



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:31 AM UTC

PDB ID : 2EGK / pdb_00002egk
Title : Crystal Structure of Tamalin PDZ-Intrinsic Ligand Fusion Protein
Authors : Sugi, T.; Oyama, T.; Muto, T.; Nakanishi, S.; Morikawa, K.; Jingami, H.
Deposited on : 2007-03-01
Resolution : 2.85 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

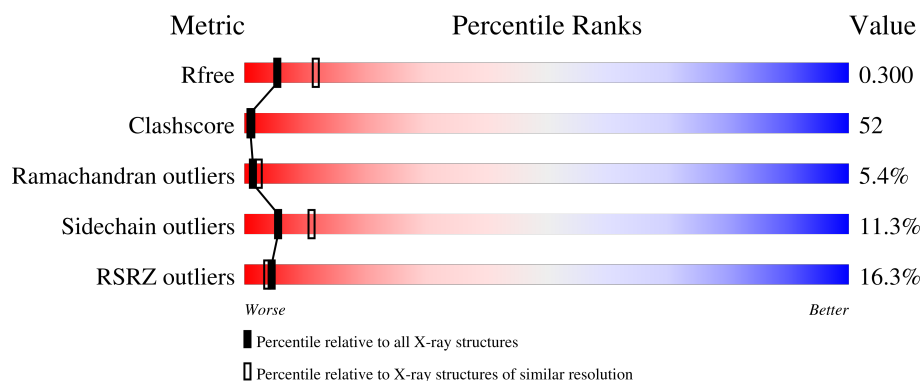
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	101	
1	B	101	
1	C	101	
1	D	101	

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	C	195	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2751 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 General receptor for phosphoinositides 1-associated scaffold protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	89	Total	C	N	O	Se	12	0	0
			670	421	113	135	1			
1	B	90	Total	C	N	O	Se	0	0	0
			686	429	123	133	1			
1	C	88	Total	C	N	O	Se	0	0	0
			676	423	120	132	1			
1	D	87	Total	C	N	O	Se	8	0	0
			666	415	117	133	1			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	GLY	-	cloning artifact	UNP Q8R4T5
A	95	SER	-	cloning artifact	UNP Q8R4T5
A	130	MSE	MET	modified residue	UNP Q8R4T5
A	135	ALA	CYS	engineered mutation	UNP Q8R4T5
B	94	GLY	-	cloning artifact	UNP Q8R4T5
B	95	SER	-	cloning artifact	UNP Q8R4T5
B	130	MSE	MET	modified residue	UNP Q8R4T5
B	135	ALA	CYS	engineered mutation	UNP Q8R4T5
C	94	GLY	-	cloning artifact	UNP Q8R4T5
C	95	SER	-	cloning artifact	UNP Q8R4T5
C	130	MSE	MET	modified residue	UNP Q8R4T5
C	135	ALA	CYS	engineered mutation	UNP Q8R4T5
D	94	GLY	-	cloning artifact	UNP Q8R4T5
D	95	SER	-	cloning artifact	UNP Q8R4T5
D	130	MSE	MET	modified residue	UNP Q8R4T5
D	135	ALA	CYS	engineered mutation	UNP Q8R4T5

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



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

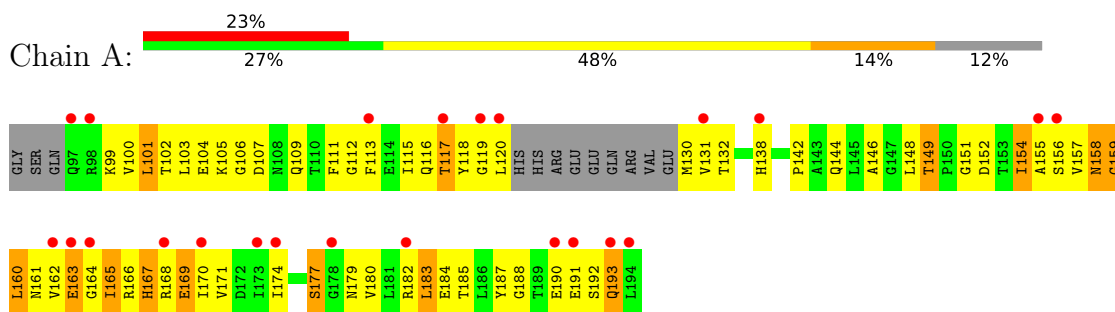
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	17	Total	O	0	0
			17	17		
3	C	13	Total	O	0	0
			13	13		
3	D	6	Total	O	0	0
			6	6		

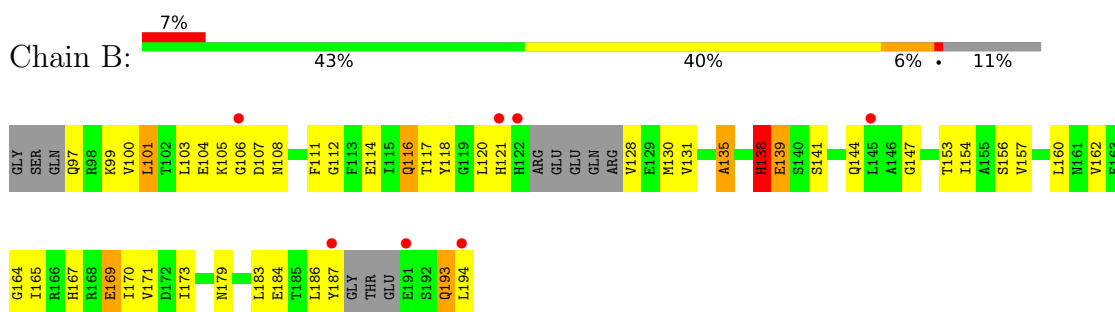
3 Residue-property plots [i](#)

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.

