



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:29 PM UTC

PDB ID : 3HIE / pdb_00003hie
Title : Structure of the membrane-binding domain of the Sec3 subunit of the Exocyst complex
Authors : Baek, K.; Dominguez, R.
Deposited on : 2009-05-19
Resolution : 2.00 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

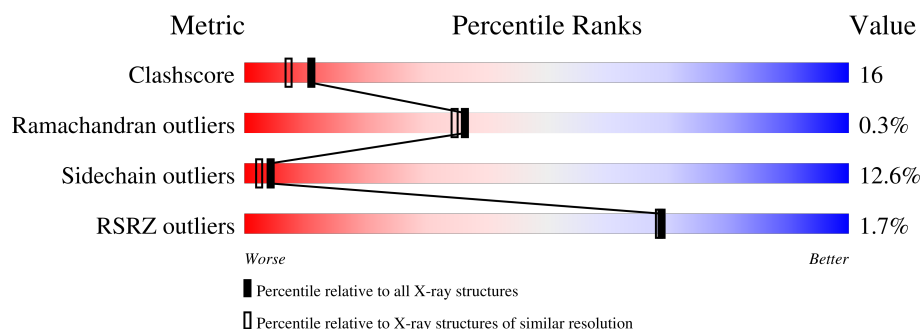
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	A	171	2% 70% 20% • 6%
1	B	171	% 66% 23% 6% 5%
1	C	171	% 64% 25% 6% • •
1	D	171	2% 62% 26% 5% 8%

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
2	PO4	A	1	-	-	X	-
2	PO4	B	2	-	-	X	-

2 Entry composition [i](#)

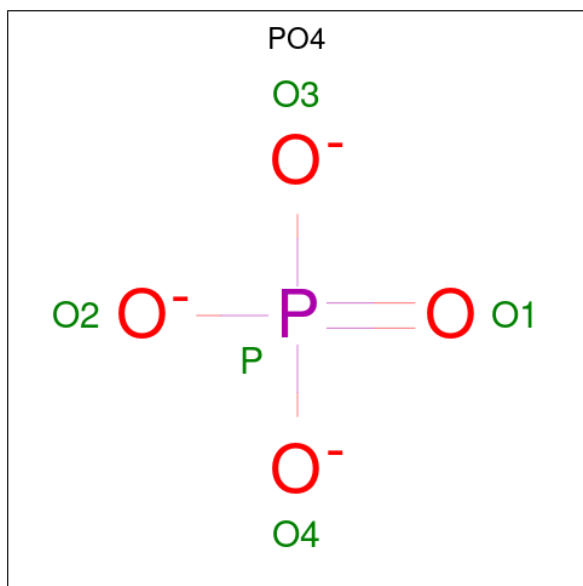
There are 3 unique types of molecules in this entry. The entry contains 5651 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Exocyst complex component SEC3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	Se	0	6	0
			1356	870	230	253	2	1			
1	B	163	Total	C	N	O	S	Se	0	1	0
			1355	867	233	252	2	1			
1	C	164	Total	C	N	O	S	Se	0	0	0
			1360	867	237	253	2	1			
1	D	158	Total	C	N	O	S	Se	0	1	0
			1321	845	229	244	2	1			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

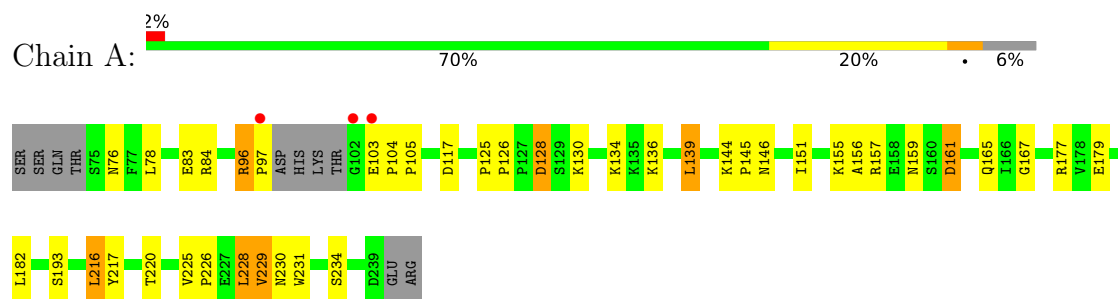
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	105	Total 105	O 105	0	0
3	B	59	Total 59	O 59	0	0
3	C	26	Total 26	O 26	0	0
3	D	59	Total 59	O 59	0	0

