



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:49 AM UTC

PDB ID : 6SS4 / pdb_00006ss4
Title : Structure of arginase-2 in complex with the inhibitory human antigen-binding fragment Fab C0021181
Authors : Burschowsky, D.; Addyman, A.; Fiedler, S.; Groves, M.; Haynes, S.; See-wooruthun, C.; Carr, M.
Deposited on : 2019-09-06
Resolution : 2.90 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

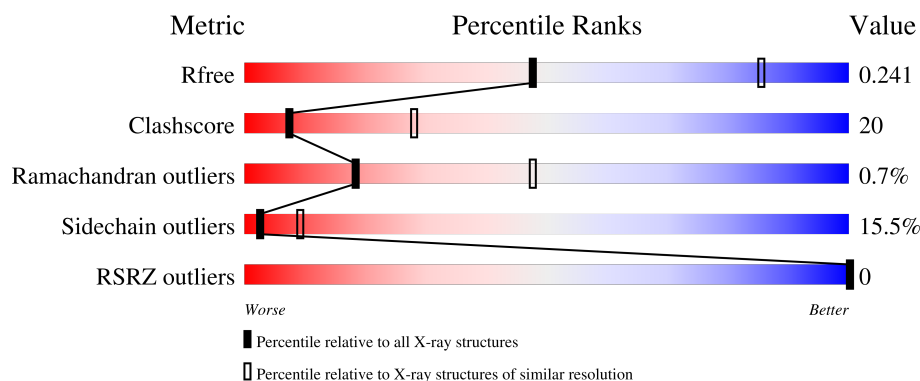
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	AAA	339	
2	HHH	233	
3	LLL	220	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	AAA	403	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11180 atoms, of which 5548 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 Arginase-2, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	316	Total	C	H	N	O	S	119	0	0
			4830	1527	2413	420	460	10			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	22	MET	-	initiating methionine	UNP P78540
AAA	355	HIS	-	expression tag	UNP P78540
AAA	356	HIS	-	expression tag	UNP P78540
AAA	357	HIS	-	expression tag	UNP P78540
AAA	358	HIS	-	expression tag	UNP P78540
AAA	359	HIS	-	expression tag	UNP P78540
AAA	360	HIS	-	expression tag	UNP P78540

- Molecule 2 is a protein called Fab C0021181 heavy chain (IgG1).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	HHH	216	Total	C	H	N	O	S	89	1	0
			3238	1027	1607	281	316	7			

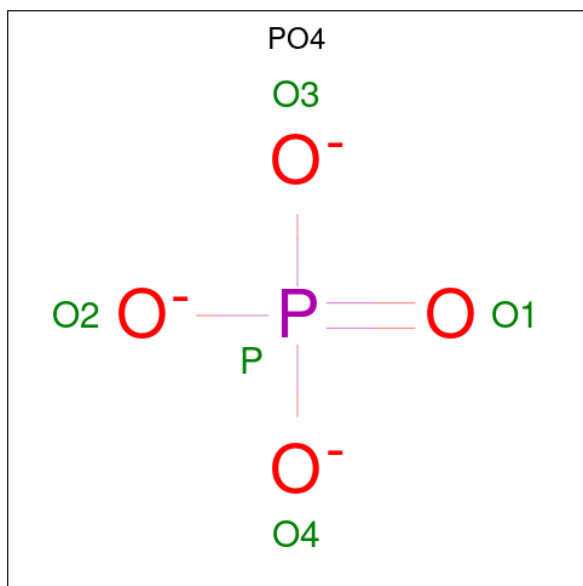
- Molecule 3 is a protein called Fab C0021181 light chain (IgG1).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	LLL	213	Total	C	H	N	O	S	100	0	0
			3105	985	1528	262	325	5			

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	2	Total	Mn	0	0
			2	2		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



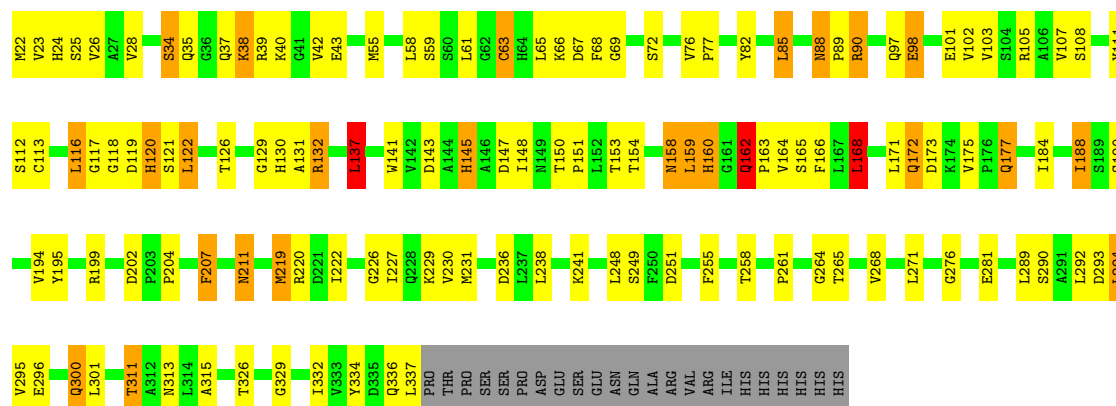
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total	O	P	0	0
			5	4	1		