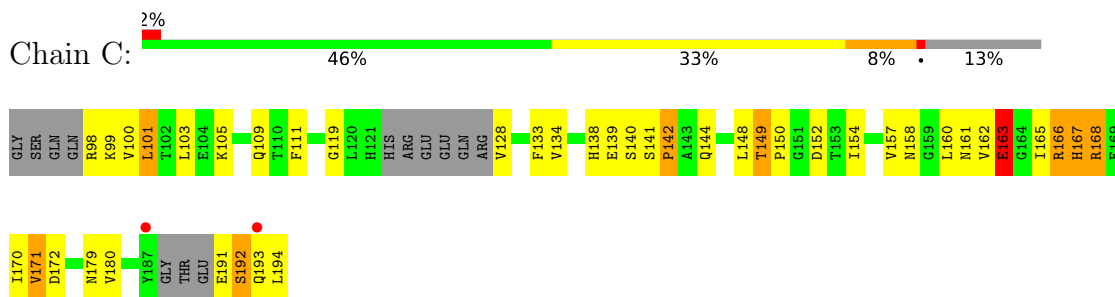
- Molecule 1: General receptor for phosphoinositides 1-associated scaffold protein



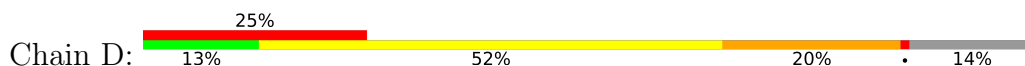
- Molecule 1: General receptor for phosphoinositides 1-associated scaffold protein

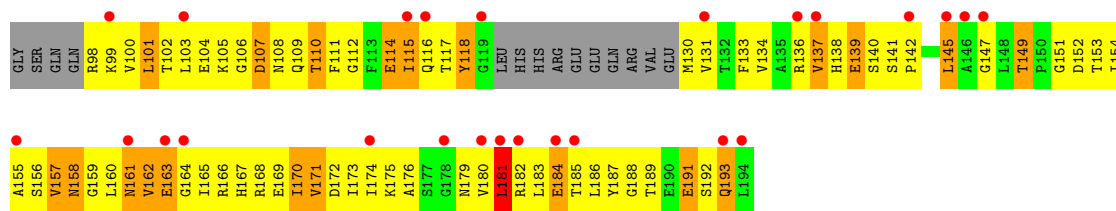


- Molecule 1: General receptor for phosphoinositides 1-associated scaffold protein



- Molecule 1: General receptor for phosphoinositides 1-associated scaffold protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.56Å 114.07Å 125.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.85 50.00 – 2.87	Depositor EDS
% Data completeness (in resolution range)	97.2 (50.00-2.85) 92.6 (50.00-2.87)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.86Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.269 , 0.291 0.278 , 0.300	Depositor DCC
R_{free} test set	1478 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 64.5	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	0.87	EDS
Total number of atoms	2751	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.81% 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: 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	0.59	1/677 (0.1%)	1.12	5/915 (0.5%)
1	B	0.67	1/691 (0.1%)	1.07	5/929 (0.5%)
1	C	0.59	0/681	1.01	3/915 (0.3%)
1	D	0.76	3/673 (0.4%)	1.19	9/907 (1.0%)
All	All	0.66	5/2722 (0.2%)	1.10	22/3666 (0.6%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	193	GLN	CA-C	-8.87	1.42	1.52
1	D	193	GLN	N-CA	-7.02	1.37	1.45
1	B	193	GLN	CD-OE1	6.13	1.35	1.23
1	D	193	GLN	C-N	-5.97	1.25	1.33
1	A	193	GLN	CA-C	-5.24	1.45	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	GLN	OE1-CD-NE2	-10.48	112.12	122.60
1	D	193	GLN	OE1-CD-NE2	-9.94	112.66	122.60
1	D	193	GLN	CG-CD-NE2	6.94	126.81	116.40
1	D	175	LYS	N-CA-C	-6.82	103.87	111.71
1	A	193	GLN	CG-CD-NE2	6.73	126.50	116.40
1	B	164	GLY	N-CA-C	-6.08	107.84	115.08
1	D	131	VAL	N-CA-C	6.04	116.54	108.27
1	D	161	ASN	N-CA-C	5.97	118.46	108.96
1	B	138	HIS	N-CA-C	5.79	117.76	110.24
1	C	138	HIS	N-CA-C	5.68	118.25	110.24
1	D	181	LEU	N-CA-C	5.63	117.70	108.52
1	D	189	THR	N-CA-C	5.62	118.22	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	170	ILE	N-CA-C	5.61	115.80	110.42
1	B	106	GLY	N-CA-C	5.59	121.41	112.58
1	A	117	THR	N-CA-C	-5.41	102.52	110.52
1	C	192	SER	N-CA-C	5.27	117.09	108.55
1	D	162	VAL	N-CA-C	5.25	119.54	112.98
1	B	170	ILE	N-CA-C	-5.24	105.27	110.62
1	B	107	ASP	N-CA-C	-5.22	102.66	110.23
1	C	119	GLY	N-CA-C	-5.13	101.02	113.18
1	A	183	LEU	N-CA-C	5.04	117.66	109.24
1	A	158	ASN	N-CA-C	-5.04	104.72	111.02