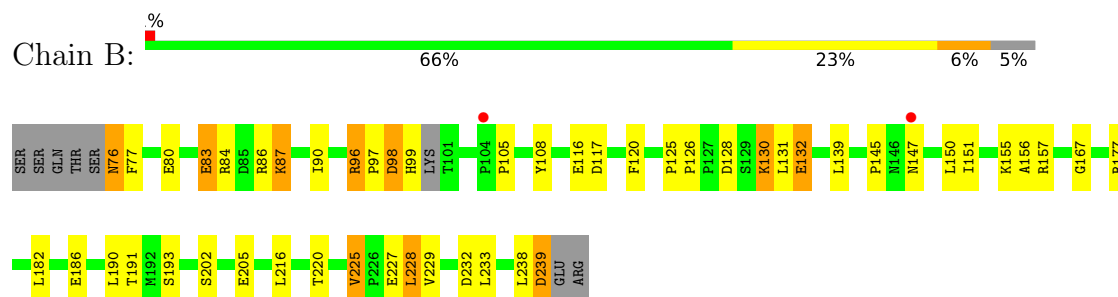
3 Residue-property plots [i](#)

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.

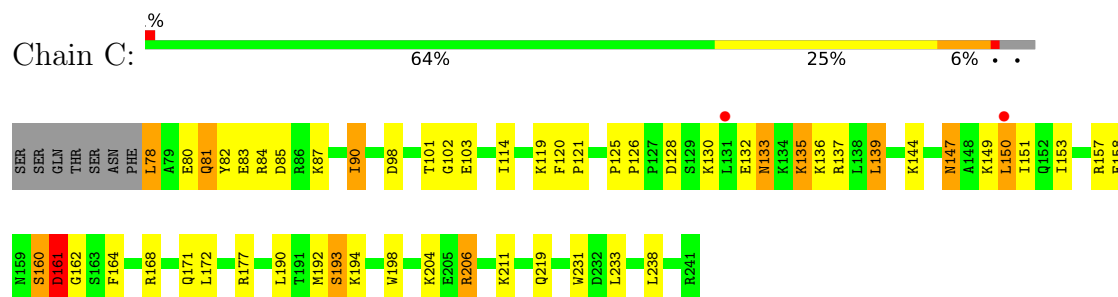
• Molecule 1: Exocyst complex component SEC3



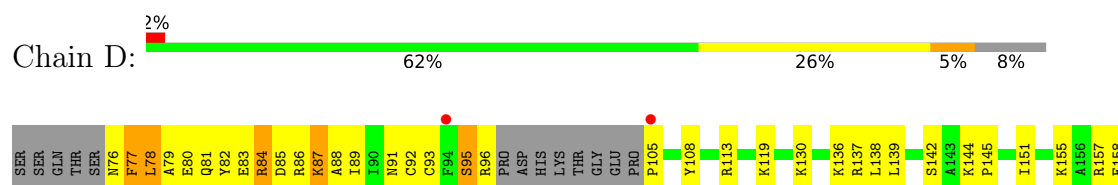
• Molecule 1: Exocyst complex component SEC3



• Molecule 1: Exocyst complex component SEC3



• Molecule 1: Exocyst complex component SEC3





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	40.70Å 68.49Å 68.04Å 89.90° 82.17° 71.79°	Depositor
Resolution (Å)	38.74 – 2.00 38.74 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.5 (38.74-2.00) 93.5 (38.74-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.202 , 0.248 0.207 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.007 for -h,-h+k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5651	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% 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: 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	A	1.46	3/1403 (0.2%)	0.88	1/1891 (0.1%)
1	B	1.36	0/1388	0.85	2/1873 (0.1%)
1	C	0.77	0/1390	0.94	6/1874 (0.3%)
1	D	0.64	0/1351	0.87	2/1817 (0.1%)
All	All	1.12	3/5532 (0.1%)	0.89	11/7455 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	LEU	C-O	-5.76	1.17	1.24
1	A	125	PRO	C-O	-5.35	1.20	1.24
1	A	83	GLU	C-O	-5.22	1.17	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	193	SER	N-CA-C	-9.39	101.95	113.97
1	C	102	GLY	N-CA-C	-8.33	103.31	115.30
1	C	193	SER	N-CA-C	-8.10	103.19	113.23
1	B	193	SER	N-CA-C	-7.73	104.37	113.88
1	A	193	SER	N-CA-C	-6.50	105.89	113.88
1	B	77	PHE	N-CA-C	-6.42	104.37	111.82
1	C	192	MSE	N-CA-C	6.31	118.89	108.48
1	C	192	MSE	CB-CA-C	-5.98	103.70	114.52
1	C	90	ILE	CB-CA-C	-5.92	104.39	111.97
1	C	125	PRO	O-C-N	5.35	123.67	121.15
1	D	162	GLY	N-CA-C	-5.11	101.06	113.18

