



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:29 AM UTC

PDB ID : 9FQ1 / pdb_00009fq1
Title : Structure of the disease-causing mutant P20S of human KCTD1
Authors : Balasco, N.; Ruggiero, A.; Smaldone, G.; Esposito, L.; Berisio, R.; Vitagliano, L.
Deposited on : 2024-06-14
Resolution : 2.60 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

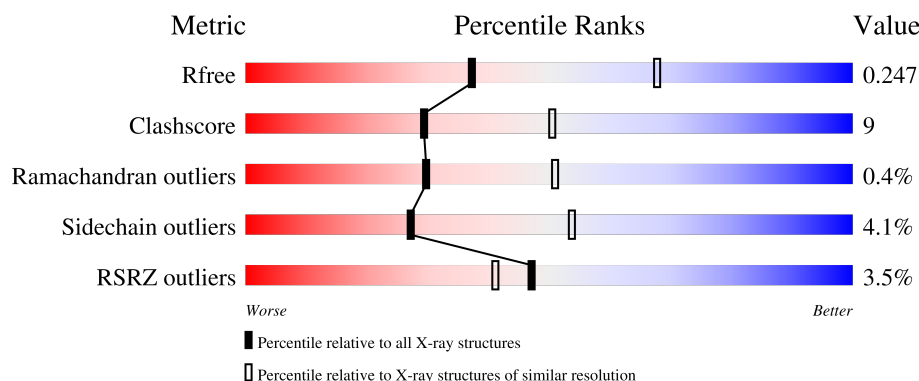
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	257	5% 66% 17% • 14%
1	B	257	% 67% 16% 17%
1	C	257	4% 60% 18% • 21%
1	D	257	3% 67% 18% • 14%
1	E	257	% 64% 15% • 21%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8561 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 BTB/POZ domain-containing protein KCTD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	1	0
			1758	1116	304	328	10			
1	B	213	Total	C	N	O	S	0	0	0
			1688	1072	290	316	10			
1	C	204	Total	C	N	O	S	0	0	0
			1634	1037	286	301	10			
1	D	221	Total	C	N	O	S	0	1	0
			1755	1112	304	329	10			
1	E	204	Total	C	N	O	S	0	0	0
			1633	1036	282	305	10			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	SER	PRO	engineered mutation	UNP Q719H9
B	20	SER	PRO	engineered mutation	UNP Q719H9
C	20	SER	PRO	engineered mutation	UNP Q719H9
D	20	SER	PRO	engineered mutation	UNP Q719H9
E	20	SER	PRO	engineered mutation	UNP Q719H9

- 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	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		

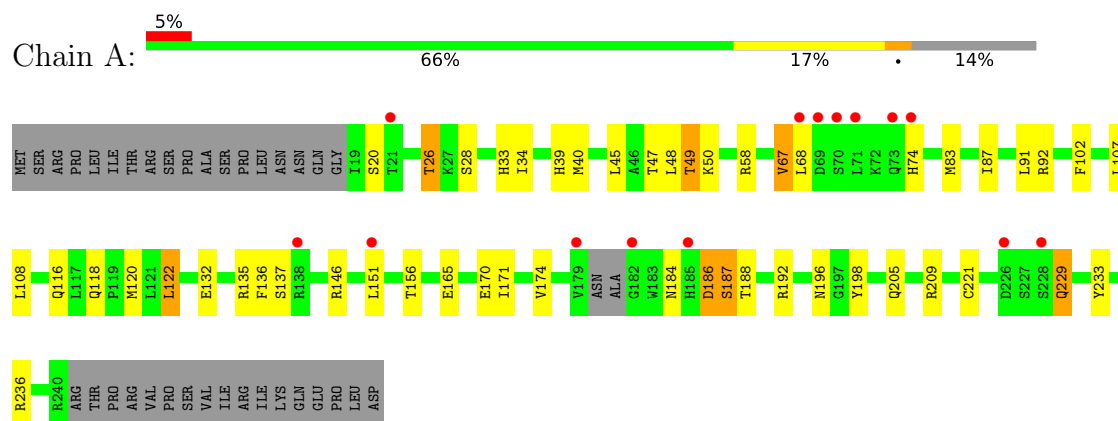
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	O	0	0
			15	15		
4	B	17	Total	O	0	0
			17	17		
4	C	12	Total	O	0	0
			12	12		
4	D	21	Total	O	0	0
			21	21		
4	E	17	Total	O	0	0
			17	17		