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	670	0	661	90	0
1	B	686	0	685	44	0
1	C	676	0	679	51	0
1	D	666	0	661	113	0
2	B	5	0	0	0	0
2	C	5	0	0	2	0
3	A	7	0	0	4	0
3	B	17	0	0	3	0
3	C	13	0	0	0	0
3	D	6	0	0	9	0
All	All	2751	0	2686	276	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 52.

All (276) 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:D:157:VAL:HG23	3:D:16:HOH:O	1.10	1.23
1:D:170:ILE:HA	1:D:173:ILE:HD12	1.31	1.12
1:A:107:ASP:HA	1:A:179:ASN:HD21	1.04	1.11
1:C:101:LEU:HD23	1:C:101:LEU:H	1.10	1.10
1:B:139:GLU:HG2	3:B:9:HOH:O	1.55	1.05
1:D:109:GLN:HA	3:D:24:HOH:O	1.58	1.04
1:A:166:ARG:HH11	1:A:168:ARG:H	1.05	1.02
1:C:166:ARG:HB2	1:C:166:ARG:HH11	1.25	1.00
1:A:177:SER:O	3:A:14:HOH:O	1.78	1.00
1:D:156:SER:HB3	1:D:184:GLU:HB2	1.40	1.00
1:D:162:VAL:HG13	3:D:16:HOH:O	1.62	0.99
1:B:139:GLU:CG	3:B:9:HOH:O	2.09	0.98
1:D:158:ASN:HA	1:D:182:ARG:HB3	1.46	0.98
1:A:107:ASP:HA	1:A:179:ASN:ND2	1.79	0.97
1:D:112:GLY:HA3	1:D:141:SER:HB2	1.47	0.96
1:D:158:ASN:ND2	1:D:182:ARG:H	1.66	0.94
1:D:136:ARG:HG2	1:D:137:VAL:H	1.32	0.94
1:D:161:ASN:HB3	1:D:163:GLU:OE1	1.68	0.94
1:A:174:ILE:HG21	1:B:194:LEU:HD13	1.50	0.93
1:D:156:SER:HB3	1:D:184:GLU:CB	1.99	0.93
1:D:158:ASN:HD22	1:D:182:ARG:HB3	1.31	0.93
1:A:162:VAL:HB	1:A:170:ILE:HD13	1.56	0.86
1:D:136:ARG:HG2	1:D:137:VAL:N	1.87	0.86
1:C:101:LEU:HD23	1:C:101:LEU:N	1.91	0.86
1:C:166:ARG:HB2	1:C:166:ARG:NH1	1.92	0.85
1:D:107:ASP:HA	1:D:179:ASN:ND2	1.93	0.82
1:A:144:GLN:HE22	1:C:139:GLU:HB2	1.45	0.82
1:B:105:LYS:O	1:B:179:ASN:HB3	1.80	0.81
1:A:111:PHE:O	1:A:142:PRO:HD2	1.82	0.80
1:B:156:SER:HB3	1:B:184:GLU:HB2	1.63	0.79
1:D:107:ASP:HA	1:D:179:ASN:HD21	1.45	0.78
1:A:99:LYS:HZ1	1:A:187:TYR:CA	1.97	0.78
1:D:99:LYS:NZ	1:D:187:TYR:HB2	1.99	0.78
1:A:154:ILE:HD12	1:A:154:ILE:H	1.50	0.77
1:D:151:GLY:O	1:D:188:GLY:HA3	1.86	0.76
1:C:191:GLU:HG2	1:D:116:GLN:HE21	1.48	0.76
1:A:156:SER:HB3	1:A:161:ASN:HA	1.68	0.76
1:D:154:ILE:HD12	1:D:183:LEU:HD22	1.69	0.75
1:A:151:GLY:O	1:A:188:GLY:HA3	1.87	0.75
1:D:109:GLN:CA	3:D:24:HOH:O	2.19	0.74
1:D:167:HIS:O	1:D:171:VAL:HG12	1.88	0.74
1:B:97:GLN:HG2	1:B:187:TYR:H	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:ILE:O	1:D:174:ILE:HG13	1.88	0.73
1:A:99:LYS:HZ1	1:A:187:TYR:N	1.87	0.72
1:A:165:ILE:HB	1:A:170:ILE:HD11	1.72	0.71
1:A:154:ILE:HD12	1:A:154:ILE:N	2.05	0.71
1:D:158:ASN:HD21	1:D:182:ARG:H	1.38	0.71
1:D:101:LEU:HD12	1:D:183:LEU:O	1.90	0.71
1:D:103:LEU:HD13	1:D:183:LEU:HD12	1.72	0.70
1:D:163:GLU:H	1:D:163:GLU:CD	1.99	0.70
1:D:101:LEU:HD11	1:D:185:THR:HG23	1.72	0.70
1:A:111:PHE:HB2	1:B:194:LEU:OXT	1.91	0.69
1:C:193:GLN:C	1:C:194:LEU:HD12	2.18	0.69
1:B:121:HIS:CE1	1:B:128:VAL:HG22	2.28	0.69
1:B:193:GLN:O	1:B:194:LEU:HD23	1.93	0.69
1:A:106:GLY:HA3	1:A:109:GLN:HE21	1.58	0.69
1:D:99:LYS:HZ2	1:D:187:TYR:HB2	1.57	0.68
1:C:101:LEU:H	1:C:101:LEU:CD2	1.91	0.68
1:D:161:ASN:HB3	1:D:163:GLU:CD	2.19	0.68
1:C:168:ARG:HE	2:C:195:PO4:P	2.17	0.68
1:A:156:SER:HB3	1:A:161:ASN:ND2	2.09	0.67
1:D:156:SER:CB	1:D:184:GLU:HB2	2.20	0.66
1:A:118:TYR:N	1:A:131:VAL:O	2.28	0.65
1:D:166:ARG:O	1:D:170:ILE:HG13	1.95	0.65
