



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2017 – 04:49 AM EDT

PDB ID : 5VKP
Title : K2P2.1(TREK-1):ML402 complex
Authors : Lolicato, M.; Minor, D.L.
Deposited on : unknown
Resolution : 2.80 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

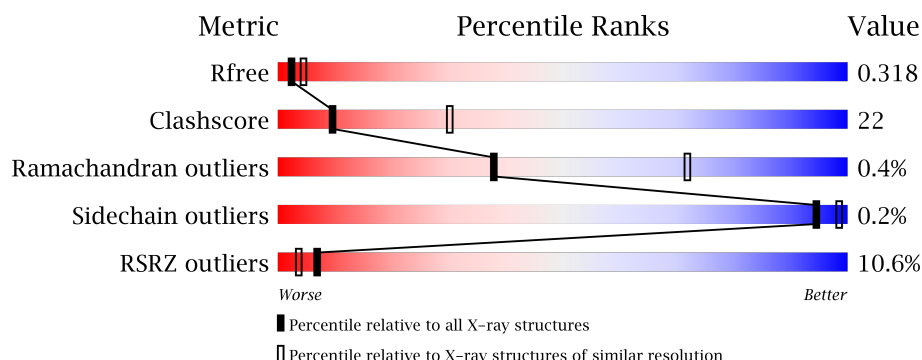
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	312	<div> <div>9%</div> <div>51%</div> <div>37%</div> <div>12%</div> </div>
1	B	312	<div> <div>10%</div> <div>52%</div> <div>38%</div> <div>10%</div> </div>

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	K	A	410	-	-	-	X
4	R16	B	407	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4557 atoms, of which 56 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 Potassium channel subfamily K member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2155	1436	340	374	5			
1	B	282	Total	C	N	O	S	0	0	0
			2173	1442	346	380	5			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP P97438
A	84	ARG	LYS	engineered mutation	UNP P97438
A	85	GLU	GLN	engineered mutation	UNP P97438
A	86	LYS	THR	engineered mutation	UNP P97438
A	88	LEU	ILE	engineered mutation	UNP P97438
A	89	ARG	ALA	engineered mutation	UNP P97438
A	90	ALA	GLN	engineered mutation	UNP P97438
A	92	PRO	ALA	engineered mutation	UNP P97438
A	95	SER	ASN	engineered mutation	UNP P97438
A	96	ASP	SER	engineered mutation	UNP P97438
A	97	GLN	THR	engineered mutation	UNP P97438
A	119	ALA	ASN	engineered mutation	UNP P97438
A	300	ALA	SER	engineered mutation	UNP P97438
A	306	ALA	GLU	engineered mutation	UNP P97438
A	323	SER	-	expression tag	UNP P97438
A	324	ASN	-	expression tag	UNP P97438
A	325	SER	-	expression tag	UNP P97438
A	326	LEU	-	expression tag	UNP P97438
A	327	GLU	-	expression tag	UNP P97438
A	328	VAL	-	expression tag	UNP P97438
A	329	LEU	-	expression tag	UNP P97438
A	330	PHE	-	expression tag	UNP P97438
A	331	GLN	-	expression tag	UNP P97438
B	20	MET	-	initiating methionine	UNP P97438
B	84	ARG	LYS	engineered mutation	UNP P97438

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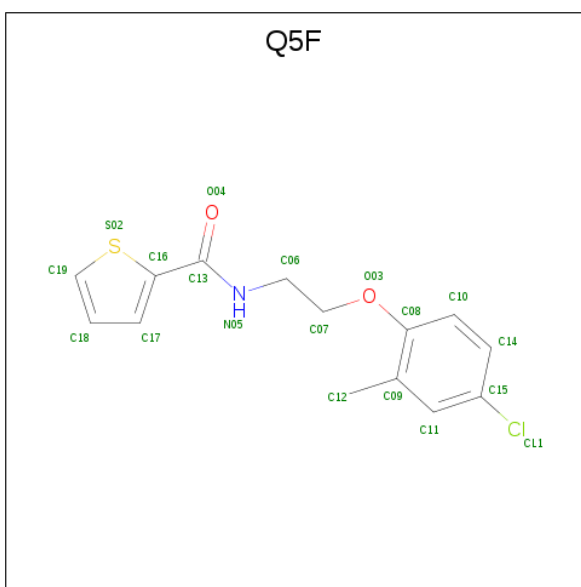
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Chain	Residue	Modelled	Actual	Comment	Reference
B	85	GLU	GLN	engineered mutation	UNP P97438
B	86	LYS	THR	engineered mutation	UNP P97438
B	88	LEU	ILE	engineered mutation	UNP P97438
B	89	ARG	ALA	engineered mutation	UNP P97438
B	90	ALA	GLN	engineered mutation	UNP P97438
B	92	PRO	ALA	engineered mutation	UNP P97438
B	95	SER	ASN	engineered mutation	UNP P97438
B	96	ASP	SER	engineered mutation	UNP P97438
B	97	GLN	THR	engineered mutation	UNP P97438
B	119	ALA	ASN	engineered mutation	UNP P97438
B	300	ALA	SER	engineered mutation	UNP P97438
B	306	ALA	GLU	engineered mutation	UNP P97438
B	323	SER	-	expression tag	UNP P97438
B	324	ASN	-	expression tag	UNP P97438
B	325	SER	-	expression tag	UNP P97438
B	326	LEU	-	expression tag	UNP P97438
B	327	GLU	-	expression tag	UNP P97438
B	328	VAL	-	expression tag	UNP P97438
B	329	LEU	-	expression tag	UNP P97438
B	330	PHE	-	expression tag	UNP P97438
B	331	GLN	-	expression tag	UNP P97438