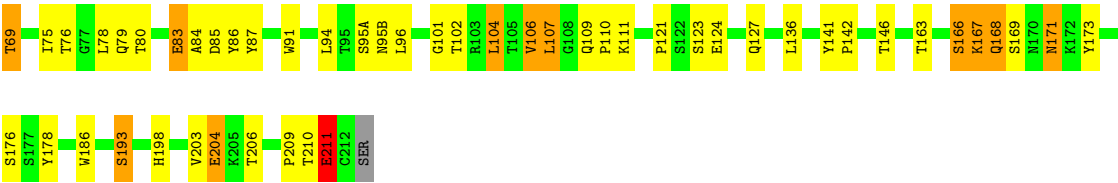
3 Residue-property plots

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: Arginase-2, mitochondrial

Chain AAA: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.38Å 150.38Å 110.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.98 – 2.90 44.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.98-2.90) 90.2 (44.98-2.90)	Depositor EDS
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.45 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.266 , 0.318 0.191 , 0.241	Depositor DCC
R_{free} test set	1602 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	64.4	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.468 for -h,-k,l	Xtriage
Reported twinning fraction	0.505 for H, K, L 0.495 for -h,-k,l	Depositor
Outliers	1 of 32382 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11180	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	AAA	1.32	9/2469 (0.4%)	1.72	16/3358 (0.5%)
2	HHH	1.22	2/1668 (0.1%)	1.61	17/2268 (0.7%)
3	LLL	1.26	0/1615	1.55	6/2208 (0.3%)
All	All	1.28	11/5752 (0.2%)	1.64	39/7834 (0.5%)

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
1	AAA	0	2
3	LLL	0	1
All	All	0	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	145	HIS	CE1-NE2	7.75	1.40	1.32
1	AAA	89	PRO	C-O	-5.87	1.16	1.24
2	HHH	64	LYS	C-O	5.86	1.31	1.23
1	AAA	34	SER	CA-CB	-5.40	1.45	1.53
1	AAA	164	VAL	C-O	-5.38	1.17	1.24
1	AAA	85	LEU	C-O	-5.27	1.17	1.24
1	AAA	98	GLU	CD-OE2	5.25	1.35	1.25
1	AAA	131	ALA	C-O	5.20	1.30	1.24
1	AAA	258	THR	C-O	-5.16	1.17	1.24
1	AAA	300	GLN	C-O	5.14	1.30	1.24
2	HHH	184	VAL	N-CA	5.00	1.50	1.46

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	311	THR	CA-CB-OG1	-10.07	94.49	109.60
1	AAA	159	LEU	N-CA-C	-8.89	103.27	114.56
1	AAA	162	GLN	CA-C-N	8.11	127.75	119.56
1	AAA	162	GLN	C-N-CA	8.11	127.75	119.56
3	LLL	80	THR	CA-CB-OG1	-7.28	98.68	109.60
3	LLL	101	GLY	CA-C-O	-7.02	117.66	122.22
1	AAA	122	LEU	N-CA-C	-6.62	104.46	112.54
1	AAA	137	LEU	CA-C-O	-6.34	114.90	121.87
2	HHH	209	LYS	CA-C-N	6.28	130.47	121.50
2	HHH	209	LYS	C-N-CA	6.28	130.47	121.50
1	AAA	231	MET	N-CA-C	-6.23	104.57	111.36
2	HHH	133	GLY	CA-C-N	6.16	126.95	119.99
2	HHH	133	GLY	C-N-CA	6.16	126.95	119.99
2	HHH	192	GLN	CA-C-N	6.10	129.54	120.87
2	HHH	192	GLN	C-N-CA	6.10	129.54	120.87
2	HHH	91	TYR	CA-C-O	-5.93	113.73	120.32
1	AAA	43	GLU	N-CA-C	-5.50	106.34	113.16
1	AAA	166	PHE	N-CA-C	-5.48	106.95	113.97
3	LLL	110	PRO	N-CA-C	5.40	119.96	111.38
3	LLL	168	GLN	CB-CA-C	-5.36	101.17	110.45
2	HHH	113	SER	CA-C-N	5.32	129.86	121.56
2	HHH	113	SER	C-N-CA	5.32	129.86	121.56
2	HHH	92	CYS	N-CA-CB	5.30	118.51	110.45
3	LLL	121	PRO	CA-C-O	-5.27	115.33	121.34
2	HHH	94	ARG	CA-C-O	-5.24	114.90	120.92
1	AAA	168	LEU	CA-C-O	-5.22	116.02	121.55
2	HHH	97	ALA	O-C-N	5.20	129.63	123.24
2	HHH	113	SER	O-C-N	5.20	128.07	122.15
1	AAA	281	GLU	O-C-N	5.11	127.53	122.12
2	HHH	24	ALA	CA-C-O	-5.08	115.27	121.36
2	HHH	90	TYR	CA-C-O	-5.07	114.86	120.38
1	AAA	69	GLY	CA-C-O	-5.07	116.17	122.65
1	AAA	107	VAL	CA-C-O	-5.07	116.00	121.27
3	LLL	204	GLU	CB-CA-C	5.07	118.02	110.62
2	HHH	50	ALA	CA-C-O	-5.05	114.33	120.54
1	AAA	24	HIS	CB-CA-C	5.04	117.19	109.03
1	AAA	132	ARG	CB-CA-C	5.02	118.84	110.81
2	HHH	208	ASP	CB-CA-C	5.02	118.03	109.75
1	AAA	160	HIS	N-CA-C	-5.01	105.92	112.23