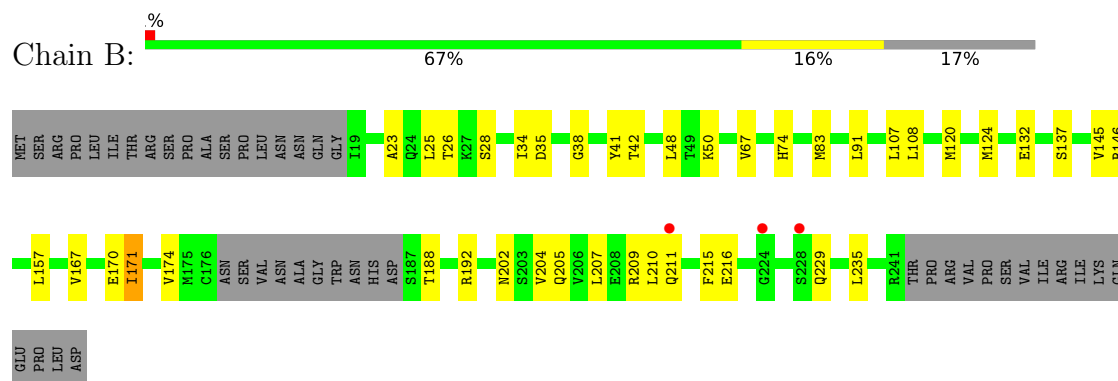
3 Residue-property plots [i](#)

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.

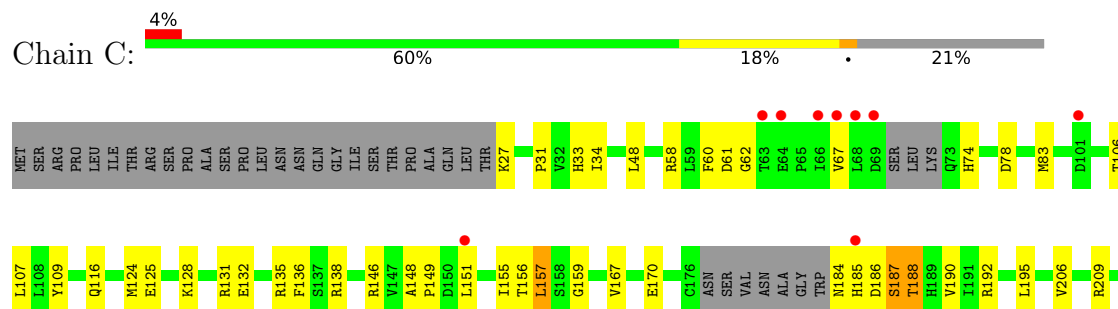
- Molecule 1: BTB/POZ domain-containing protein KCTD1



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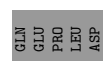


- Molecule 1: BTB/POZ domain-containing protein KCTD1

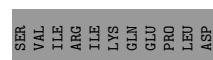
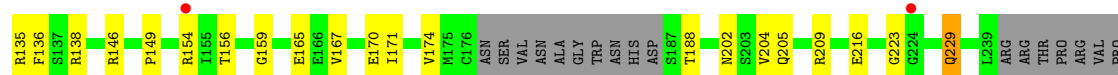
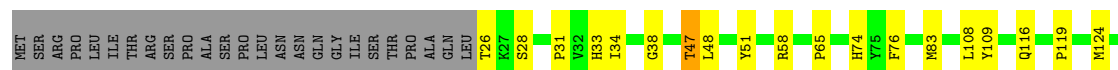




- Molecule 1: BTB/POZ domain-containing protein KCTD1



- Molecule 1: BTB/POZ domain-containing protein KCTD1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.05Å 96.00Å 116.81Å 90.00° 98.20° 90.00°	Depositor
Resolution (Å)	14.99 – 2.60 14.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (14.99-2.60) 98.9 (14.99-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.194 , 0.243 0.200 , 0.247	Depositor DCC
R_{free} test set	2186 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	63.2	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 70.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8561	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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: K, 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	0.29	0/1798	0.58	0/2432
1	B	0.29	0/1723	0.55	0/2331
1	C	0.27	0/1668	0.56	1/2251 (0.0%)
1	D	0.36	1/1795 (0.1%)	0.58	2/2427 (0.1%)
1	E	0.27	0/1667	0.55	1/2251 (0.0%)
All	All	0.30	1/8651 (0.0%)	0.56	4/11692 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	224	GLY	C-N	7.36	1.43	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	228	SER	CA-C-N	-6.58	110.83	122.07
1	D	228	SER	C-N-CA	-6.58	110.83	122.07
1	E	154	ARG	CB-CG-CD	-5.32	99.06	111.30
1	C	223	GLY	O-C-N	-5.08	118.19	123.58