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

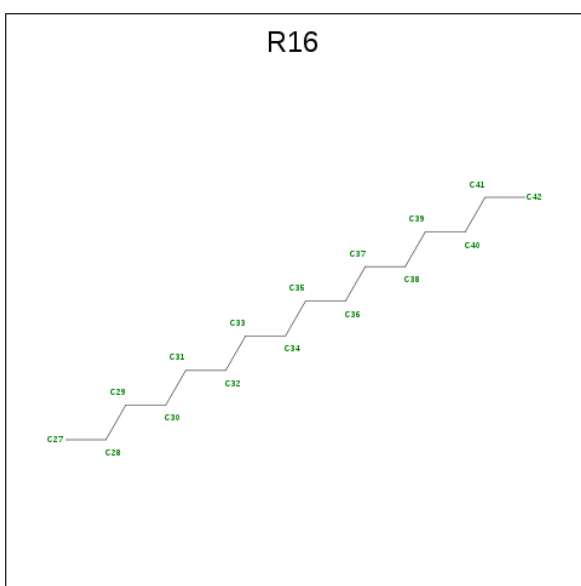
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	5	Total K 5 5	0	0

- Molecule 3 is N-[2-(4-chloro-2-methylphenoxy)ethyl]thiophene-2-carboxamide (three-letter code: Q5F) (formula: C₁₄H₁₄ClNO₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	0	0
			19	14	1	1	2	1		
3	B	1	Total	C	Cl	N	O	S	0	0
			19	14	1	1	2	1		

- Molecule 4 is HEXADECANE (three-letter code: R16) (formula: C₁₆H₃₄).



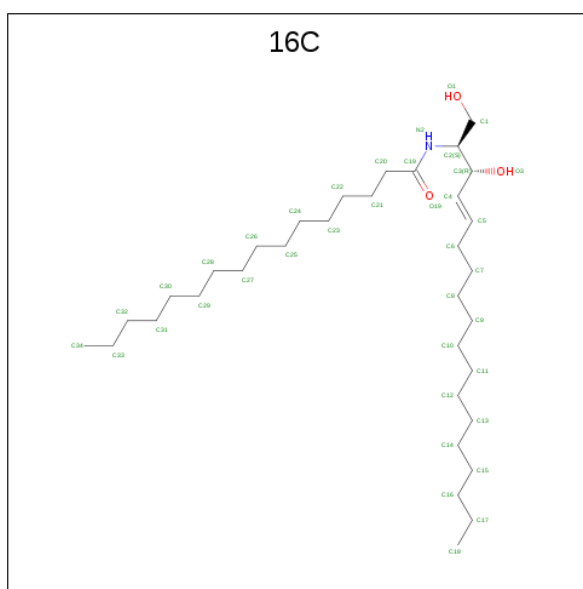
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C	0	0
			12	12		
4	A	1	Total	C	0	0
			11	11		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H 24 8 16	0	0
4	B	1	Total C 12 12	0	0
4	B	1	Total C 12 12	0	0
4	B	1	Total C 5 5	0	0
4	B	1	Total C H 15 5 10	0	0
4	B	1	Total C H 15 5 10	0	0
4	B	1	Total C 11 11	0	0
4	B	1	Total C H 30 10 20	0	0

- Molecule 5 is N-((E,2S,3R)-1,3-DIHYDROXYOCTADEC-4-EN-2-YL)PALMITAMIDE (three-letter code: 16C) (formula: $C_{34}H_{67}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 38 34 1 3	0	0

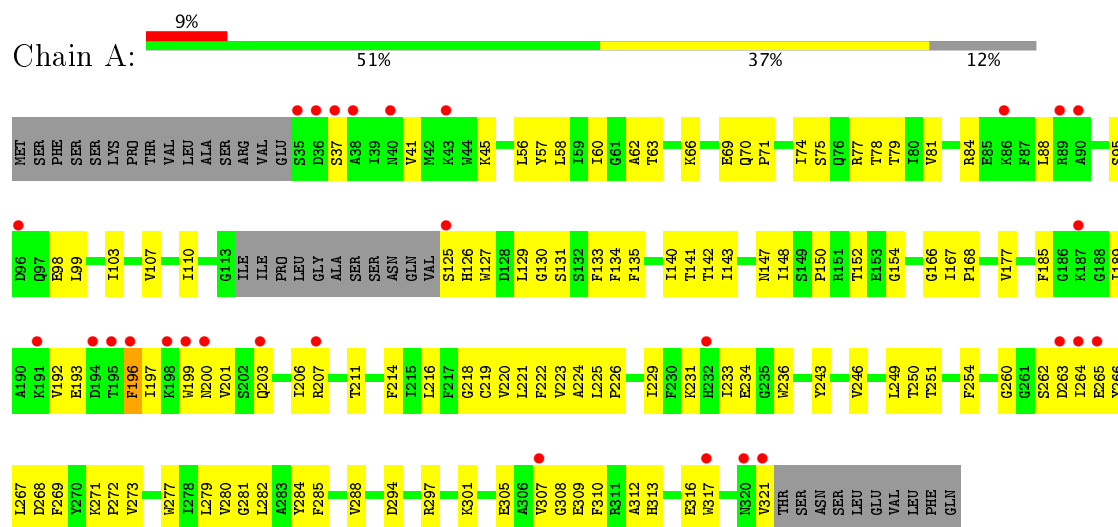
- Molecule 6 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cd	0	0
			1	1		