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1356	0	1374	40	0
1	B	1355	0	1355	53	0
1	C	1360	0	1367	57	0
1	D	1321	0	1333	39	0
2	A	5	0	0	6	0
2	B	5	0	0	8	0
3	A	105	0	0	1	0
3	B	59	0	0	4	0
3	C	26	0	0	2	0
3	D	59	0	0	2	0
All	All	5651	0	5429	178	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (178) 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:C:101:THR:HG23	1:C:103:GLU:N	1.36	1.35
1:C:219:GLN:NE2	1:D:225:VAL:HG23	1.48	1.24
1:C:101:THR:CG2	1:C:103:GLU:H	1.51	1.22
1:A:167:GLY:HA3	2:A:1:PO4:O4	1.36	1.22
1:C:101:THR:OG1	1:C:103:GLU:HG3	1.38	1.21
1:C:101:THR:CG2	1:C:103:GLU:HB2	1.76	1.13
1:C:98:ASP:HB3	1:C:101:THR:CG2	1.80	1.11
1:A:225:VAL:HG13	1:A:226:PRO:HD2	1.34	1.09
1:C:98:ASP:CB	1:C:101:THR:HG22	1.83	1.07
1:B:167:GLY:HA3	2:B:2:PO4:O1	1.56	1.06
1:B:228:LEU:HD22	1:B:228:LEU:H	1.17	1.04
1:C:101:THR:HG21	1:C:103:GLU:HB2	1.06	1.02
1:A:103:GLU:HB3	1:A:104:PRO:CD	1.92	0.99
1:B:228:LEU:H	1:B:228:LEU:CD2	1.76	0.98
1:C:101:THR:HG21	1:C:103:GLU:CB	1.92	0.98
1:C:101:THR:CG2	1:C:103:GLU:CB	2.42	0.97
1:A:103:GLU:HB3	1:A:104:PRO:HD2	1.45	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:LYS:HE2	1:D:87:LYS:HA	1.49	0.95
1:D:77:PHE:HD1	1:D:77:PHE:O	1.48	0.94
1:C:206:ARG:HH11	1:C:206:ARG:HG2	1.28	0.93
1:B:147:ASN:ND2	1:B:150:LEU:HD12	1.83	0.93
1:C:98:ASP:HB3	1:C:101:THR:HG22	0.94	0.92
1:C:219:GLN:HE21	1:D:225:VAL:HG23	1.18	0.92
1:C:219:GLN:HE21	1:D:225:VAL:CG2	1.84	0.89
1:A:167:GLY:CA	2:A:1:PO4:O4	2.21	0.89
1:A:226:PRO:HG2	1:A:228:LEU:CD2	2.02	0.88
1:C:219:GLN:NE2	1:D:225:VAL:CG2	2.37	0.88
1:D:77:PHE:C	1:D:77:PHE:CD1	2.47	0.88
1:A:226:PRO:HG2	1:A:228:LEU:HD21	1.58	0.85
1:A:217:TYR:OH	1:B:238:LEU:HD11	1.76	0.84
1:B:147:ASN:ND2	1:B:150:LEU:CD1	2.39	0.84
1:D:77:PHE:O	1:D:77:PHE:CD1	2.30	0.84
1:A:157:ARG:NE	2:A:1:PO4:O1	2.10	0.83
1:C:78:LEU:HB2	3:C:250:HOH:O	1.79	0.83
1:C:101:THR:HG23	1:C:103:GLU:CA	2.09	0.82
1:A:226:PRO:CG	1:A:228:LEU:HD21	2.12	0.79
1:C:206:ARG:HH11	1:C:206:ARG:CG	1.95	0.79
1:D:95:SER:O	1:D:96:ARG:HB2	1.84	0.77
1:C:101:THR:HG23	1:C:103:GLU:CB	2.13	0.76
1:D:87:LYS:HE2	1:D:87:LYS:CA	2.09	0.76
1:D:76:ASN:O	1:D:77:PHE:C	2.30	0.75
1:C:101:THR:HG23	1:C:103:GLU:H	0.64	0.74
1:C:101:THR:OG1	1:C:103:GLU:CG	2.30	0.74
1:B:228:LEU:CD2	1:B:228:LEU:N	2.45	0.74
1:A:155:LYS:HE3	2:A:1:PO4:O2	1.87	0.74
1:B:116:GLU:OE1	1:B:155:LYS:NZ	2.21	0.73
1:B:228:LEU:HD22	1:B:228:LEU:N	1.97	0.73
1:C:206:ARG:HG2	1:C:206:ARG:NH1	1.89	0.73
1:C:219:GLN:HE22	1:D:225:VAL:HG23	1.52	0.72
1:C:119:LYS:C	1:C:121:PRO:HD3	2.15	0.72
1:B:147:ASN:HB3	1:B:150:LEU:HB2	1.72	0.72
1:B:147:ASN:HD22	1:B:150:LEU:HD12	1.55	0.71
1:B:157:ARG:NE	2:B:2:PO4:O3	2.22	0.70
1:A:225:VAL:CG1	1:A:226:PRO:HD2	2.16	0.70
1:B:156:ALA:CA	2:B:2:PO4:O4	2.40	0.69
1:B:167:GLY:CA	2:B:2:PO4:O1	2.36	0.69