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1758	0	1715	45	0
1	B	1688	0	1639	30	0
1	C	1634	0	1583	33	0
1	D	1755	0	1704	31	0
1	E	1633	0	1589	29	0
2	A	5	0	0	1	0
2	C	5	0	0	0	0
3	A	1	0	0	0	0
4	A	15	0	0	1	0
4	B	17	0	0	0	0
4	C	12	0	0	0	0
4	D	21	0	0	2	0
4	E	17	0	0	0	0
All	All	8561	0	8230	143	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 9.

All (143) 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:A:33:HIS:O	1:A:74:HIS:HB2	1.42	1.16
1:A:33:HIS:HB2	1:A:74:HIS:CB	1.84	1.07
1:A:33:HIS:HB2	1:A:74:HIS:HB3	1.09	1.07
1:C:138:ARG:HH12	1:E:216:GLU:HG2	1.41	0.85
1:A:33:HIS:CB	1:A:74:HIS:HB3	2.02	0.84
1:A:33:HIS:CB	1:A:74:HIS:CB	2.61	0.78
1:B:171:ILE:HG23	1:B:174:VAL:HG22	1.68	0.76
1:A:33:HIS:C	1:A:74:HIS:HB2	2.11	0.75
1:D:202:ASN:H	1:D:205:GLN:HE21	1.37	0.70
1:B:204:VAL:HG21	1:E:159:GLY:HA2	1.73	0.70
1:A:87:ILE:HG12	1:A:120:MET:HE1	1.72	0.69
1:E:165:GLU:HG2	1:E:171:ILE:HD11	1.76	0.67
1:A:58:ARG:NH2	1:A:116:GLN:OE1	2.28	0.67
1:B:50:LYS:HD3	1:B:91:LEU:O	1.95	0.66
1:B:83:MET:HE2	1:B:108:LEU:HB2	1.77	0.66
1:A:40:MET:HE1	1:A:74:HIS:NE2	2.12	0.65
1:B:146:ARG:NH2	1:D:229:GLN:OE1	2.30	0.63
1:A:45:LEU:O	1:A:49:THR:HG23	1.97	0.63
1:E:146:ARG:HB2	1:E:156:THR:HG22	1.81	0.63
1:C:159:GLY:HA2	1:E:204:VAL:HG11	1.82	0.62
1:D:183:TRP:HH2	1:D:198:TYR:HH	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:LYS:HE3	1:D:132:GLU:HG3	1.82	0.61
1:D:58:ARG:NH2	1:D:116:GLN:OE1	2.34	0.61
1:A:83:MET:HE3	1:A:108:LEU:HD13	1.82	0.60
1:B:192:ARG:NH2	1:D:149:PRO:HG2	2.18	0.59
1:B:34:ILE:HD11	1:B:48:LEU:HD11	1.85	0.59
1:A:170:GLU:CD	1:A:209:ARG:HH12	2.11	0.58
1:C:138:ARG:HH12	1:E:216:GLU:CG	2.13	0.58
1:B:120:MET:HE2	1:B:124:MET:HE2	1.87	0.57
1:B:38:GLY:HA2	1:D:42:THR:HG22	1.85	0.57
1:D:83:MET:HG3	1:D:107:LEU:HG	1.86	0.57
1:D:183:TRP:HH2	1:D:198:TYR:OH	1.88	0.57
1:C:239:LEU:HG	1:C:240:ARG:H	1.70	0.56
1:B:211:GLN:HG2	1:B:215:PHE:O	2.06	0.56
1:A:50:LYS:HD3	1:A:91:LEU:O	2.05	0.55
1:C:109:TYR:HA	1:C:124:MET:HE1	1.88	0.55
1:B:137:SER:O	1:B:137:SER:OG	2.18	0.55
1:B:26:THR:O	1:B:28:SER:N	2.38	0.55
1:A:40:MET:HE1	1:A:74:HIS:CD2	2.41	0.55
1:A:40:MET:HE1	1:A:74:HIS:CE1	2.41	0.54
1:C:146:ARG:HH12	1:E:149:PRO:HG3	1.73	0.54
1:B:38:GLY:CA	1:D:42:THR:HG22	2.38	0.53
1:D:178:SER:O	1:D:179:VAL:C	2.51	0.53
1:B:23:ALA:HA	1:E:65:PRO:HB2	1.90	0.53
1:E:34:ILE:HD11	1:E:48:LEU:HD11	1.91	0.53
