:H:94:ARG:O	3:H:100(E):MET:HA	2.21	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:47:LEU:C	2:L:48:ILE:HD12	2.46	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
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%)	14	27
2	L	213/215 (99%)	189 (89%)	17 (8%)	7 (3%)	3	6
3	H	227/229 (99%)	198 (87%)	23 (10%)	6 (3%)	4	9
All	All	675/681 (99%)	603 (89%)	57 (8%)	15 (2%)	5	11

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	95(H)	PHE
2	L	169	LYS
3	H	149	SER
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 [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%)	181 (88%)	24 (12%)	5	11
2	L	186/186 (100%)	162 (87%)	24 (13%)	4	8
3	H	195/195 (100%)	169 (87%)	26 (13%)	4	8
All	All	586/586 (100%)	512 (87%)	74 (13%)	4	9

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	16	ILE
1	P	17	VAL
1	P	31	VAL
1	P	35	SER
1	P	36	ARG
1	P	64	VAL
1	P	66	LEU
1	P	67	LEU
1	P	93	LEU
1	P	106	LEU
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	13	VAL
2	L	15	LEU
2	L	17	GLN
2	L	47	LEU
2	L	54	LEU
2	L	76	GLN
2	L	80	GLU
2	L	107	LYS
2	L	121	SER

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Mol	Chain	Res	Type
2	L	122	SER
2	L	127	SER
2	L	134	CYS
2	L	144	ILE
2	L	167	ASP
2	L	170	ASP
2	L	181	LEU
2	L	183	LYS
2	L	185	GLU
2	L	190	ASN
2	L	197	THR
2	L	200	THR
2	L	202	THR
2	L	210	ASN
3	H	1	GLN
3	H	2	VAL
3	H	9	ASP
3	H	17	SER
3	H	31	THR
3	H	43	GLN
3	H	50	ARG
3	H	51	ILE
3	H	56	THR
3	H	60	SER
3	H	110	THR
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	204	THR
3	H	205	LYS
3	H	211	VAL
3	H	217	CYS
3	H	218	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	27	GLN
1	P	30	GLN
1	P	50	GLN
1	P	75	HIS
1	P	95(F)	ASN
1	P	128	GLN
1	P	156	GLN
1	P	202	ASN
1	P	233	HIS
2	L	17	GLN
2	L	53	ASN
2	L	76	GLN
2	L	89	GLN
2	L	92	ASN
2	L	157	ASN
2	L	161	ASN
2	L	198	HIS
2	L	210	ASN
3	H	3	GLN
3	H	35	ASN
3	H	81	GLN
3	H	100	ASN
3	H	171	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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	$\# Z > 2$
4	NDG	P	403	-	15,15,15	1.01	1 (6%)	21,21,21	1.95	4 (19%)
4	NDG	P	401	-	15,15,15	1.16	1 (6%)	21,21,21	3.14	9 (42%)
6	PO4	H	1001	-	4,4,4	0.99	0	6,6,6	0.98	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
4	NDG	P	403	-	-	5/6/26/26	0/1/1/1
4	NDG	P	401	-	-	4/6/26/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	401	NDG	O1-C1	3.79	1.51	1.39
4	P	403	NDG	C2-N2	2.47	1.49	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	401	NDG	C1-C2-C3	-6.83	101.23	110.54
4	P	401	NDG	C1-C2-N2	6.62	118.40	110.73
4	P	401	NDG	O5-C1-C2	6.55	116.09	109.52
4	P	403	NDG	O5-C1-C2	6.49	116.03	109.52
4	P	401	NDG	C1-O5-C5	-4.25	105.43	113.65
4	P	401	NDG	C4-C3-C2	3.42	115.38	110.40
4	P	401	NDG	O1-C1-C2	3.01	115.47	109.22
4	P	403	NDG	C3-C2-N2	2.98	116.11	110.62
4	P	401	NDG	C3-C2-N2	2.71	115.61	110.62
4	P	401	NDG	O7-C7-C8	-2.60	117.42	122.05
4	P	401	NDG	C3-C4-C5	2.57	114.89	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	403	NDG	O7-C7-C8	-2.24	118.06	122.05
4	P	403	NDG	O5-C5-C6	2.02	111.45	106.44

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	401	NDG	C8-C7-N2-C2
4	P	401	NDG	O7-C7-N2-C2
4	P	403	NDG	C3-C2-N2-C7
4	P	403	NDG	C8-C7-N2-C2
4	P	403	NDG	O7-C7-N2-C2
4	P	403	NDG	C4-C5-C6-O6
4	P	403	NDG	O5-C5-C6-O6
4	P	401	NDG	O5-C5-C6-O6
4	P	401	NDG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	403	NDG	1	0
4	P	401	NDG	6	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 ⓘ

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%)	-0.06	3 (1%) 75 69	23, 34, 53, 63	0
2	L	215/215 (100%)	0.35	13 (6%) 27 21	25, 42, 76, 82	0
3	H	229/229 (100%)	0.21	11 (4%) 35 29	26, 39, 64, 82	0
All	All	681/681 (100%)	0.16	27 (3%) 42 33	23, 38, 70, 82	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	131	THR	4.0
3	H	127	VAL	3.9
3	H	217	CYS	3.6
2	L	204	PRO	3.3
1	P	95(H)	PHE	3.1
1	P	147	GLU	3.0
2	L	184	ASP	3.0
2	L	197	THR	2.8
3	H	129	GLY	2.8
3	H	61	GLU	2.8
2	L	200	THR	2.7
3	H	133	GLY	2.7
2	L	202	THR	2.5
3	H	114	ALA	2.5
2	L	211	ARG	2.4
2	L	205	ILE	2.3
3	H	216	GLY	2.3
2	L	150	ILE	2.3
2	L	153	SER	2.3
2	L	203	SER	2.2
1	P	128	GLN	2.2
2	L	198	HIS	2.2
2	L	154	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
3	H	115	LYS	2.1
3	H	116	THR	2.1
2	L	170	ASP	2.1
3	H	128	CYS	2.1

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 oligosaccharides 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, 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($\text{\AA}^2$)	Q<0.9
4	NDG	P	403	15/15	0.46	0.17	107,109,110,110	0
4	NDG	P	401	15/15	0.61	0.17	94,96,98,98	0
5	CL	P	2001	1/1	0.95	0.09	64,64,64,64	0
6	PO4	H	1001	5/5	0.95	0.16	13,13,15,15	5

6.5 Other polymers [i](#)

There are no such residues in this entry.