1:C:130:LYS:O	1:C:133:ASN:ND2	2.27	0.68
1:D:218:ILE:HG23	1:D:225:VAL:HG21	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:LYS:HG2	1:C:132:GLU:HG2	1.74	0.68
1:B:147:ASN:CG	1:B:150:LEU:HD12	2.18	0.68
1:D:96:ARG:H	1:D:105:PRO:HG3	1.58	0.67
1:D:85:ASP:O	1:D:89:ILE:HG13	1.94	0.67
1:C:160:SER:C	1:C:162:GLY:N	2.48	0.67
1:C:160:SER:O	1:C:161:ASP:C	2.36	0.65
1:B:98:ASP:OD2	1:B:99:HIS:N	2.30	0.65
1:C:160:SER:O	1:C:162:GLY:N	2.30	0.65
1:C:161:ASP:N	1:C:161:ASP:OD1	2.30	0.65
1:B:130:LYS:HG2	1:B:132:GLU:OE1	1.97	0.64
1:C:114:ILE:HD13	1:C:139:LEU:HD13	1.80	0.63
1:A:226:PRO:HG2	1:A:228:LEU:HD22	1.79	0.63
1:B:76:ASN:O	1:B:76:ASN:CG	2.42	0.62
1:A:161:ASP:OD2	1:A:161:ASP:N	2.29	0.62
1:C:78:LEU:N	3:C:263:HOH:O	2.33	0.62
1:C:101:THR:CB	1:C:103:GLU:HG3	2.29	0.61
1:D:86:ARG:NH1	3:D:282:HOH:O	2.30	0.60
1:B:147:ASN:CB	1:B:150:LEU:HD12	2.32	0.60
1:B:156:ALA:C	2:B:2:PO4:O4	2.45	0.59
1:A:156:ALA:CA	2:A:1:PO4:O3	2.51	0.59
1:B:84:ARG:HD2	3:B:284:HOH:O	2.01	0.59
1:A:105:PRO:O	1:A:145:PRO:HG3	2.03	0.59
1:A:226:PRO:HB2	1:A:228:LEU:CD1	2.33	0.58
1:C:101:THR:CG2	1:C:103:GLU:CG	2.82	0.58
1:D:88:ALA:O	1:D:92:CYS:SG	2.56	0.58
1:A:225:VAL:HG13	1:A:226:PRO:CD	2.22	0.57
1:D:87:LYS:HB3	1:D:87:LYS:NZ	2.19	0.57
1:C:147:ASN:HB3	1:C:150:LEU:HB2	1.86	0.57
1:A:226:PRO:CG	1:A:228:LEU:CD2	2.76	0.57
1:A:103:GLU:HB3	1:A:104:PRO:HD3	1.86	0.57
1:C:160:SER:C	1:C:162:GLY:H	2.13	0.57
1:A:228:LEU:H	1:A:228:LEU:HD13	1.69	0.56
1:B:87:LYS:NZ	3:B:281:HOH:O	2.25	0.56
1:B:225:VAL:O	1:B:228:LEU:HD21	2.05	0.56
1:C:80:GLU:O	1:C:81:GLN:C	2.46	0.55
1:C:98:ASP:CB	1:C:101:THR:CG2	2.61	0.55
1:B:156:ALA:HA	2:B:2:PO4:O4	2.06	0.54
1:A:226:PRO:HB2	1:A:228:LEU:HD13	1.88	0.54
1:A:177:ARG:HG2	1:A:179[B]:GLU:HG2	1.89	0.54
1:B:83[B]:GLU:CD	1:B:86:ARG:HH11	2.15	0.54
1:B:98:ASP:OD2	1:B:98:ASP:C	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:GLN:HG2	1:C:82:TYR:N	2.19	0.53
1:A:234[B]:SER:HB2	1:B:232:ASP:OD2	2.08	0.53
1:D:158:GLU:C	1:D:159:ASN:O	2.47	0.52
1:D:161:ASP:OD1	1:D:161:ASP:N	2.29	0.52
1:A:216:LEU:O	1:A:220:THR:HG23	2.10	0.52
1:B:225:VAL:HG12	1:B:227:GLU:OE1	2.09	0.52
1:C:120:PHE:N	1:C:121:PRO:HD3	2.21	0.52
1:D:233:LEU:C	1:D:233:LEU:HD23	2.35	0.52
1:A:156:ALA:HA	2:A:1:PO4:O3	2.11	0.51
1:C:101:THR:CG2	1:C:103:GLU:HG3	2.39	0.51
1:B:202:SER:OG	1:B:205:GLU:OE2	2.20	0.51
1:B:157:ARG:HH21	2:B:2:PO4:P	2.34	0.51
1:D:142:SER:O	1:D:151:ILE:HG23	2.10	0.51
1:C:133:ASN:HA	1:C:135:LYS:NZ	2.26	0.51
1:D:95:SER:O	1:D:96:ARG:CB	2.57	0.51
1:B:233:LEU:C	1:B:233:LEU:HD23	2.37	0.50
1:D:130:LYS:HG3	3:D:276:HOH:O	2.11	0.50
1:D:137:ARG:O	1:D:138:LEU:HD12	2.12	0.50
1:B:128:ASP:O	1:B:128:ASP:OD2	2.30	0.49
1:C:153:ILE:HD11	1:C:172:LEU:HD12	1.95	0.49
1:D:80:GLU:O	1:D:81:GLN:C	2.55	0.49
1:D:216:LEU:O	1:D:220:THR:HG23	2.13	0.49