1:C:146:ARG:HH11	1:C:192:ARG:HD3	1.71	0.53
1:E:83:MET:HE2	1:E:108:LEU:HB2	1.90	0.52
1:A:170:GLU:OE2	1:A:209:ARG:NH1	2.33	0.52
1:B:83:MET:HE3	1:B:108:LEU:HD13	1.91	0.52
1:D:87:ILE:HG12	1:D:120:MET:HE1	1.91	0.52
1:C:187:SER:OG	1:C:188:THR:N	2.40	0.52
1:B:35:ASP:OD2	1:D:42:THR:HG21	2.10	0.52
1:A:33:HIS:HB3	1:A:74:HIS:CD2	2.45	0.51
1:E:51:TYR:CE2	1:E:119:PRO:HG2	2.45	0.51
1:E:33:HIS:O	1:E:74:HIS:HB2	2.11	0.51
1:A:174:VAL:HG21	1:A:198:TYR:CD2	2.46	0.50
1:B:170:GLU:CD	1:B:209:ARG:HH12	2.18	0.50
1:C:132:GLU:O	1:C:135:ARG:HG2	2.11	0.50
1:A:67:VAL:HG11	1:C:31:PRO:HD3	1.93	0.50
1:A:205:GLN:HE21	1:D:189:HIS:CE1	2.30	0.50
2:A:301:PO4:O2	1:C:220:SER:HB2	2.12	0.50
1:A:137:SER:O	1:A:137:SER:OG	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ASP:OD2	1:E:47:THR:OG1	2.31	0.49
1:D:34:ILE:HD11	1:D:48:LEU:HD11	1.95	0.49
1:B:145:VAL:HG11	1:B:207:LEU:HD21	1.94	0.49
1:C:58:ARG:NH2	1:C:116:GLN:OE1	2.42	0.49
1:C:135:ARG:HG3	1:C:136:PHE:CD1	2.47	0.49
1:C:34:ILE:HD11	1:C:48:LEU:HD11	1.94	0.49
1:C:223:GLY:HA3	1:E:223:GLY:HA2	1.95	0.48
1:E:167:VAL:HG12	1:E:209:ARG:HD2	1.94	0.48
1:A:40:MET:CE	1:A:74:HIS:NE2	2.76	0.48
1:D:217:ILE:HD13	1:D:235:LEU:HG	1.95	0.48
1:E:109:TYR:HA	1:E:124:MET:HE1	1.96	0.48
1:D:26:THR:O	1:D:28:SER:N	2.45	0.47
1:A:49:THR:O	1:A:49:THR:OG1	2.32	0.47
1:C:83:MET:HG3	1:C:107:LEU:HG	1.95	0.47
1:C:185:HIS:HA	1:C:190:VAL:HG23	1.97	0.47
1:D:122:LEU:O	1:D:126:ARG:HG3	2.15	0.46
1:B:41:TYR:HA	1:E:38:GLY:HA3	1.95	0.46
1:D:32:VAL:HG21	1:D:48:LEU:HD12	1.98	0.46
1:C:155:ILE:HG21	1:C:206:VAL:HG21	1.96	0.46
1:A:122:LEU:HD11	4:A:402:HOH:O	2.15	0.46
1:A:83:MET:CE	1:A:108:LEU:HB2	2.45	0.46
1:A:184:ASN:HD21	1:A:192:ARG:NH2	2.14	0.46
1:B:202:ASN:OD1	1:B:205:GLN:HG3	2.16	0.46
1:C:157:LEU:CD2	1:C:195:LEU:HB2	2.46	0.46
1:D:53:GLU:HG2	4:D:321:HOH:O	2.15	0.46
1:A:33:HIS:CB	1:A:74:HIS:CG	2.99	0.46
1:B:42:THR:HG22	1:E:76:PHE:CE1	2.49	0.46
1:D:187:SER:O	1:D:189:HIS:N	2.43	0.46
1:E:26:THR:O	1:E:28:SER:N	2.45	0.45
1:B:83:MET:HE2	1:B:108:LEU:CB	2.46	0.45
1:C:61:ASP:OD1	1:C:62:GLY:N	2.49	0.45
1:D:33:HIS:HB2	1:D:74:HIS:HB3	1.97	0.45
1:C:48:LEU:HD13	1:C:60:PHE:CZ	2.52	0.45
1:C:170:GLU:CD	1:C:209:ARG:HH12	2.24	0.45
1:E:58:ARG:NH2	1:E:116:GLN:OE1	2.49	0.45
1:A:165:GLU:HG2	1:A:171:ILE:HD11	1.99	0.44
1:C:67:VAL:HG11	1:E:31:PRO:HD3	2.00	0.44