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	117	GLY	Peptide
1	AAA	334	TYR	Peptide
3	LLL	211	GLU	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	AAA	2417	2413	2398	97	2
2	HHH	1631	1607	1601	74	2
3	LLL	1577	1528	1524	72	0
4	AAA	2	0	0	0	0
5	AAA	5	0	0	2	0
All	All	5632	5548	5523	227	2

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 20.

All (227) 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:AAA:38:LYS:HE2	2:HHH:98:ASP:HA	1.36	1.02
3:LLL:167:LYS:HD3	3:LLL:171:ASN:HA	1.36	1.01
2:HHH:48:VAL:HG13	2:HHH:63:VAL:HG11	1.44	0.97
3:LLL:83:GLU:HB3	3:LLL:106:VAL:HG12	1.48	0.95
3:LLL:171:ASN:O	3:LLL:171:ASN:ND2	2.01	0.94
1:AAA:162:GLN:H	1:AAA:163:PRO:CD	1.82	0.92
2:HHH:197:ASN:H	2:HHH:197:ASN:HD22	1.15	0.92
3:LLL:83:GLU:HA	3:LLL:104:LEU:HD23	1.54	0.90
3:LLL:51:ASN:HD21	3:LLL:66:LYS:HE3	1.39	0.87
2:HHH:119:PRO:HB3	2:HHH:145:TYR:HB3	1.57	0.84
3:LLL:193:SER:OG	3:LLL:206:THR:OG1	1.93	0.84
1:AAA:42:VAL:HG22	1:AAA:118:GLY:HA2	1.59	0.82
2:HHH:157:GLY:O	2:HHH:160:THR:CG2	2.27	0.82
2:HHH:157:GLY:O	2:HHH:160:THR:HG22	1.80	0.82
2:HHH:212:GLU:H	2:HHH:213:PRO:HD3	1.43	0.82
1:AAA:261:PRO:HD2	1:AAA:311:THR:OG1	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:LLL:18:LYS:HB2	3:LLL:76:THR:HA	1.62	0.80
2:HHH:195:ILE:HG23	2:HHH:209:LYS:C	2.07	0.80
1:AAA:130:HIS:CE1	1:AAA:290:SER:HB3	2.17	0.79
1:AAA:177:GLN:NE2	1:AAA:177:GLN:HA	1.93	0.78
2:HHH:179:SER:OG	3:LLL:178:TYR:OH	1.92	0.78
1:AAA:40:LYS:HG3	1:AAA:40:LYS:O	1.83	0.77
1:AAA:162:GLN:H	1:AAA:163:PRO:HD3	1.50	0.76
3:LLL:83:GLU:HA	3:LLL:104:LEU:CD2	2.16	0.76
3:LLL:109:GLN:OE1	3:LLL:171:ASN:ND2	2.19	0.76
2:HHH:3:GLN:N	2:HHH:25:SER:HG	1.84	0.75
1:AAA:226:GLY:O	1:AAA:230:VAL:HG23	1.88	0.74
1:AAA:42:VAL:HG22	1:AAA:118:GLY:CA	2.18	0.74
1:AAA:120:HIS:CE1	1:AAA:251:ASP:HB2	2.23	0.73
2:HHH:197:ASN:H	2:HHH:197:ASN:ND2	1.85	0.73
2:HHH:126:PRO:HG3	2:HHH:138:LEU:HB3	1.70	0.73
3:LLL:25:GLY:HA3	3:LLL:28:ILE:HD12	1.72	0.72
1:AAA:162:GLN:N	1:AAA:163:PRO:CD	2.51	0.70
1:AAA:39:ARG:NH1	1:AAA:160:HIS:CE1	2.60	0.70
3:LLL:5:LEU:HD22	3:LLL:28:ILE:HD11	1.75	0.69
2:HHH:6:GLU:N	2:HHH:6:GLU:OE1	2.23	0.69
3:LLL:167:LYS:CD	3:LLL:171:ASN:HA	2.20	0.69
2:HHH:197:ASN:HD22	2:HHH:197:ASN:N	1.91	0.69
3:LLL:96:LEU:HD12	3:LLL:96:LEU:H	1.58	0.68