1:C:191:GLU:CG	1:D:116:GLN:HE21	2.09	0.65
1:D:102:THR:HA	1:D:181:LEU:O	1.97	0.64
1:A:192:SER:O	3:A:3:HOH:O	2.14	0.64
1:C:191:GLU:CB	1:D:116:GLN:HG3	2.28	0.64
1:D:130:MSE:HB3	1:D:164:GLY:HA2	1.79	0.64
1:C:105:LYS:HG2	1:C:111:PHE:CE1	2.33	0.64
1:D:153:THR:HB	1:D:186:LEU:HB2	1.80	0.63
1:D:145:LEU:N	1:D:145:LEU:HD23	2.11	0.63
1:A:105:LYS:HG2	1:A:179:ASN:HA	1.80	0.63
1:D:158:ASN:C	1:D:182:ARG:HD2	2.24	0.62
1:D:158:ASN:ND2	1:D:182:ARG:HB3	2.10	0.62
1:D:111:PHE:O	1:D:142:PRO:HD2	1.99	0.62
1:A:102:THR:HG22	1:A:182:ARG:HG3	1.81	0.62
1:A:166:ARG:HH11	1:A:168:ARG:N	1.89	0.62
1:D:158:ASN:HD22	1:D:182:ARG:CB	2.10	0.62
1:A:117:THR:HG23	1:A:132:THR:OG1	2.00	0.62
1:A:166:ARG:NH1	1:A:168:ARG:H	1.89	0.61
1:D:101:LEU:HD11	1:D:185:THR:CG2	2.31	0.61
1:B:108:ASN:N	1:B:108:ASN:HD22	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:VAL:HG23	1:C:162:VAL:HG11	1.83	0.61
1:D:155:ALA:O	1:D:162:VAL:HG22	2.00	0.61
1:A:99:LYS:NZ	1:A:187:TYR:N	2.48	0.61
1:A:99:LYS:HZ1	1:A:187:TYR:HB2	1.66	0.61
1:C:166:ARG:HE	1:C:168:ARG:HB2	1.66	0.60
1:D:109:GLN:CB	3:D:24:HOH:O	2.46	0.60
1:D:157:VAL:CG2	3:D:16:HOH:O	1.91	0.60
1:A:156:SER:CB	1:A:161:ASN:HA	2.31	0.60
1:A:166:ARG:HD3	1:A:167:HIS:N	2.16	0.60
1:D:99:LYS:HB2	3:D:5:HOH:O	2.01	0.59
1:D:154:ILE:HD12	1:D:183:LEU:CD2	2.32	0.59
1:D:105:LYS:HG3	1:D:179:ASN:OD1	2.02	0.59
1:D:157:VAL:C	1:D:159:GLY:N	2.59	0.59
1:A:165:ILE:HB	1:A:170:ILE:CG1	2.32	0.59
1:C:193:GLN:O	1:C:194:LEU:HD12	2.02	0.59
1:A:106:GLY:H	1:A:109:GLN:CD	2.11	0.58
1:A:158:ASN:O	1:A:160:LEU:N	2.36	0.58
1:D:109:GLN:HB2	3:D:24:HOH:O	2.03	0.58
1:D:157:VAL:O	1:D:159:GLY:N	2.35	0.58
1:D:157:VAL:O	1:D:160:LEU:HD23	2.02	0.58
1:A:99:LYS:HZ1	1:A:187:TYR:CB	2.15	0.58
1:A:149:THR:HB	1:A:152:ASP:OD2	2.04	0.58
1:D:169:GLU:O	1:D:173:ILE:HG13	2.04	0.58
1:A:100:VAL:HG12	1:A:101:LEU:N	2.19	0.58
1:A:118:TYR:O	1:A:131:VAL:HG12	2.04	0.58
1:A:106:GLY:H	1:A:109:GLN:CG	2.18	0.57
1:A:156:SER:HB3	1:A:161:ASN:HD22	1.69	0.57
1:A:156:SER:CB	1:A:161:ASN:HD22	2.17	0.57
1:D:130:MSE:HE3	1:D:130:MSE:C	2.29	0.57
1:C:139:GLU:HA	1:C:144:GLN:OE1	2.04	0.57
1:A:116:GLN:C	1:A:132:THR:HG23	2.29	0.57
1:A:165:ILE:HB	1:A:170:ILE:CD1	2.33	0.57
1:B:117:THR:CG2	1:B:130:MSE:HE3	2.35	0.57
1:A:115:ILE:HD12	1:A:132:THR:HG21	1.86	0.57
1:A:165:ILE:HG22	1:A:166:ARG:N	2.19	0.57
1:A:167:HIS:O	1:A:171:VAL:HG23	2.05	0.57
1:B:97:GLN:HG2	1:B:187:TYR:N	2.19	0.57
1:B:112:GLY:HA3	1:B:141:SER:HB2	1.85	0.57
1:D:166:ARG:NE	1:D:169:GLU:HB2	2.20	0.57
1:D:156:SER:HB3	1:D:184:GLU:HB3	1.83	0.57
1:A:106:GLY:CA	1:A:109:GLN:HE21	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:VAL:HA	1:A:165:ILE:HD12	1.87	0.56
1:D:158:ASN:HD22	1:D:182:ARG:H	1.54	0.55
1:C:158:ASN:O	1:C:160:LEU:HG	2.07	0.55
1:C:161:ASN:OD1	1:C:163:GLU:HB2	2.06	0.54
1:A:99:LYS:NZ	1:A:187:TYR:HB2	2.22	0.54
1:A:106:GLY:H	1:A:109:GLN:NE2	2.05	0.54
1:A:106:GLY:CA	1:A:109:GLN:HG2	2.38	0.54
1:B:157:VAL:HG22	1:B:183:LEU:HD23	1.89	0.54
1:B:138:HIS:ND1	1:B:138:HIS:N	2.56	0.53
1:C:191:GLU:HB2	1:D:116:GLN:HG3	1.90	0.53
1:D:185:THR:C	1:D:186:LEU:HD12	2.33	0.53
1:B:154:ILE:HG22	1:B:162:VAL:HG21	1.89	0.53