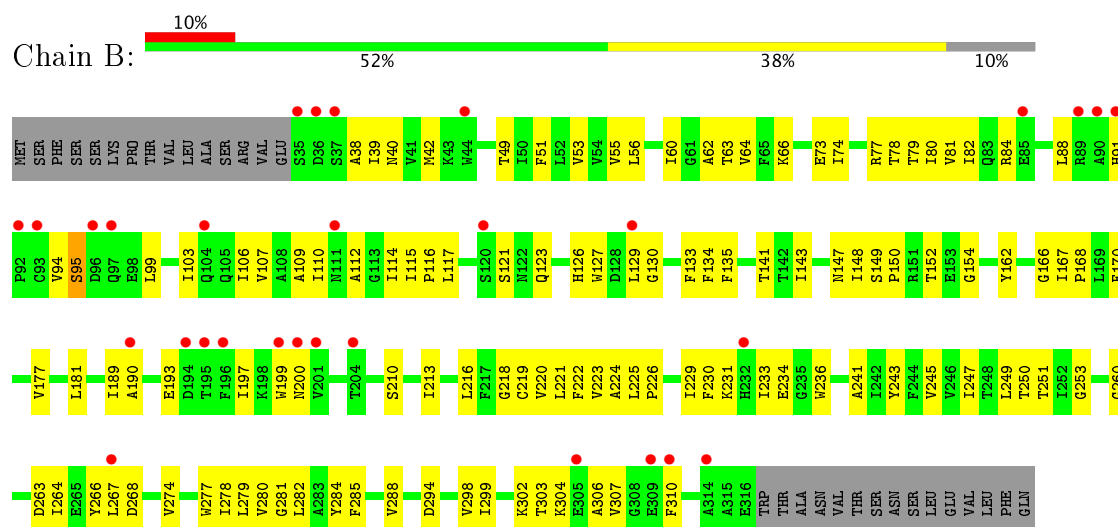
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Potassium channel subfamily K member 2



• Molecule 1: Potassium channel subfamily K member 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.09Å 119.56Å 127.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.98 – 2.80 14.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.4 (14.98-2.80) 99.8 (14.98-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.269 , 0.314 0.280 , 0.318	Depositor DCC
R_{free} test set	1236 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	97.9	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 132.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4557	wwPDB-VP
Average B, all atoms (Å ²)	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: R16, K, Q5F, CD, 16C

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	0.28	0/2208	0.39	0/3003
1	B	0.24	0/2226	0.38	0/3027
All	All	0.26	0/4434	0.39	0/6030

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	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	TRP	Peptide
1	B	263	ASP	Peptide
1	B	95	SER	Peptide

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	2155	0	2201	109	4
1	B	2173	0	2196	102	0
2	A	5	0	0	0	0
3	A	19	0	0	1	0
3	B	19	0	0	3	0
4	A	31	16	50	0	0
4	B	60	40	92	3	0
5	A	38	0	67	2	0
6	B	1	0	0	0	0
All	All	4501	56	4606	197	4

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 22.