2:HHH:212:GLU:HA	2:HHH:214:LYS:HE3	1.76	0.68
1:AAA:39:ARG:NH1	1:AAA:160:HIS:HE1	1.91	0.68
2:HHH:196:CYS:SG	2:HHH:196:CYS:O	2.54	0.65
3:LLL:11:VAL:HG23	3:LLL:104:LEU:HB2	1.77	0.65
2:HHH:150:VAL:CG2	2:HHH:178:LEU:HD21	2.27	0.64
1:AAA:137:LEU:HD12	1:AAA:137:LEU:C	2.23	0.64
3:LLL:171:ASN:C	3:LLL:171:ASN:HD22	2.06	0.63
3:LLL:167:LYS:HE2	3:LLL:171:ASN:CG	2.24	0.63
3:LLL:37:GLN:HB2	3:LLL:86:TYR:CE2	2.35	0.62
2:HHH:181:VAL:HG21	3:LLL:136:LEU:HD12	1.82	0.62
3:LLL:14:ALA:O	3:LLL:17:GLN:HG2	2.00	0.62
3:LLL:38:GLN:HB3	3:LLL:85:ASP:HB2	1.82	0.61
1:AAA:162:GLN:N	1:AAA:163:PRO:HD2	2.16	0.61
3:LLL:83:GLU:HB3	3:LLL:106:VAL:CG1	2.27	0.61
3:LLL:17:GLN:NE2	3:LLL:17:GLN:HA	2.15	0.60
3:LLL:27:SER:O	3:LLL:30:SER:OG	2.15	0.60
1:AAA:66:LYS:HG2	1:AAA:68:PHE:CE1	2.36	0.60
1:AAA:137:LEU:HD12	1:AAA:137:LEU:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:194:VAL:HG23	1:AAA:238:LEU:HD21	1.82	0.60
2:HHH:212:GLU:N	2:HHH:213:PRO:CD	2.64	0.60
3:LLL:17:GLN:HA	3:LLL:17:GLN:HE21	1.66	0.59
1:AAA:162:GLN:H	1:AAA:163:PRO:HD2	1.66	0.59
3:LLL:62:PHE:CD2	3:LLL:75:ILE:HG12	2.37	0.59
3:LLL:13:ALA:HB3	3:LLL:78:LEU:HD13	1.84	0.59
2:HHH:150:VAL:HG22	2:HHH:178:LEU:HD21	1.85	0.59
2:HHH:94:ARG:NH1	2:HHH:101:ASP:OD2	2.35	0.59
1:AAA:294:LEU:HD22	1:AAA:315:ALA:HB1	1.84	0.59
1:AAA:116:LEU:CD1	1:AAA:116:LEU:N	2.66	0.59
2:HHH:67:PHE:CZ	2:HHH:82:MET:HG2	2.38	0.59
1:AAA:148:ILE:HG23	1:AAA:148:ILE:O	2.03	0.59
1:AAA:220:ARG:HG3	1:AAA:220:ARG:HH11	1.67	0.59
3:LLL:211:GLU:H	3:LLL:211:GLU:CD	2.10	0.58
2:HHH:212:GLU:N	2:HHH:213:PRO:HD3	2.14	0.58
2:HHH:208:ASP:OD2	2:HHH:208:ASP:N	2.36	0.58
1:AAA:88:ASN:OD1	1:AAA:88:ASN:N	2.37	0.57
1:AAA:255:PHE:CZ	1:AAA:276:GLY:HA3	2.40	0.57
2:HHH:104:GLY:O	3:LLL:43:ALA:CB	2.52	0.57
3:LLL:96:LEU:HD12	3:LLL:96:LEU:N	2.19	0.57
1:AAA:98:GLU:O	1:AAA:102:VAL:HG23	2.04	0.57
2:HHH:67:PHE:CE1	2:HHH:82:MET:HG2	2.39	0.57
2:HHH:195:ILE:HG23	2:HHH:209:LYS:O	2.03	0.57
3:LLL:166:SER:O	3:LLL:173:TYR:HA	2.05	0.57
2:HHH:156:SER:H	2:HHH:197:ASN:HD21	1.53	0.57
1:AAA:122:LEU:HD12	1:AAA:122:LEU:C	2.30	0.56
1:AAA:154:THR:HG21	1:AAA:158:ASN:HB3	1.86	0.56
2:HHH:212:GLU:H	2:HHH:213:PRO:CD	2.14	0.56
1:AAA:158:ASN:O	1:AAA:162:GLN:NE2	2.36	0.56
1:AAA:337:LEU:N	1:AAA:337:LEU:HD23	2.21	0.56