1:A:100:VAL:HA	1:A:184:GLU:HA	1.90	0.53
1:A:156:SER:CB	1:A:161:ASN:ND2	2.72	0.53
1:A:112:GLY:O	1:A:138:HIS:HD2	1.91	0.53
1:D:191:GLU:C	1:D:193:GLN:H	2.17	0.52
1:C:105:LYS:HE3	1:C:179:ASN:HA	1.91	0.52
1:A:103:LEU:N	1:A:103:LEU:HD12	2.25	0.52
1:A:144:GLN:NE2	1:C:139:GLU:HB2	2.22	0.52
1:A:112:GLY:O	1:A:138:HIS:CD2	2.61	0.52
1:D:100:VAL:HG22	1:D:184:GLU:HG3	1.92	0.52
1:B:138:HIS:HA	1:D:139:GLU:OE2	2.10	0.52
1:A:105:LYS:HG3	1:A:106:GLY:O	2.10	0.51
1:D:99:LYS:HG3	1:D:185:THR:OG1	2.11	0.51
1:D:151:GLY:C	1:D:188:GLY:HA3	2.36	0.51
1:D:158:ASN:ND2	1:D:182:ARG:N	2.48	0.51
1:D:173:ILE:O	1:D:176:ALA:HB3	2.10	0.51
1:C:128:VAL:HG13	1:C:128:VAL:O	2.09	0.51
1:D:157:VAL:O	1:D:158:ASN:C	2.52	0.51
1:B:144:GLN:O	1:B:147:GLY:N	2.39	0.51
1:C:191:GLU:HA	1:D:116:GLN:HG3	1.94	0.51
1:D:133:PHE:HD1	1:D:134:VAL:O	1.95	0.50
1:A:180:VAL:O	3:A:14:HOH:O	2.20	0.50
1:B:160:LEU:HD12	1:B:173:ILE:CG2	2.42	0.50
1:B:160:LEU:HD12	1:B:173:ILE:HG21	1.93	0.50
1:D:162:VAL:O	1:D:164:GLY:N	2.44	0.50
1:B:117:THR:HG21	1:B:130:MSE:HE3	1.94	0.50
1:C:105:LYS:O	1:C:179:ASN:HB3	2.12	0.50
1:A:118:TYR:O	1:A:131:VAL:N	2.45	0.49
1:C:166:ARG:HH22	1:D:191:GLU:CD	2.20	0.49
1:B:165:ILE:HG23	1:B:169:GLU:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:LEU:HD23	1:C:111:PHE:HB3	1.93	0.49
1:A:165:ILE:CG2	1:A:166:ARG:N	2.76	0.49
1:A:151:GLY:C	1:A:188:GLY:HA3	2.38	0.49
1:A:101:LEU:HD12	1:A:146:ALA:O	2.12	0.49
1:A:154:ILE:HA	1:A:185:THR:HG22	1.95	0.49
1:A:157:VAL:HG12	1:A:158:ASN:ND2	2.28	0.49
1:A:165:ILE:CG2	1:A:169:GLU:HB3	2.43	0.49
1:B:167:HIS:O	1:B:171:VAL:HG23	2.13	0.48
1:B:120:LEU:O	1:B:128:VAL:HA	2.13	0.48
1:C:166:ARG:NH2	1:C:167:HIS:HB3	2.28	0.48
1:D:99:LYS:HZ1	1:D:187:TYR:HB2	1.79	0.48
1:D:138:HIS:O	1:D:141:SER:HB3	2.13	0.48
1:A:166:ARG:NH1	1:A:168:ARG:CB	2.76	0.48
1:B:99:LYS:O	1:B:101:LEU:HD12	2.14	0.48
1:A:116:GLN:O	1:A:132:THR:HA	2.14	0.48
1:C:191:GLU:CA	1:D:116:GLN:HG3	2.43	0.48
1:D:117:THR:HG22	1:D:118:TYR:N	2.29	0.48
1:A:100:VAL:HG22	1:A:184:GLU:HG2	1.96	0.47
1:A:102:THR:HG22	1:A:182:ARG:HA	1.96	0.47
1:B:103:LEU:CD2	1:B:111:PHE:HB3	2.43	0.47
1:B:169:GLU:O	1:B:173:ILE:HG13	2.14	0.47
1:D:139:GLU:O	1:D:141:SER:N	2.47	0.47
1:C:105:LYS:HE3	1:C:179:ASN:OD1	2.13	0.47
1:A:106:GLY:N	1:A:109:GLN:NE2	2.62	0.47
1:D:149:THR:O	1:D:152:ASP:OD2	2.33	0.47
1:C:191:GLU:HG2	1:D:114:GLU:OE2	2.15	0.47
1:A:159:GLY:O	1:A:160:LEU:C	2.58	0.47
1:B:114:GLU:O	1:B:135:ALA:N	2.44	0.47
1:C:194:LEU:HD13	1:D:115:ILE:HG12	1.96	0.46
1:C:162:VAL:HB	1:C:170:ILE:HD11	1.97	0.46
1:D:166:ARG:CZ	1:D:169:GLU:HB2	2.46	0.46
1:C:171:VAL:CG2	1:C:172:ASP:N	2.77	0.46
1:A:106:GLY:HA3	1:A:109:GLN:HG2	1.98	0.46
1:A:100:VAL:CG1	1:A:101:LEU:N	2.77	0.46
1:A:118:TYR:CE2	1:B:131:VAL:HG11	2.51	0.46
1:C:191:GLU:CG	1:D:116:GLN:NE2	2.76	0.46
1:B:108:ASN:N	1:B:108:ASN:ND2	2.60	0.46
1:B:139:GLU:OE1	1:B:139:GLU:HA	2.16	0.46
1:D:100:VAL:HG22	1:D:184:GLU:CG	2.46	0.46
1:A:154:ILE:N	1:A:154:ILE:CD1	2.76	0.46
1:B:100:VAL:C	1:B:101:LEU:HD12	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:PHE:C	1:A:142:PRO:HD2	2.41	0.45
1:B:169:GLU:HA	1:B:169:GLU:OE1	2.16	0.45
1:B:139:GLU:HG3	3:B:9:HOH:O	1.98	0.45