All (197) 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:197:ILE:HG23	1:A:206:ILE:HD13	1.33	1.08
1:A:197:ILE:HD12	1:A:206:ILE:HG21	1.48	0.93
1:A:193:GLU:HA	1:A:197:ILE:HG13	1.53	0.90
1:A:262:SER:O	1:A:266:TYR:OH	1.88	0.90
1:B:229:ILE:HG23	1:B:233:ILE:HD13	1.56	0.88
1:A:203:GLN:HA	1:A:206:ILE:HD12	1.57	0.86
1:A:63:THR:HA	1:A:66:LYS:HE2	1.61	0.83
1:A:229:ILE:HG23	1:A:233:ILE:HD13	1.64	0.80
1:A:263:ASP:OD1	1:A:264:ILE:HG13	1.83	0.79
1:A:197:ILE:HG23	1:A:206:ILE:CD1	2.14	0.77
1:B:126:HIS:HB3	1:B:148:ILE:HD13	1.66	0.76
1:B:221:LEU:HA	1:B:225:LEU:HD12	1.68	0.75
1:B:63:THR:HA	1:B:66:LYS:HE2	1.68	0.74
1:B:91:HIS:HB2	1:B:94:VAL:HG23	1.69	0.74
1:A:308:GLY:O	1:A:312:ALA:N	2.21	0.74
1:A:84:ARG:NH1	1:B:116:PRO:HA	2.03	0.73
1:A:152:THR:HG22	1:A:154:GLY:H	1.54	0.73
1:B:260:GLY:HA2	1:B:266:TYR:CZ	2.23	0.73
1:A:88:LEU:HD11	1:A:99:LEU:HD13	1.69	0.72
1:A:193:GLU:HA	1:A:197:ILE:CG1	2.18	0.72
1:A:135:PHE:CZ	1:A:150:PRO:HD3	2.24	0.71
1:A:197:ILE:HD12	1:A:206:ILE:CG2	2.21	0.70
1:B:152:THR:HG22	1:B:154:GLY:H	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:SER:N	1:B:77:ARG:HH12	1.89	0.70
1:B:181:LEU:HD22	1:B:280:VAL:HG13	1.74	0.69
1:B:167:ILE:HB	1:B:168:PRO:HD3	1.76	0.68
1:A:37:SER:O	1:A:41:VAL:HG23	1.95	0.67
1:A:77:ARG:HD3	1:B:123:GLN:OE1	1.95	0.67
1:B:84:ARG:O	1:B:88:LEU:HG	1.96	0.65
1:A:126:HIS:HB2	1:A:148:ILE:CD1	2.26	0.65
1:A:127:TRP:HB2	1:B:73:GLU:OE1	1.97	0.65
1:A:249:LEU:HA	1:A:282:LEU:HD23	1.78	0.65
1:B:229:ILE:CG2	1:B:233:ILE:HD13	2.26	0.64
1:A:229:ILE:CG2	1:A:233:ILE:HD13	2.28	0.62
1:A:95:SER:OG	1:A:98:GLU:OE1	2.17	0.62
1:B:60:ILE:O	1:B:64:VAL:HG23	1.99	0.62
1:B:299:ILE:O	1:B:303:THR:HG22	1.99	0.62
1:A:264:ILE:HG23	1:A:265:GLU:HG3	1.82	0.61
1:B:303:THR:HG23	1:B:304:LYS:N	2.15	0.61
1:B:302:LYS:O	1:B:307:VAL:HG23	2.00	0.61
1:A:74:ILE:O	1:A:78:THR:HG23	2.02	0.59
1:B:91:HIS:HB2	1:B:94:VAL:CG2	2.31	0.59
1:B:106:ILE:O	1:B:110:ILE:HG13	2.03	0.59
1:B:303:THR:HG23	1:B:304:LYS:H	1.67	0.58
1:B:306:ALA:O	1:B:310:PHE:HD2	1.87	0.58
1:B:219:CYS:O	1:B:223:VAL:HB	2.03	0.58
1:A:249:LEU:HB2	1:A:285:PHE:CD2	2.39	0.58
1:A:200:ASN:OD1	1:A:201:VAL:N	2.36	0.58
1:A:126:HIS:HB2	1:A:148:ILE:HD13	1.85	0.58
1:B:107:VAL:HA	1:B:110:ILE:HD12	1.86	0.58
1:A:309:GLU:HA	1:A:312:ALA:HB3	1.86	0.57
1:A:231:LYS:HG3	1:A:236:TRP:O	2.04	0.57
1:B:126:HIS:HB3	1:B:148:ILE:CD1	2.31	0.57
1:A:84:ARG:HH11	1:B:116:PRO:HA	1.67	0.57
1:A:129:LEU:HD12	1:A:130:GLY:N	2.19	0.57
1:A:249:LEU:HB2	1:A:285:PHE:CE2	2.40	0.56
1:B:103:ILE:HD12	1:B:103:ILE:H	1.71	0.56
1:B:210:SER:O	1:B:213:ILE:HG22	2.05	0.56
1:B:129:LEU:HD12	1:B:130:GLY:N	2.21	0.56
1:A:41:VAL:HG12	1:A:45:LYS:HE3	1.87	0.56
1:B:216:LEU:O	1:B:220:VAL:HG23	2.06	0.56
1:A:70:GLN:HB3	1:A:71:PRO:HD3	1.87	0.56
1:B:234:GLU:HG2	1:B:236:TRP:CE2	2.42	0.56
1:A:218:GLY:HA3	1:A:284:TYR:CZ	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ASP:HA	1:A:297:ARG:HG2	1.89	0.55