2:HHH:36:TRP:NE1	2:HHH:80:LEU:HB2	2.21	0.55
3:LLL:211:GLU:N	3:LLL:211:GLU:OE1	2.39	0.55
3:LLL:11:VAL:HG23	3:LLL:104:LEU:HA	1.88	0.55
2:HHH:201:LYS:N	2:HHH:202:PRO:HD2	2.23	0.54
2:HHH:189:LEU:HD23	2:HHH:190:GLY:H	1.70	0.54
1:AAA:165:SER:O	1:AAA:175:VAL:HG21	2.07	0.54
2:HHH:146:PHE:HB2	2:HHH:175:LEU:HD23	1.89	0.54
3:LLL:5:LEU:HD22	3:LLL:28:ILE:CD1	2.37	0.53
3:LLL:38:GLN:NE2	3:LLL:42:THR:O	2.40	0.53
2:HHH:22:CYS:HB3	2:HHH:78:LEU:HB3	1.90	0.53
1:AAA:23:VAL:O	1:AAA:23:VAL:HG22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:220:ARG:HG3	1:AAA:220:ARG:NH1	2.24	0.53
3:LLL:107:LEU:O	3:LLL:107:LEU:HD12	2.09	0.53
1:AAA:147:ASP:HB3	1:AAA:163:PRO:HD2	1.91	0.52
1:AAA:122:LEU:HD21	1:AAA:295:VAL:HG12	1.92	0.52
2:HHH:189:LEU:HB2	2:HHH:214:LYS:NZ	2.25	0.51
1:AAA:103:VAL:HG21	1:AAA:126:THR:HA	1.91	0.51
1:AAA:219:MET:HE1	1:AAA:271:LEU:HD23	1.93	0.51
1:AAA:337:LEU:HD23	1:AAA:337:LEU:H	1.74	0.51
1:AAA:177:GLN:NE2	1:AAA:177:GLN:CA	2.70	0.51
2:HHH:181:VAL:HG21	3:LLL:136:LEU:CD1	2.41	0.51
1:AAA:326:THR:OG1	1:AAA:329:GLY:O	2.23	0.50
1:AAA:148:ILE:O	1:AAA:148:ILE:HG12	2.11	0.50
1:AAA:168:LEU:HD12	1:AAA:188:ILE:HG22	1.93	0.50
2:HHH:179:SER:HB2	3:LLL:136:LEU:HD21	1.94	0.50
1:AAA:66:LYS:HE3	1:AAA:68:PHE:CZ	2.46	0.50
1:AAA:76:VAL:O	1:AAA:88:ASN:ND2	2.44	0.50
3:LLL:17:GLN:NE2	3:LLL:17:GLN:CA	2.73	0.50
1:AAA:120:HIS:HE1	1:AAA:251:ASP:HB2	1.75	0.50
3:LLL:7:GLN:NE2	3:LLL:86:TYR:O	2.43	0.50
2:HHH:157:GLY:O	2:HHH:160:THR:HG23	2.09	0.50
1:AAA:35:GLN:NE2	1:AAA:159:LEU:HB2	2.26	0.50
1:AAA:82:TYR:CD1	1:AAA:82:TYR:C	2.89	0.50
1:AAA:336:GLN:HA	1:AAA:336:GLN:OE1	2.11	0.49
2:HHH:189:LEU:H	2:HHH:189:LEU:HD22	1.77	0.49
3:LLL:91:TRP:CZ2	3:LLL:95(A):SER:HA	2.48	0.49
2:HHH:179:SER:CB	3:LLL:136:LEU:HD21	2.42	0.49
2:HHH:48:VAL:HG13	2:HHH:63:VAL:CG1	2.30	0.49
2:HHH:154:TRP:CH2	2:HHH:196:CYS:HB3	2.48	0.49
1:AAA:137:LEU:C	1:AAA:137:LEU:CD1	2.86	0.49
2:HHH:121:VAL:HB	2:HHH:207:VAL:HG11	1.94	0.49
2:HHH:151:THR:HG23	2:HHH:199:ASN:HB3	1.95	0.48
3:LLL:142:PRO:O	3:LLL:198:HIS:HE1	1.96	0.48
1:AAA:130:HIS:HE1	1:AAA:290:SER:HB3	1.70	0.48
1:AAA:168:LEU:HD23	1:AAA:171:LEU:CD1	2.44	0.48
1:AAA:211:ASN:C	1:AAA:211:ASN:HD22	2.22	0.48
2:HHH:154:TRP:CZ3	2:HHH:196:CYS:HB3	2.49	0.48
1:AAA:227:ILE:HD12	1:AAA:227:ILE:HA	1.78	0.47