1:D:166:ARG:HE	1:D:169:GLU:HB2	1.80	0.45
1:B:118:TYR:O	1:B:130:MSE:HA	2.15	0.45
1:C:154:ILE:HG22	1:C:162:VAL:HG21	1.99	0.45
1:A:159:GLY:O	1:A:161:ASN:ND2	2.49	0.45
1:C:149:THR:HA	1:C:150:PRO:HD3	1.85	0.45
1:D:106:GLY:O	1:D:109:GLN:HG2	2.17	0.45
1:D:130:MSE:HE2	1:D:165:ILE:O	2.17	0.45
1:C:192:SER:OG	1:D:167:HIS:NE2	2.50	0.44
1:D:104:GLU:HG2	1:D:180:VAL:HG22	2.00	0.44
1:D:165:ILE:CB	1:D:170:ILE:HD11	2.47	0.44
1:A:119:GLY:O	1:A:120:LEU:HG	2.17	0.44
1:B:114:GLU:HG2	1:D:192:SER:O	2.18	0.44
1:C:166:ARG:NH2	2:C:195:PO4:O2	2.49	0.44
1:D:137:VAL:O	1:D:137:VAL:HG12	2.17	0.44
1:D:153:THR:HG22	1:D:154:ILE:N	2.32	0.44
1:C:101:LEU:N	1:C:101:LEU:CD2	2.62	0.44
1:D:98:ARG:HG3	1:D:99:LYS:H	1.82	0.44
1:D:166:ARG:NH2	1:D:169:GLU:HB2	2.33	0.44
1:B:116:GLN:HA	1:B:116:GLN:NE2	2.31	0.44
1:C:140:SER:N	1:C:144:GLN:OE1	2.48	0.43
1:D:110:THR:N	3:D:24:HOH:O	2.49	0.43
1:D:145:LEU:C	1:D:147:GLY:N	2.76	0.43
1:D:159:GLY:O	1:D:160:LEU:C	2.60	0.43
1:A:130:MSE:HB2	1:A:164:GLY:O	2.19	0.43
1:D:169:GLU:O	1:D:172:ASP:HB3	2.17	0.43
1:C:165:ILE:HG22	1:C:166:ARG:N	2.32	0.43
1:C:167:HIS:O	1:C:168:ARG:C	2.61	0.43
1:C:141:SER:O	1:C:142:PRO:C	2.61	0.43
1:C:191:GLU:HA	1:D:116:GLN:HA	2.01	0.43
1:C:105:LYS:HB2	1:C:109:GLN:OE1	2.18	0.43
1:A:167:HIS:O	1:A:168:ARG:C	2.61	0.43
1:D:159:GLY:N	1:D:182:ARG:HD2	2.34	0.43
1:D:167:HIS:C	1:D:171:VAL:HG12	2.44	0.43
1:A:156:SER:HB2	1:A:159:GLY:O	2.18	0.43
1:C:133:PHE:HA	1:C:152:ASP:O	2.19	0.42
1:B:154:ILE:HG22	1:B:162:VAL:CG2	2.49	0.42
1:A:101:LEU:HD23	1:A:183:LEU:O	2.20	0.42
1:D:136:ARG:O	1:D:137:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ILE:HB	1:A:170:ILE:HG12	2.01	0.42
1:B:117:THR:HG22	1:B:130:MSE:HE3	2.00	0.42
1:C:101:LEU:HD11	1:C:148:LEU:HA	2.02	0.42
1:A:101:LEU:HA	3:A:39:HOH:O	2.19	0.42
1:A:113:PHE:O	1:B:194:LEU:N	2.51	0.42
1:D:98:ARG:NH2	1:D:161:ASN:HD21	2.18	0.42
1:A:155:ALA:HA	1:A:163:GLU:HG3	2.01	0.42
1:A:190:GLU:O	1:A:193:GLN:HG2	2.20	0.42
1:A:103:LEU:HG	1:A:146:ALA:CB	2.50	0.41
1:B:186:LEU:HA	1:B:186:LEU:HD23	1.73	0.41
1:C:162:VAL:HB	1:C:170:ILE:CD1	2.50	0.41
1:D:139:GLU:C	1:D:141:SER:N	2.77	0.41
1:D:145:LEU:C	1:D:147:GLY:H	2.27	0.41
1:D:186:LEU:HD12	1:D:186:LEU:N	2.35	0.41
1:B:103:LEU:HD22	1:B:111:PHE:HB3	2.02	0.41
1:D:168:ARG:O	1:D:171:VAL:HG13	2.21	0.41
1:D:137:VAL:O	1:D:138:HIS:C	2.64	0.41
1:B:117:THR:HA	1:B:131:VAL:O	2.20	0.41
1:D:157:VAL:C	1:D:159:GLY:H	2.26	0.41
1:A:148:LEU:HD23	1:A:148:LEU:HA	1.89	0.41
1:B:105:LYS:HG3	1:B:111:PHE:CE1	2.56	0.41
1:C:134:VAL:HG21	1:C:148:LEU:HD11	2.02	0.41
1:C:191:GLU:N	1:D:167:HIS:CE1	2.89	0.41
1:D:99:LYS:HG2	1:D:185:THR:O	2.21	0.41
1:A:105:LYS:HG2	1:A:179:ASN:CA	2.47	0.40
1:A:144:GLN:HE22	1:C:139:GLU:CB	2.25	0.40
1:D:106:GLY:O	1:D:108:ASN:N	2.54	0.40
1:D:161:ASN:ND2	1:D:163:GLU:OE2	2.54	0.40
1:D:155:ALA:HB1	1:D:163:GLU:OE2	2.20	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	85/101 (84%)	73 (86%)	7 (8%)	5 (6%)	1	2
1	B	84/101 (83%)	77 (92%)	6 (7%)	1 (1%)	10	22
1	C	82/101 (81%)	72 (88%)	5 (6%)	5 (6%)	1	2
1	D	83/101 (82%)	61 (74%)	15 (18%)	7 (8%)	0	1
All	All	334/404 (83%)	283 (85%)	33 (10%)	18 (5%)	1	2