1:B:238:LEU:O	3:B:247:HOH:O	2.20	0.48
1:C:80:GLU:HA	1:C:80:GLU:OE1	2.13	0.48
1:A:159:ASN:ND2	1:A:165:GLN:OE1	2.46	0.48
1:A:217:TYR:OH	3:A:263:HOH:O	2.20	0.48
1:D:231:TRP:C	1:D:231:TRP:CD1	2.92	0.47
1:B:147:ASN:ND2	1:B:150:LEU:HD11	2.26	0.47
1:B:87:LYS:HB3	1:B:87:LYS:HE2	1.62	0.47
1:B:105:PRO:O	1:B:145:PRO:HG3	2.14	0.47
1:A:217:TYR:OH	1:B:238:LEU:CD1	2.57	0.47
1:D:89:ILE:O	1:D:93:CYS:HB2	2.14	0.47
1:A:229:VAL:HA	1:B:238:LEU:HD23	1.96	0.47
1:A:117:ASP:OD1	1:A:134:LYS:NZ	2.44	0.47
1:B:120:PHE:CZ	1:B:126:PRO:HG2	2.50	0.46
1:C:177:ARG:HG3	1:D:237:TYR:HB3	1.97	0.46
1:C:233:LEU:C	1:C:233:LEU:HD23	2.40	0.46
1:D:78:LEU:O	1:D:79:ALA:C	2.56	0.46
1:A:231:TRP:C	1:A:231:TRP:CD1	2.93	0.46
1:B:216:LEU:O	1:B:220:THR:HG23	2.17	0.45
1:C:114:ILE:HG13	1:C:137:ARG:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:LEU:CD2	1:D:81:GLN:HE21	2.30	0.45
1:D:83:GLU:O	1:D:84:ARG:C	2.56	0.45
1:D:105:PRO:O	1:D:145:PRO:HG3	2.16	0.44
1:A:230:ASN:HD21	1:B:239:ASP:HB2	1.82	0.44
1:B:228:LEU:N	1:B:228:LEU:HD23	2.32	0.44
1:D:78:LEU:HD23	1:D:81:GLN:HE21	1.82	0.44
1:A:96:ARG:O	1:A:105:PRO:HB3	2.18	0.44
1:A:177:ARG:HD3	1:A:179[B]:GLU:CD	2.42	0.44
1:C:101:THR:CG2	1:C:103:GLU:N	2.30	0.44
1:C:136:LYS:O	1:C:137:ARG:HD3	2.18	0.43
1:A:96:ARG:HA	1:A:97:PRO:HD3	1.66	0.43
1:B:177:ARG:HB3	1:B:191:THR:HB	2.01	0.43
1:B:177:ARG:HD2	3:B:245:HOH:O	2.19	0.43
1:D:165:GLN:O	1:D:165:GLN:HG2	2.19	0.43
1:B:120:PHE:CE2	1:B:126:PRO:HD3	2.53	0.43
1:C:101:THR:C	1:C:103:GLU:N	2.68	0.43
1:D:81:GLN:OE1	1:D:113:ARG:NH2	2.52	0.43
1:C:114:ILE:HD12	1:C:198:TRP:CD1	2.53	0.42
1:D:86:ARG:HG3	1:D:108:TYR:CZ	2.54	0.42
1:B:120:PHE:CD2	1:B:126:PRO:HD3	2.55	0.42
1:B:151:ILE:HD12	1:B:220:THR:CG2	2.49	0.42
1:C:231:TRP:C	1:C:231:TRP:CD1	2.97	0.42
1:B:108:TYR:CD2	1:B:108:TYR:C	2.98	0.42
1:C:101:THR:HG1	1:C:103:GLU:HG3	1.72	0.42
1:B:96:ARG:HB2	1:B:97:PRO:HD2	2.01	0.42
1:C:84:ARG:O	1:C:85:ASP:C	2.62	0.42
1:B:117:ASP:C	1:B:117:ASP:OD2	2.61	0.42
1:A:103:GLU:CB	1:A:104:PRO:CD	2.70	0.41
1:A:126:PRO:C	1:A:128[A]:ASP:H	2.29	0.41
1:B:125:PRO:HA	1:B:126:PRO:HD3	1.92	0.41
1:C:83:GLU:O	1:C:84:ARG:C	2.62	0.41
1:C:158:GLU:HB2	1:C:164:PHE:CE1	2.55	0.41
1:C:126:PRO:C	1:C:128:ASP:N	2.78	0.41
1:D:79:ALA:O	1:D:82:TYR:HB3	2.21	0.41
1:A:225:VAL:CG1	1:A:226:PRO:CD	2.92	0.40
1:A:139:LEU:HD12	1:A:139:LEU:HA	1.87	0.40
1:B:157:ARG:HE	2:B:2:PO4:P	2.41	0.40
1:B:86:ARG:HG3	1:B:108:TYR:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	163/171 (95%)	160 (98%)	3 (2%)	0	100	100
1	B	160/171 (94%)	155 (97%)	5 (3%)	0	100	100
1	C	162/171 (95%)	157 (97%)	4 (2%)	1 (1%)	21	17
1	D	155/171 (91%)	145 (94%)	9 (6%)	1 (1%)	21	17
All	All	640/684 (94%)	617 (96%)	21 (3%)	2 (0%)	36	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	159	ASN
1	C	161	ASP