1:A:189:ILE:O	1:A:193:GLU:HG3	2.07	0.55
1:A:75:SER:O	1:A:79:THR:HG23	2.06	0.54
1:B:250:THR:O	1:B:251:THR:OG1	2.22	0.54
1:A:77:ARG:O	1:A:81:VAL:HG23	2.07	0.54
1:B:231:LYS:HG3	1:B:236:TRP:O	2.07	0.54
1:A:264:ILE:CG2	1:A:265:GLU:HG3	2.38	0.54
1:A:218:GLY:HA3	1:A:284:TYR:CE1	2.43	0.54
1:B:249:LEU:HD11	1:B:277:TRP:CZ2	2.43	0.54
1:A:234:GLU:HG2	1:A:236:TRP:CE2	2.43	0.53
1:B:141:THR:HG22	1:B:170:PHE:CE2	2.43	0.53
1:B:218:GLY:HA3	1:B:284:TYR:CZ	2.44	0.53
1:B:221:LEU:O	1:B:226:PRO:HD3	2.07	0.53
1:B:141:THR:HG22	1:B:170:PHE:CZ	2.44	0.53
1:A:301:LYS:O	1:A:305:GLU:HG2	2.09	0.53
1:B:260:GLY:HA2	1:B:266:TYR:CE2	2.43	0.53
1:B:56:LEU:HD21	1:B:60:ILE:HD11	1.91	0.52
1:A:222:PHE:CE1	1:A:280:VAL:HG12	2.43	0.52
1:A:192:VAL:HG12	1:A:196:PHE:HE1	1.75	0.52
1:B:149:SER:HB2	1:B:150:PRO:HD2	1.92	0.52
1:A:125:SER:HA	1:B:73:GLU:OE2	2.10	0.51
1:A:131:SER:O	1:A:134:PHE:HB3	2.10	0.51
1:A:267:LEU:HD23	1:A:269:PHE:CE1	2.46	0.51
1:B:278:ILE:HD13	3:B:402:Q5F:C15	2.41	0.51
1:A:310:PHE:HA	1:A:313:HIS:CD2	2.46	0.51
1:B:77:ARG:O	1:B:81:VAL:HG23	2.10	0.51
1:A:196:PHE:H	1:A:196:PHE:HD1	1.57	0.51
1:A:234:GLU:HG2	1:A:236:TRP:CZ2	2.46	0.51
1:A:250:THR:O	1:A:251:THR:OG1	2.29	0.50
1:B:294:ASP:O	1:B:298:VAL:HG23	2.11	0.50
1:A:307:VAL:HG23	1:A:307:VAL:O	2.10	0.50
1:A:126:HIS:HB2	1:A:148:ILE:HD11	1.92	0.50
1:B:39:ILE:HD12	1:B:40:ASN:N	2.26	0.50
1:B:49:THR:O	1:B:53:VAL:HG23	2.11	0.50
1:B:94:VAL:HG11	1:B:99:LEU:HD22	1.94	0.50
1:B:249:LEU:HB2	1:B:285:PHE:CE2	2.47	0.49
1:B:303:THR:O	1:B:307:VAL:HB	2.12	0.49
1:A:66:LYS:O	1:A:70:GLN:HB2	2.12	0.49
1:B:245:VAL:HG13	1:B:277:TRP:HZ2	1.78	0.49
1:A:192:VAL:CG1	1:A:196:PHE:HE1	2.27	0.48
1:A:277:TRP:O	1:A:281:GLY:N	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LEU:O	1:A:103:ILE:HG12	2.12	0.48
1:A:98:GLU:HG2	1:B:91:HIS:NE2	2.29	0.48
1:A:177:VAL:HG21	1:A:279:LEU:HD11	1.96	0.48
1:A:192:VAL:CG1	1:A:196:PHE:CE1	2.96	0.48
1:A:317:TRP:O	1:A:321:VAL:HG22	2.14	0.48
1:A:58:LEU:HB3	1:B:133:PHE:CE1	2.48	0.48
1:A:260:GLY:HA2	1:A:266:TYR:CE1	2.49	0.47
1:A:62:ALA:HB2	1:B:133:PHE:HA	1.96	0.47
1:B:135:PHE:CZ	1:B:150:PRO:HD3	2.49	0.47
1:B:229:ILE:HG23	1:B:233:ILE:CD1	2.35	0.47
1:B:306:ALA:O	1:B:310:PHE:CD2	2.68	0.47
1:B:218:GLY:HA3	1:B:284:TYR:CE1	2.49	0.47
1:B:79:THR:HA	1:B:82:ILE:HD12	1.97	0.47
1:B:177:VAL:HG21	1:B:279:LEU:HD21	1.95	0.47
1:B:274:VAL:O	1:B:278:ILE:HG13	2.14	0.47
1:B:121:SER:O	1:B:123:GLN:HG3	2.15	0.47
1:B:249:LEU:HD22	1:B:281:GLY:C	2.34	0.46
1:A:88:LEU:HD11	1:A:99:LEU:CD1	2.40	0.46
1:B:266:TYR:O	1:B:268:ASP:N	2.48	0.46
1:A:147:ASN:OD1	1:A:148:ILE:N	2.49	0.46
1:A:185:PHE:CZ	1:A:214:PHE:HB2	2.51	0.46
1:A:110:ILE:HD11	1:B:110:ILE:HD13	1.98	0.46
1:B:304:LYS:HD3	4:B:404:R16:H291	1.98	0.46
1:A:193:GLU:O	1:A:197:ILE:HB	2.16	0.45
1:B:220:VAL:HA	1:B:224:ALA:HB3	1.98	0.45
1:B:249:LEU:HB2	1:B:285:PHE:CD2	2.51	0.45