1:AAA:296:GLU:OE2	5:AAA:403:PO4:O4	2.33	0.47
2:HHH:167:PRO:HG3	3:LLL:166:SER:OG	2.14	0.47
3:LLL:52:SER:HB3	3:LLL:64:GLY:O	2.14	0.47
1:AAA:207:PHE:C	1:AAA:207:PHE:CD2	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:LLL:38:GLN:O	3:LLL:84:ALA:HB1	2.15	0.47
1:AAA:23:VAL:HG21	1:AAA:289:LEU:O	2.15	0.47
1:AAA:264:GLY:HA2	1:AAA:301:LEU:HD12	1.97	0.46
2:HHH:100(B):TYR:CE1	2:HHH:101:ASP:HB3	2.51	0.46
2:HHH:154:TRP:O	2:HHH:159:LEU:HB3	2.15	0.46
3:LLL:83:GLU:CB	3:LLL:106:VAL:HG12	2.31	0.46
3:LLL:11:VAL:CG2	3:LLL:104:LEU:HB2	2.44	0.46
1:AAA:261:PRO:HD2	1:AAA:311:THR:HG1	1.79	0.46
1:AAA:76:VAL:HA	1:AAA:77:PRO:HA	1.68	0.46
3:LLL:26:SER:C	3:LLL:69:THR:HG22	2.41	0.46
1:AAA:34:SER:HB2	1:AAA:42:VAL:CG1	2.46	0.46
2:HHH:145:TYR:HB2	2:HHH:200:HIS:CE1	2.50	0.46
3:LLL:109:GLN:HB2	3:LLL:141:TYR:CZ	2.51	0.46
3:LLL:34:SER:HA	3:LLL:48:ILE:O	2.13	0.46
2:HHH:145:TYR:CE1	2:HHH:150:VAL:HG13	2.50	0.46
1:AAA:66:LYS:HD3	1:AAA:111:TYR:CE2	2.50	0.46
1:AAA:66:LYS:HB2	1:AAA:111:TYR:OH	2.16	0.45
1:AAA:120:HIS:CG	1:AAA:295:VAL:HG21	2.52	0.45
1:AAA:130:HIS:NE2	1:AAA:290:SER:HB3	2.32	0.45
2:HHH:178:LEU:HD12	2:HHH:178:LEU:C	2.42	0.45
1:AAA:28:VAL:HG21	1:AAA:55:MET:SD	2.57	0.45
2:HHH:99:LEU:HB3	3:LLL:32:TYR:CZ	2.52	0.45
2:HHH:122:PHE:HD1	3:LLL:124:GLU:HB2	1.82	0.45
1:AAA:85:LEU:HD13	2:HHH:100(A):LEU:HD22	1.99	0.44
1:AAA:116:LEU:N	1:AAA:116:LEU:HD13	2.32	0.44
1:AAA:154:THR:HG21	1:AAA:162:GLN:HG3	1.98	0.44
2:HHH:184:VAL:HB	2:HHH:185:PRO:HD2	1.99	0.44
2:HHH:45:LEU:HD12	3:LLL:87:TYR:CD2	2.52	0.44
2:HHH:189:LEU:HD23	2:HHH:190:GLY:N	2.33	0.44
3:LLL:27(B):ASN:O	3:LLL:31:HIS:N	2.50	0.44
3:LLL:167:LYS:HE2	3:LLL:171:ASN:CB	2.47	0.44
1:AAA:90:ARG:O	1:AAA:90:ARG:HG3	2.10	0.44
1:AAA:129:GLY:O	1:AAA:132:ARG:HB3	2.18	0.44
2:HHH:169:VAL:HA	3:LLL:163:THR:HG22	2.00	0.44
3:LLL:168:GLN:HE21	3:LLL:168:GLN:HB3	1.44	0.44
3:LLL:51:ASN:ND2	3:LLL:66:LYS:HE3	2.20	0.44
2:HHH:122:PHE:HD1	3:LLL:124:GLU:CB	2.31	0.43
1:AAA:199:ARG:HD3	1:AAA:219:MET:HG2	2.01	0.43
2:HHH:99:LEU:HG	3:LLL:50:ASP:OD2	2.17	0.43
1:AAA:67:ASP:OD1	1:AAA:67:ASP:C	2.62	0.43
3:LLL:186:TRP:CZ2	3:LLL:209:PRO:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:294:LEU:CD2	1:AAA:315:ALA:HB1	2.47	0.43
2:HHH:146:PHE:HA	2:HHH:147:PRO:HA	1.84	0.43