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	156/159 (98%)	140 (90%)	16 (10%)	7	4
1	B	153/159 (96%)	134 (88%)	19 (12%)	4	2
1	C	153/159 (96%)	129 (84%)	24 (16%)	2	1
1	D	149/159 (94%)	130 (87%)	19 (13%)	4	2
All	All	611/636 (96%)	533 (87%)	78 (13%)	4	2

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	78	LEU
1	A	84	ARG
1	A	96	ARG
1	A	128[A]	ASP
1	A	128[B]	ASP
1	A	130	LYS
1	A	136	LYS
1	A	139	LEU
1	A	144	LYS
1	A	146	ASN
1	A	151	ILE
1	A	161	ASP
1	A	182	LEU
1	A	228	LEU
1	A	229	VAL
1	B	76	ASN
1	B	80	GLU
1	B	83[A]	GLU
1	B	83[B]	GLU
1	B	87	LYS
1	B	90	ILE
1	B	96	ARG
1	B	98	ASP
1	B	130	LYS
1	B	131	LEU
1	B	132	GLU
1	B	139	LEU
1	B	182	LEU
1	B	186	GLU
1	B	190	LEU
1	B	225	VAL
1	B	228	LEU
1	B	229	VAL
1	B	239	ASP
1	C	78	LEU
1	C	81	GLN
1	C	87	LYS
1	C	90	ILE
1	C	133	ASN
1	C	135	LYS
1	C	139	LEU
1	C	144	LYS