1:A:236:ARG:NH2	1:C:216:GLU:OE2	2.47	0.44
1:B:67:VAL:HG13	1:D:25:LEU:HD21	1.99	0.44
1:B:216:GLU:HG3	1:E:138:ARG:HH12	1.81	0.44
1:E:202:ASN:OD1	1:E:205:GLN:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:CYS:SG	1:C:231:SER:HB3	2.58	0.44
1:D:183:TRP:CZ3	1:D:194:PRO:HD2	2.52	0.43
1:A:186:ASP:HB3	1:A:187:SER:H	1.66	0.43
1:B:202:ASN:OD1	1:B:204:VAL:HG22	2.19	0.43
1:C:186:ASP:N	1:C:186:ASP:OD1	2.51	0.43
1:D:157:LEU:HD11	1:D:195:LEU:HD22	2.00	0.43
1:A:132:GLU:O	1:A:135:ARG:HG2	2.19	0.43
1:A:136:PHE:CZ	1:C:239:LEU:HD12	2.53	0.43
1:E:109:TYR:CD2	1:E:124:MET:HE3	2.53	0.43
1:E:135:ARG:HG3	1:E:136:PHE:CD1	2.54	0.43
1:A:83:MET:HE1	1:A:102:PHE:HZ	1.83	0.43
1:A:83:MET:HE2	1:A:108:LEU:HB2	2.01	0.42
1:A:229:GLN:HE21	1:A:229:GLN:HB2	1.64	0.42
1:A:39:HIS:HE1	4:D:312:HOH:O	2.02	0.42
1:B:137:SER:HA	1:D:212:GLN:O	2.20	0.42
1:A:135:ARG:HG3	1:A:136:PHE:CD1	2.55	0.42
1:A:233:TYR:OH	1:D:232:GLU:OE2	2.35	0.42
1:D:180:ASN:C	1:D:182:GLY:H	2.28	0.42
1:E:83:MET:HE2	1:E:108:LEU:CB	2.50	0.42
1:E:51:TYR:CD2	1:E:119:PRO:HG2	2.55	0.42
1:A:26:THR:O	1:A:28:SER:N	2.48	0.41
1:A:83:MET:HG3	1:A:107:LEU:HG	2.02	0.41
1:B:83:MET:HG3	1:B:107:LEU:HG	2.02	0.41
1:A:34:ILE:HD11	1:A:48:LEU:HD11	2.02	0.41
1:B:167:VAL:HG11	1:B:210:LEU:HD23	2.03	0.41
1:C:109:TYR:OH	1:C:125:GLU:OE2	2.25	0.41
1:C:157:LEU:HD22	1:C:195:LEU:HB2	2.02	0.41
1:A:33:HIS:HB2	1:A:74:HIS:CG	2.51	0.41
1:A:33:HIS:HB3	1:A:74:HIS:CG	2.56	0.41
1:D:168:PHE:O	1:D:171:ILE:HG12	2.21	0.41
1:E:229:GLN:HE21	1:E:229:GLN:HB2	1.64	0.41
1:D:225:VAL:HG23	1:D:227:SER:H	1.86	0.41
1:A:47:THR:HG21	1:A:92:ARG:HG2	2.03	0.40
1:D:154:ARG:CZ	1:D:154:ARG:HB3	2.50	0.40
1:C:33:HIS:O	1:C:74:HIS:HB2	2.22	0.40
1:B:83:MET:CE	1:B:108:LEU:HB2	2.48	0.40
1:C:128:LYS:NZ	1:C:131:ARG:NH2	2.70	0.40
1:C:148:ALA:HA	1:C:149:PRO:HD3	1.79	0.40
1:E:83:MET:CE	1:E:108:LEU:HD13	2.52	0.40
1:B:215:PHE:HB3	1:B:235:LEU:HB3	2.03	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	217/257 (84%)	197 (91%)	19 (9%)	1 (0%)	24	46
1	B	209/257 (81%)	196 (94%)	13 (6%)	0	100	100
1	C	198/257 (77%)	184 (93%)	13 (7%)	1 (0%)	24	46
1	D	218/257 (85%)	198 (91%)	19 (9%)	1 (0%)	24	46
1	E	200/257 (78%)	189 (94%)	10 (5%)	1 (0%)	24	46
All	All	1042/1285 (81%)	964 (92%)	74 (7%)	4 (0%)	30	51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	180	ASN
1	E	188	THR
1	C	187	SER
1	A	187	SER