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	GLU
1	C	163	GLU
1	D	107	ASP
1	D	140	SER
1	D	163	GLU
1	A	165	ILE
1	D	158	ASN
1	A	159	GLY
1	A	160	LEU
1	A	167	HIS
1	B	135	ALA
1	C	168	ARG
1	C	99	LYS
1	D	137	VAL
1	D	139	GLU
1	D	191	GLU
1	C	167	HIS
1	C	100	VAL

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	72/85 (85%)	65 (90%)	7 (10%)	8	17
1	B	74/85 (87%)	67 (90%)	7 (10%)	8	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	74/85 (87%)	66 (89%)	8 (11%)	6	12
1	D	72/85 (85%)	61 (85%)	11 (15%)	3	5
All	All	292/340 (86%)	259 (89%)	33 (11%)	5	11

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	LEU
1	A	104	GLU
1	A	149	THR
1	A	154	ILE
1	A	169	GLU
1	A	177	SER
1	A	191	GLU
1	B	101	LEU
1	B	104	GLU
1	B	116	GLN
1	B	138	HIS
1	B	139	GLU
1	B	153	THR
1	B	169	GLU
1	C	98	ARG
1	C	101	LEU
1	C	142	PRO
1	C	149	THR
1	C	163	GLU
1	C	166	ARG
1	C	171	VAL
1	C	180	VAL
1	D	101	LEU
1	D	110	THR
1	D	114	GLU
1	D	115	ILE
1	D	118	TYR
1	D	145	LEU
1	D	149	THR
1	D	157	VAL
1	D	171	VAL
1	D	181	LEU
1	D	184	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	138	HIS
1	A	144	GLN
1	A	161	ASN
1	B	108	ASN
1	B	121	HIS
1	C	116	GLN
1	D	108	ASN
1	D	116	GLN
1	D	158	ASN
1	D	161	ASN
1	D	193	GLN