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Mol	Chain	Res	Type
1	C	147	ASN
1	C	149	LYS
1	C	150	LEU
1	C	151	ILE
1	C	157	ARG
1	C	160	SER
1	C	161	ASP
1	C	168	ARG
1	C	171	GLN
1	C	190	LEU
1	C	193	SER
1	C	194	LYS
1	C	204	LYS
1	C	206	ARG
1	C	211	LYS
1	C	238	LEU
1	D	77	PHE
1	D	78	LEU
1	D	84	ARG
1	D	87	LYS
1	D	91	ASN
1	D	95	SER
1	D	119	LYS
1	D	136	LYS
1	D	139	LEU
1	D	144	LYS
1	D	155	LYS
1	D	157	ARG
1	D	161	ASP
1	D	165	GLN
1	D	168	ARG
1	D	190	LEU
1	D	222	GLU
1	D	229	VAL
1	D	235	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	106	ASN
1	A	107	ASN

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Mol	Chain	Res	Type
1	A	152	GLN
1	A	230	ASN
1	B	106	ASN
1	B	147	ASN
1	C	81	GLN
1	C	146	ASN
1	C	171	GLN
1	C	201	ASN
1	C	219	GLN
1	D	81	GLN
1	D	107	ASN
1	D	224	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no 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	$\# Z > 2$
2	PO4	A	1	-	4,4,4	2.62	3 (75%)	6,6,6	0.93	0
2	PO4	B	2	-	4,4,4	2.54	3 (75%)	6,6,6	1.11	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	PO4	P-O3	-3.17	1.45	1.54
2	B	2	PO4	P-O4	-3.00	1.45	1.54
2	B	2	PO4	P-O2	-2.87	1.46	1.54
2	A	1	PO4	P-O2	-2.84	1.46	1.54
2	B	2	PO4	P-O3	-2.34	1.47	1.54
2	A	1	PO4	P-O4	-2.33	1.47	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	PO4	6	0
2	B	2	PO4	8	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	A	160/171 (93%)	-0.15	3 (1%) 66 66	20, 40, 80, 116	6 (3%)
1	B	162/171 (94%)	0.00	2 (1%) 76 76	31, 51, 84, 124	1 (0%)
1	C	163/171 (95%)	0.24	2 (1%) 76 76	33, 65, 108, 138	0
1	D	157/171 (91%)	0.26	4 (2%) 58 58	28, 64, 130, 153	1 (0%)
All	All	642/684 (93%)	0.09	11 (1%) 69 68	20, 54, 108, 153	8 (1%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	GLU	5.9
1	A	102	GLY	4.5
1	B	147	ASN	3.7
1	D	229	VAL	2.6
1	D	94	PHE	2.5
1	C	150	LEU	2.3
1	D	105	PRO	2.3
1	A	97	PRO	2.2
1	D	224	HIS	2.1
1	C	131	LEU	2.1
1	B	104	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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
2	PO4	B	2	5/5	0.86	0.19	47,47,47,47	5
2	PO4	A	1	5/5	0.92	0.15	40,40,40,40	5

6.5 Other polymers [i](#)

There are no such residues in this entry.