W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:50 am GMT

PDB ID	:	3UT3
Title	:	A novel PAI-I inhibitor and its structural mechanism
Authors	:	Lin, Z.H.; Hong, Z.B.; Shi, X.L.; Hu, L.H.; Andreasen, P.A.; Huang, M.D.
Deposited on	:	2011-11-25
Resolution	:	2.42 Å(reported)

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

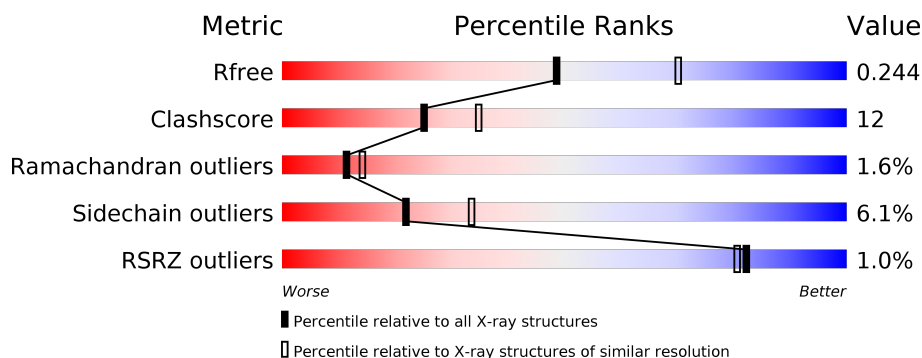|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 2.42 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	Percentile Ranks	Value
Rfree		0.244
Clashscore		12
Ramachandran outliers		1.6%
Sidechain outliers		6.1%
RSRZ outliers		1.0%

Worse ←　　　　　　　　　→ *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3709 (2.44-2.40)
Clashscore	112137	4241 (2.44-2.40)
Ramachandran outliers	110173	4178 (2.44-2.40)
Sidechain outliers	110143	4179 (2.44-2.40)
RSRZ outliers	101464	3740 (2.44-2.40)

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 <=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	375	67%　　　27%　　· ·
1	B	375	%　67%　　　26%　　· ·
1	C	375	%　74%　　　22%　　· ·
1	D	375	%　69%　　　23%　　· ·

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EMJ	B	401	-	-	-	X

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11638 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.
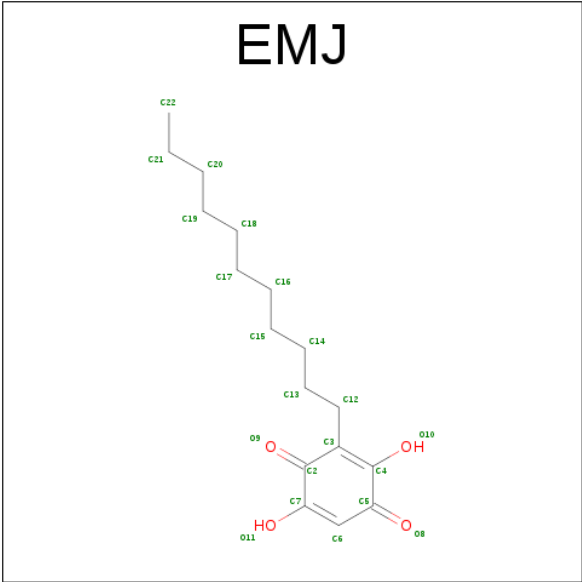
- Molecule 1 is a protein called Plasminogen activator inhibitor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2928	1881	499	533	15			
1	B	360	Total	C	N	O	S	0	0	0
			2877	1849	489	525	14			
1	C	368	Total	C	N	O	S	0	0	0
			2935	1886	500	534	15			
1	D	360	Total	C	N	O	S	0	0	0
			2877	1849	489	525	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	HIS	ASN	ENGINEERED MUTATION	UNP P05121
A	154	THR	LYS	ENGINEERED MUTATION	UNP P05121
A	319	LEU	GLN	ENGINEERED MUTATION	UNP P05121
A	354	ILE	MET	ENGINEERED MUTATION	UNP P05121
B	150	HIS	ASN	ENGINEERED MUTATION	UNP P05121
B	154	THR	LYS	ENGINEERED MUTATION	UNP P05121
B	319	LEU	GLN	ENGINEERED MUTATION	UNP P05121
B	354	ILE	MET	ENGINEERED MUTATION	UNP P05121
C	150	HIS	ASN	ENGINEERED MUTATION	UNP P05121
C	154	THR	LYS	ENGINEERED MUTATION	UNP P05121
C	319	LEU	GLN	ENGINEERED MUTATION	UNP P05121
C	354	ILE	MET	ENGINEERED MUTATION	UNP P05121
D	150	HIS	ASN	ENGINEERED MUTATION	UNP P05121
D	154	THR	LYS	ENGINEERED MUTATION	UNP P05121
D	319	LEU	GLN	ENGINEERED MUTATION	UNP P05121
D	354	ILE	MET	ENGINEERED MUTATION	UNP P05121