3:LLL:37:GLN:HG2	3:LLL:37:GLN:O	2.17	0.43
1:AAA:248:LEU:O	1:AAA:292:LEU:HA	2.19	0.43
2:HHH:63:VAL:O	2:HHH:63:VAL:HG23	2.18	0.43
1:AAA:26:VAL:HG12	1:AAA:65:LEU:HD23	2.00	0.43
1:AAA:141:TRP:HB3	1:AAA:195:TYR:CD1	2.54	0.43
1:AAA:119:ASP:C	1:AAA:121:SER:H	2.27	0.42
1:AAA:61:LEU:HB3	1:AAA:63:CYS:SG	2.59	0.42
2:HHH:18:LEU:HD12	2:HHH:18:LEU:HA	1.90	0.42
1:AAA:37:GLN:HB3	1:AAA:38:LYS:HE3	2.02	0.42
2:HHH:94:ARG:HH11	2:HHH:101:ASP:CG	2.26	0.42
2:HHH:194:TYR:HD1	2:HHH:194:TYR:HA	1.68	0.42
1:AAA:98:GLU:O	1:AAA:98:GLU:HG3	2.20	0.42
3:LLL:84:ALA:H	3:LLL:104:LEU:HD23	1.85	0.42
3:LLL:8:PRO:O	3:LLL:102:THR:OG1	2.27	0.42
3:LLL:104:LEU:HD23	3:LLL:104:LEU:O	2.20	0.42
1:AAA:61:LEU:HD12	1:AAA:61:LEU:HA	1.93	0.42
1:AAA:202:ASP:HB3	1:AAA:204:PRO:HD2	2.01	0.42
1:AAA:120:HIS:CD2	1:AAA:295:VAL:HG21	2.55	0.41
1:AAA:143:ASP:HB3	1:AAA:145:HIS:O	2.20	0.41
1:AAA:202:ASP:CB	1:AAA:204:PRO:HD2	2.50	0.41
2:HHH:64:LYS:HG3	2:HHH:65:SER:N	2.34	0.41
2:HHH:189:LEU:HB2	2:HHH:214:LYS:HZ2	1.83	0.41
3:LLL:58:ILE:H	3:LLL:58:ILE:CD1	2.32	0.41
2:HHH:83:ARG:C	2:HHH:111:VAL:HG11	2.45	0.41
1:AAA:300:GLN:HA	2:HHH:28:THR:HG22	2.02	0.41
2:HHH:82:MET:HE3	2:HHH:82:MET:HB2	1.69	0.41
3:LLL:13:ALA:HB3	3:LLL:78:LEU:CD1	2.49	0.41
1:AAA:154:THR:HG21	1:AAA:158:ASN:CB	2.49	0.41
1:AAA:42:VAL:HG22	1:AAA:118:GLY:C	2.45	0.41
1:AAA:313:ASN:HD22	1:AAA:313:ASN:HA	1.71	0.41
1:AAA:113:CYS:O	1:AAA:292:LEU:N	2.47	0.41
2:HHH:195:ILE:CG2	2:HHH:209:LYS:O	2.69	0.41
3:LLL:27(A):SER:HB3	3:LLL:94:LEU:HG	2.03	0.41
1:AAA:147:ASP:OD1	5:AAA:403:PO4:O2	2.39	0.41
1:AAA:249:SER:HA	1:AAA:293:ASP:HB2	2.03	0.41
3:LLL:96:LEU:H	3:LLL:96:LEU:CD1	2.31	0.41
1:AAA:172:GLN:OE1	1:AAA:172:GLN:N	2.53	0.40
1:AAA:42:VAL:O	1:AAA:118:GLY:HA2	2.21	0.40
2:HHH:195:ILE:HA	2:HHH:209:LYS:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:LLL:25:GLY:HA3	3:LLL:28:ILE:CD1	2.48	0.40
1:AAA:58:LEU:O	1:AAA:63:CYS:SG	2.70	0.40
2:HHH:168:ALA:HB2	2:HHH:178:LEU:HB3	2.04	0.40
2:HHH:166:PHE:N	2:HHH:166:PHE:CD1	2.89	0.40
3:LLL:26:SER:HA	3:LLL:69:THR:HG22	2.03	0.40
1:AAA:150:THR:N	1:AAA:153:THR:OG1	2.55	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:97:GLN:NE2	2:HHH:64:LYS:O[5_556]	1.88	0.32
1:AAA:97:GLN:HE22	2:HHH:64:LYS:O[5_556]	1.48	0.12