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	B	195	-	4,4,4	1.75	1 (25%)	6,6,6	0.49	0
2	PO4	C	195	-	4,4,4	1.78	1 (25%)	6,6,6	0.46	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	195	PO4	P-O3	-2.10	1.48	1.54
2	B	195	PO4	P-O2	-2.09	1.48	1.54

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
2	C	195	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

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	A	88/101 (87%)	1.40	23 (26%) 1 1	4, 52, 63, 69	2 (2%)
1	B	89/101 (88%)	0.72	7 (7%) 18 14	10, 27, 50, 53	0
1	C	87/101 (86%)	0.44	2 (2%) 61 52	8, 22, 46, 54	0
1	D	86/101 (85%)	1.64	25 (29%) 1 1	4, 53, 64, 70	1 (1%)
All	All	350/404 (86%)	1.05	57 (16%) 4 4	4, 38, 62, 70	3 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	194	LEU	6.0
1	D	163	GLU	4.6
1	D	131	VAL	4.5
1	B	122	HIS	4.0
1	B	187	TYR	3.8
1	C	187	TYR	3.7
1	D	142	PRO	3.7
1	D	164	GLY	3.7
1	A	194	LEU	3.6
1	A	98	ARG	3.6
1	D	147	GLY	3.2
1	D	161	ASN	3.1
1	D	99	LYS	3.1
1	A	131	VAL	2.8
1	A	163	GLU	2.7
1	B	194	LEU	2.7
1	D	185	THR	2.7
1	A	182	ARG	2.6
1	A	97	GLN	2.6
1	D	136	ARG	2.6
1	D	119	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	120	LEU	2.6
1	A	156	SER	2.6
1	A	164	GLY	2.5
1	A	190	GLU	2.5
1	B	191	GLU	2.5
1	D	146	ALA	2.5
1	D	145	LEU	2.4
1	A	162	VAL	2.4
1	A	168	ARG	2.4
1	A	113	PHE	2.4
1	A	117	THR	2.4
1	A	138	HIS	2.4
1	D	103	LEU	2.3
1	A	170	ILE	2.3
1	A	191	GLU	2.3
1	D	193	GLN	2.3
1	B	145	LEU	2.3
1	A	155	ALA	2.3
1	C	193	GLN	2.3
1	D	174	ILE	2.3
1	D	115	ILE	2.2
1	D	178	GLY	2.2
1	A	178	GLY	2.2
1	B	106	GLY	2.2
1	D	181	LEU	2.2
1	D	184	GLU	2.2
1	A	119	GLY	2.1
1	A	174	ILE	2.1
1	D	182	ARG	2.1
1	A	173	ILE	2.1
1	D	137	VAL	2.1
1	D	116	GLN	2.0
1	A	193	GLN	2.0
1	B	121	HIS	2.0
1	D	180	VAL	2.0
1	D	155	ALA	2.0

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 [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
2	PO4	B	195	5/5	0.96	0.09	18,19,20,23	0
2	PO4	C	195	5/5	0.98	0.07	17,17,18,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.