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	193/233 (83%)	179 (93%)	14 (7%)	13	29
1	B	184/233 (79%)	177 (96%)	7 (4%)	29	56
1	C	177/233 (76%)	167 (94%)	10 (6%)	19	40
1	D	191/233 (82%)	188 (98%)	3 (2%)	55	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	179/233 (77%)	175 (98%)	4 (2%)	45	72
All	All	924/1165 (79%)	886 (96%)	38 (4%)	27	54

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	SER
1	A	26	THR
1	A	49	THR
1	A	67	VAL
1	A	68	LEU
1	A	118	GLN
1	A	122	LEU
1	A	146	ARG
1	A	151	LEU
1	A	156	THR
1	A	186	ASP
1	A	188	THR
1	A	196	ASN
1	A	229	GLN
1	B	25	LEU
1	B	74	HIS
1	B	132	GLU
1	B	157	LEU
1	B	171	ILE
1	B	188	THR
1	B	229	GLN
1	C	27	LYS
1	C	106	THR
1	C	151	LEU
1	C	156	THR
1	C	157	LEU
1	C	167	VAL
1	C	184	ASN
1	C	188	THR
1	C	231	SER
1	C	240	ARG
1	D	174	VAL
1	D	199	CYS
1	D	229	GLN
1	E	47	THR
1	E	170	GLU

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Mol	Chain	Res	Type
1	E	174	VAL
1	E	229	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	118	GLN
1	A	205	GLN
1	B	196	ASN
1	D	196	ASN
1	E	33	HIS
1	E	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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z > 2$
2	PO4	A	301	-	4,4,4	1.08	0	6,6,6	0.49	0
2	PO4	C	301	3	4,4,4	0.94	0	6,6,6	0.57	0

There are no bond length outliers.

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 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	PO4	1	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	220/257 (85%)	0.03	14 (6%) 25 20	31, 83, 134, 178	1 (0%)
1	B	213/257 (82%)	-0.29	3 (1%) 73 69	39, 74, 125, 151	0
1	C	204/257 (79%)	-0.05	10 (4%) 35 29	47, 82, 138, 167	0
1	D	221/257 (85%)	-0.19	8 (3%) 46 40	41, 74, 131, 147	1 (0%)
1	E	204/257 (79%)	-0.22	2 (0%) 79 76	51, 76, 122, 140	0
All	All	1062/1285 (82%)	-0.14	37 (3%) 47 41	31, 78, 132, 178	2 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	ASP	5.4
1	B	211	GLN	4.8
1	A	185	HIS	4.6
1	A	74	HIS	4.2
1	C	69	ASP	4.1
1	D	180	ASN	3.7
1	B	224	GLY	3.5
1	D	181	ALA	3.2
1	C	63	THR	3.0
1	D	177	ASN	3.0
1	C	67	VAL	3.0
1	D	179	VAL	2.9
1	D	24	GLN	2.9
1	A	179	VAL	2.8
1	D	226	ASP	2.7
1	C	66	ILE	2.7
1	A	68	LEU	2.6
1	A	226	ASP	2.5
1	C	68	LEU	2.5
1	A	71	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	70	SER	2.4
1	B	228	SER	2.4
1	E	154	ARG	2.3
1	C	226	ASP	2.2
1	C	64	GLU	2.2
1	C	185	HIS	2.2
1	A	151	LEU	2.2
1	C	151	LEU	2.2
1	D	178	SER	2.1
1	A	182	GLY	2.1
1	C	101	ASP	2.1
1	A	228	SER	2.1
1	A	138	ARG	2.0
1	D	187	SER	2.0
1	E	224	GLY	2.0
1	A	21	THR	2.0
1	A	73	GLN	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($\text{\AA}^2$)	Q<0.9
2	PO4	A	301	5/5	0.86	0.20	56,57,66,73	5
2	PO4	C	301	5/5	0.97	0.10	69,73,81,88	0
3	K	A	302	1/1	0.98	0.04	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.