1:B:304:LYS:HD3	4:B:404:R16:C29	2.46	0.45
1:A:310:PHE:HA	1:A:313:HIS:HD2	1.79	0.45
1:A:219:CYS:O	1:A:223:VAL:HB	2.15	0.45
1:A:41:VAL:O	1:A:45:LYS:HG3	2.16	0.45
1:B:241:ALA:O	1:B:245:VAL:HG23	2.17	0.45
1:A:134:PHE:HE1	3:A:404:Q5F:C09	2.30	0.45
1:A:269:PHE:O	1:A:273:VAL:HG23	2.16	0.45
1:B:193:GLU:O	1:B:197:ILE:HB	2.16	0.45
1:B:147:ASN:OD1	1:B:148:ILE:N	2.50	0.45
1:A:260:GLY:HA2	1:A:266:TYR:CZ	2.52	0.45
1:B:115:ILE:O	1:B:115:ILE:HG22	2.15	0.45
1:A:167:ILE:HB	1:A:168:PRO:HD3	1.98	0.45
1:A:140:ILE:HG22	1:A:166:GLY:HA3	1.99	0.44
1:B:189:ILE:HD12	1:B:190:ALA:N	2.31	0.44
1:A:135:PHE:HZ	1:A:150:PRO:HD3	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:PHE:CE1	1:B:280:VAL:HG12	2.52	0.44
1:B:189:ILE:O	1:B:193:GLU:HG3	2.17	0.44
1:B:134:PHE:HE1	3:B:402:Q5F:C09	2.31	0.44
5:A:406:16C:H151	5:A:406:16C:H183	1.67	0.44
1:A:69:GLU:HG3	1:B:127:TRP:CH2	2.53	0.44
1:B:94:VAL:HG12	1:B:95:SER:N	2.33	0.43
1:B:181:LEU:HD22	1:B:280:VAL:CG1	2.45	0.43
1:A:192:VAL:HG13	1:A:196:PHE:CE1	2.53	0.43
1:B:143:ILE:O	1:B:253:GLY:HA3	2.18	0.43
1:A:133:PHE:HA	1:B:62:ALA:HB2	1.99	0.43
1:A:312:ALA:O	1:A:316:GLU:HG3	2.18	0.43
1:A:196:PHE:N	1:A:196:PHE:CD1	2.87	0.42
1:B:278:ILE:HD13	3:B:402:Q5F:C11	2.49	0.42
1:B:162:TYR:O	1:B:166:GLY:N	2.47	0.42
1:B:304:LYS:HD3	4:B:404:R16:C28	2.49	0.42
1:B:284:TYR:CE2	1:B:288:VAL:HG21	2.54	0.42
1:A:41:VAL:CG1	1:A:45:LYS:HE3	2.48	0.42
1:A:56:LEU:HD21	1:A:60:ILE:HD11	2.02	0.42
1:B:249:LEU:HD22	1:B:282:LEU:N	2.35	0.42
1:A:220:VAL:HA	1:A:224:ALA:HB3	2.01	0.42
1:B:38:ALA:O	1:B:42:MET:HG2	2.19	0.42
1:A:221:LEU:HA	1:A:225:LEU:HD12	2.00	0.42
1:A:243:TYR:HH	1:A:254:PHE:HD2	1.67	0.42
1:B:109:ALA:HB1	1:B:114:ILE:HG21	2.01	0.42
1:B:74:ILE:O	1:B:78:THR:HG23	2.20	0.42
1:A:57:TYR:CE1	5:A:406:16C:H162	2.55	0.42
1:A:141:THR:O	1:A:142:THR:OG1	2.32	0.42
1:A:143:ILE:HG12	1:A:251:THR:HA	2.02	0.42
1:B:51:PHE:O	1:B:55:VAL:HG23	2.20	0.42
1:A:63:THR:CA	1:A:66:LYS:HE2	2.41	0.41
1:A:225:LEU:N	1:A:226:PRO:HD2	2.35	0.41
1:A:284:TYR:O	1:A:288:VAL:HG23	2.19	0.41
1:A:249:LEU:CB	1:A:285:PHE:CD2	3.03	0.41
1:A:310:PHE:O	1:A:313:HIS:CD2	2.74	0.41
1:B:112:ALA:O	1:B:114:ILE:HG23	2.21	0.41
1:B:243:TYR:O	1:B:247:ILE:HG12	2.19	0.41
1:A:216:LEU:O	1:A:220:VAL:HG23	2.20	0.41
1:A:246:VAL:O	1:A:250:THR:HG23	2.21	0.41
1:A:264:ILE:HG22	1:A:265:GLU:HB2	2.02	0.41
1:A:129:LEU:HA	1:B:66:LYS:HD3	2.01	0.41
1:B:303:THR:CG2	1:B:304:LYS:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:PHE:O	1:B:234:GLU:HB3	2.21	0.41
1:A:207:ARG:O	1:A:211:THR:HG23	2.21	0.41
1:A:271:LYS:HB2	1:A:272:PRO:HD3	2.03	0.41
1:A:103:ILE:HB	1:B:117:LEU:HD21	2.03	0.41
1:A:249:LEU:HA	1:A:282:LEU:CD2	2.48	0.40
1:A:69:GLU:HG3	1:B:127:TRP:CZ2	2.56	0.40
1:A:103:ILE:O	1:A:107:VAL:HG23	2.21	0.40
1:B:199:TRP:CE3	1:B:200:ASN:HB2	2.56	0.40
1:B:77:ARG:HA	1:B:80:ILE:HG22	2.03	0.40
1:B:222:PHE:CE1	1:B:280:VAL:CG1	3.04	0.40