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	AAA	314/339 (93%)	288 (92%)	24 (8%)	2 (1%)	21	51	
2	HHH	213/233 (91%)	199 (93%)	12 (6%)	2 (1%)	14	41	
3	LLL	211/220 (96%)	199 (94%)	11 (5%)	1 (0%)	24	54	
All	All	738/792 (93%)	686 (93%)	47 (6%)	5 (1%)	18	48	

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	162	GLN
1	AAA	120	HIS
2	HHH	98	ASP
2	HHH	212	GLU
3	LLL	68	GLY

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	AAA	266/288 (92%)	231 (87%)	35 (13%)	4	13
2	HHH	181/193 (94%)	153 (84%)	28 (16%)	2	9
3	LLL	178/184 (97%)	144 (81%)	34 (19%)	1	5
All	All	625/665 (94%)	528 (84%)	97 (16%)	2	9

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	22	MET
1	AAA	25	SER
1	AAA	38	LYS
1	AAA	59	SER
1	AAA	63	CYS
1	AAA	72	SER
1	AAA	88	ASN
1	AAA	90	ARG
1	AAA	101	GLU
1	AAA	105	ARG
1	AAA	108	SER
1	AAA	112	SER
1	AAA	116	LEU
1	AAA	137	LEU
1	AAA	151	PRO
1	AAA	158	ASN
1	AAA	162	GLN
1	AAA	168	LEU
1	AAA	172	GLN
1	AAA	173	ASP
1	AAA	177	GLN
1	AAA	184	ILE
1	AAA	188	ILE
1	AAA	190	SER
1	AAA	207	PHE
1	AAA	211	ASN

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Mol	Chain	Res	Type
1	AAA	219	MET
1	AAA	222	ILE
1	AAA	229	LYS
1	AAA	236	ASP
1	AAA	241	LYS
1	AAA	265	THR
1	AAA	268	VAL
1	AAA	294	LEU
1	AAA	332	ILE
2	HHH	26	GLU
2	HHH	30	ARG
2	HHH	32	ASP
2	HHH	56	SER
2	HHH	63	VAL
2	HHH	74	SER
2	HHH	76	ASN
2	HHH	85	GLU
2	HHH	105	ARG
2	HHH	110	THR
2	HHH	117	LYS
2	HHH	121	VAL
2	HHH	147	PRO
2	HHH	151	THR
2	HHH	153	SER
2	HHH	164	HIS
2	HHH	179	SER
2	HHH	181	VAL
2	HHH	189	LEU
2	HHH	191	THR
2	HHH	192	GLN
2	HHH	197	ASN
2	HHH	205	THR
2	HHH	206	LYS
2	HHH	208	ASP
2	HHH	209	LYS
2	HHH	212	GLU
2	HHH	214	LYS
3	LLL	11	VAL
3	LLL	18	LYS
3	LLL	19	VAL
3	LLL	27(B)	ASN
3	LLL	37	GLN

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Mol	Chain	Res	Type
3	LLL	38	GLN
3	LLL	47	LEU
3	LLL	48	ILE
3	LLL	52	SER
3	LLL	55	THR
3	LLL	58	ILE
3	LLL	60	ASP
3	LLL	63	SER
3	LLL	69	THR
3	LLL	79	GLN
3	LLL	83	GLU
3	LLL	95(B)	ASN
3	LLL	104	LEU
3	LLL	106	VAL
3	LLL	107	LEU
3	LLL	111	LYS
3	LLL	123	SER
3	LLL	127	GLN
3	LLL	146	THR
3	LLL	166	SER
3	LLL	167	LYS
3	LLL	169	SER
3	LLL	171	ASN
3	LLL	176	SER
3	LLL	193	SER
3	LLL	203	VAL
3	LLL	204	GLU
3	LLL	210	THR
3	LLL	211	GLU

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z > 2$
5	PO4	AAA	403	4	4,4,4	1.17	1 (25%)	6,6,6	0.50	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AAA	403	PO4	P-O1	2.06	1.55	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	AAA	403	PO4	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, 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	AAA	316/339 (93%)	-1.27	0 100 100	43, 62, 86, 114	0
2	HHH	216/233 (92%)	-1.03	0 100 100	50, 82, 145, 155	1 (0%)
3	LLL	213/220 (96%)	-0.97	0 100 100	57, 99, 151, 182	0
All	All	745/792 (94%)	-1.12	0 100 100	43, 74, 143, 182	1 (0%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
5	PO4	AAA	403	5/5	0.99	0.05	62,81,88,94	0
4	MN	AAA	402	1/1	1.00	0.02	63,63,63,63	0
4	MN	AAA	401	1/1	1.00	0.01	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.