All (4) 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:A:37:SER:CA	1:A:268:ASP:OD2[1_455]	1.93	0.27
1:A:37:SER:OG	1:A:268:ASP:CG[1_455]	2.13	0.07
1:A:37:SER:OG	1:A:268:ASP:OD1[1_455]	2.17	0.03
1:A:37:SER:OG	1:A:268:ASP:OD2[1_455]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	272/312 (87%)	264 (97%)	8 (3%)	0	100	100
1	B	280/312 (90%)	264 (94%)	14 (5%)	2 (1%)	25	59
All	All	552/624 (88%)	528 (96%)	22 (4%)	2 (0%)	38	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	264	ILE
1	B	267	LEU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	226/260 (87%)	225 (100%)	1 (0%)	93	98
1	B	224/260 (86%)	224 (100%)	0	100	100
All	All	450/520 (86%)	449 (100%)	1 (0%)	94	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	313	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 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
3	Q5F	A	404	-	19,20,20	2.51	10 (52%)	21,26,26	2.18	5 (23%)
4	R16	A	405	-	11,11,15	0.30	0	10,10,14	0.81	0
5	16C	A	406	-	36,37,37	1.12	2 (5%)	36,39,39	1.22	2 (5%)
4	R16	A	407	-	10,10,15	0.30	0	9,9,14	0.80	0
4	R16	A	408	-	7,7,15	0.30	0	6,6,14	0.71	0
3	Q5F	B	402	-	19,20,20	2.52	10 (52%)	21,26,26	2.09	4 (19%)
4	R16	B	403	-	11,11,15	0.30	0	10,10,14	0.82	0
4	R16	B	404	-	11,11,15	0.30	0	10,10,14	0.81	0
4	R16	B	405	-	4,4,15	0.32	0	3,3,14	0.54	0
4	R16	B	406	-	4,4,15	0.31	0	3,3,14	0.55	0
4	R16	B	407	-	4,4,15	0.32	0	3,3,14	0.53	0
4	R16	B	408	-	10,10,15	0.30	0	9,9,14	0.81	0
4	R16	B	409	-	9,9,15	0.32	0	8,8,14	0.75	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	Q5F	A	404	-	-	0/9/11/11	0/2/2/2
4	R16	A	405	-	-	0/9/9/13	0/0/0/0
5	16C	A	406	-	-	0/40/40/40	0/0/0/0
4	R16	A	407	-	-	0/8/8/13	0/0/0/0
4	R16	A	408	-	-	0/5/5/13	0/0/0/0
3	Q5F	B	402	-	-	0/9/11/11	0/2/2/2
4	R16	B	403	-	-	0/9/9/13	0/0/0/0
4	R16	B	404	-	-	0/9/9/13	0/0/0/0
4	R16	B	405	-	-	0/2/2/13	0/0/0/0
4	R16	B	406	-	-	0/2/2/13	0/0/0/0
4	R16	B	407	-	-	0/2/2/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	R16	B	408	-	-	0/8/8/13	0/0/0/0
4	R16	B	409	-	-	0/7/7/13	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	406	16C	O19-C19	-2.14	1.18	1.23
3	A	404	Q5F	C10-C14	2.09	1.42	1.38
3	A	404	Q5F	C18-C17	2.14	1.46	1.39
3	A	404	Q5F	C14-C15	2.17	1.42	1.38
3	B	402	Q5F	C18-C17	2.17	1.47	1.39
3	A	404	Q5F	C10-C08	2.23	1.44	1.39
3	B	402	Q5F	C10-C14	2.32	1.42	1.38
3	B	402	Q5F	C10-C08	2.37	1.44	1.39
3	B	402	Q5F	C14-C15	2.45	1.42	1.38
3	B	402	Q5F	C11-C09	2.73	1.43	1.39
3	A	404	Q5F	C11-C09	2.83	1.43	1.39
3	A	404	Q5F	C11-C15	3.21	1.43	1.38
3	B	402	Q5F	C15-CL1	3.23	1.81	1.74
3	B	402	Q5F	C11-C15	3.29	1.43	1.38
3	A	404	Q5F	C15-CL1	3.35	1.81	1.74
3	A	404	Q5F	C06-C07	3.54	1.63	1.50
3	B	402	Q5F	C06-C07	3.69	1.63	1.50
3	B	402	Q5F	C08-C09	3.82	1.48	1.39
3	A	404	Q5F	C08-C09	4.17	1.49	1.39
3	A	404	Q5F	C13-N05	5.51	1.46	1.33
5	A	406	16C	C19-N2	5.66	1.45	1.34
3	B	402	Q5F	C13-N05	5.68	1.46	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	406	16C	C3-C4-C5	-3.86	120.03	125.22
3	B	402	Q5F	O04-C13-N05	-3.34	115.70	122.59
3	A	404	Q5F	O04-C13-N05	-3.26	115.86	122.59
3	B	402	Q5F	O03-C08-C09	2.07	119.23	115.14
3	A	404	Q5F	C07-O03-C08	2.14	122.92	117.70
5	A	406	16C	C20-C19-N2	2.54	120.29	115.82
3	A	404	Q5F	O03-C08-C09	2.71	120.50	115.14
3	B	402	Q5F	O03-C07-C06	4.88	118.69	107.87
3	A	404	Q5F	O03-C07-C06	5.24	119.48	107.87
3	A	404	Q5F	C16-C13-N05	5.56	123.13	115.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	Q5F	C16-C13-N05	5.88	123.57	115.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	404	Q5F	1	0
5	A	406	16C	2	0
3	B	402	Q5F	3	0
4	B	404	R16	3	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	276/312 (88%)	0.22	29 (10%) 7 4	80, 127, 237, 286	0
1	B	282/312 (90%)	0.42	30 (10%) 7 4	72, 134, 242, 335	0
All	All	558/624 (89%)	0.32	59 (10%) 7 4	72, 131, 241, 335	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	92	PRO	27.2
1	B	93	CYS	15.0
1	B	199	TRP	8.8
1	B	97	GLN	7.7
1	A	199	TRP	7.4
1	A	36	ASP	7.3
1	B	35	SER	6.7
1	A	264	ILE	6.6
1	B	200	ASN	6.5
1	B	310	PHE	6.4
1	A	194	ASP	6.0
1	B	91	HIS	6.0
1	A	203	GLN	5.5
1	A	195	THR	5.4
1	B	195	THR	5.4
1	B	89	ARG	5.1
1	B	104	GLN	5.1
1	A	265	GLU	5.0
1	B	85	GLU	4.9
1	B	194	ASP	4.1
1	B	305	GLU	3.8
1	A	89	ARG	3.7
1	B	36	ASP	3.6
1	A	40	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	232	HIS	3.6
1	B	196	PHE	3.5
1	A	196	PHE	3.4
1	A	37	SER	3.4
1	B	309	GLU	3.3
1	A	317	TRP	3.3
1	A	187	LYS	3.3
1	A	38	ALA	3.1
1	A	207	ARG	3.1
1	B	204	THR	3.1
1	A	263	ASP	3.0
1	B	96	ASP	3.0
1	B	120	SER	3.0
1	A	90	ALA	2.9
1	A	200	ASN	2.8
1	B	314	ALA	2.8
1	A	307	VAL	2.8
1	B	44	TRP	2.7
1	B	111	ASN	2.7
1	B	37	SER	2.7
1	B	190	ALA	2.7
1	A	232	HIS	2.6
1	B	267	LEU	2.6
1	B	90	ALA	2.4
1	A	35	SER	2.4
1	B	129	LEU	2.3
1	A	86	LYS	2.3
1	A	198	LYS	2.3
1	A	96	ASP	2.2
1	A	125	SER	2.2
1	A	191	LYS	2.2
1	A	43	LYS	2.2
1	A	320	ASN	2.2
1	B	201	VAL	2.1
1	A	321	VAL	2.1

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	R16	B	407	5/16	0.71	0.41	10.76	121,146,163,163	0
2	K	A	410	1/1	0.86	0.39	6.30	134,134,134,134	0
4	R16	B	409	10/16	0.74	0.24	1.07	99,144,182,196	0
3	Q5F	A	404	19/19	0.92	0.18	0.71	79,119,139,145	0
5	16C	A	406	38/38	0.69	0.23	0.60	96,118,150,194	0
3	Q5F	B	402	19/19	0.91	0.19	0.58	76,103,145,147	0
4	R16	B	403	12/16	0.91	0.18	0.37	92,114,127,128	0
2	K	A	409	1/1	0.95	0.16	0.21	105,105,105,105	0
4	R16	B	404	12/16	0.83	0.16	-0.04	79,110,124,125	0
4	R16	B	406	5/16	0.88	0.16	-0.36	111,134,158,158	0
4	R16	A	405	12/16	0.86	0.14	-0.62	97,120,136,137	0
2	K	A	403	1/1	0.96	0.12	-1.35	121,121,121,121	0
4	R16	B	408	11/16	0.90	0.09	-1.47	107,113,132,134	0
4	R16	A	408	8/16	0.87	0.10	-1.78	107,159,189,191	0
4	R16	A	407	11/16	0.92	0.12	-1.97	86,103,125,127	0
2	K	A	402	1/1	0.97	0.06	-3.36	105,105,105,105	0
6	CD	B	401	1/1	0.98	0.09	-	144,144,144,144	0
4	R16	B	405	5/16	0.89	0.14	-	94,97,113,116	0
2	K	A	401	1/1	0.85	0.16	-	152,152,152,152	0

6.5 Other polymers ⓘ

There are no such residues in this entry.