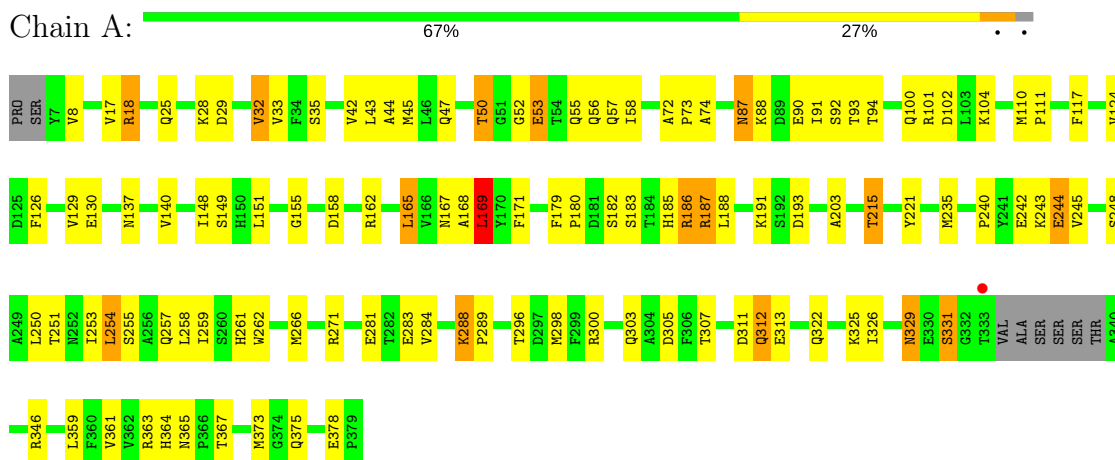- Molecule 2 is 2,5-DIHYDROXY-3-UNDECYLCYCLOHEXA-2,5-DIENE-1,4-DIONE (three-letter code: EMJ) (formula: $C_{17}H_{26}O_4$).

EMJ

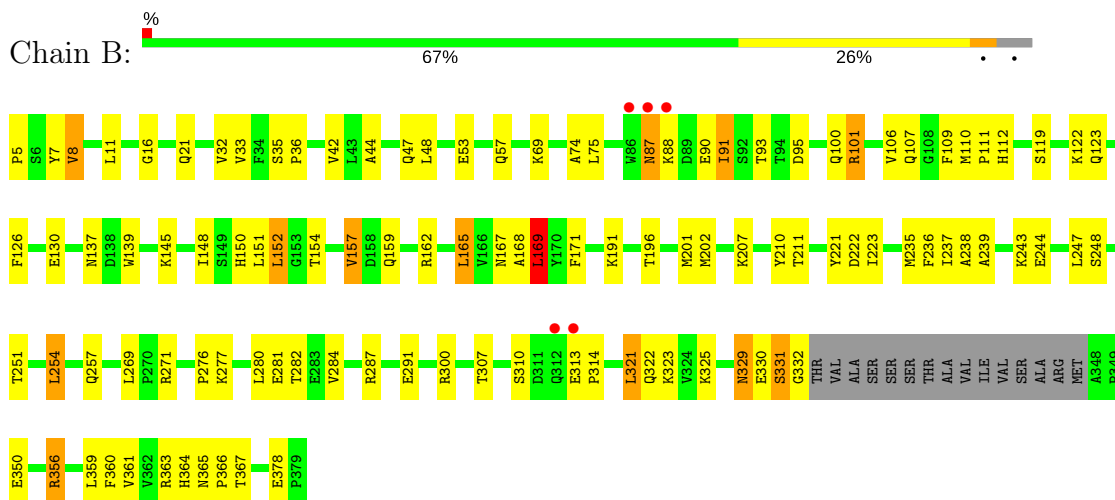| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 21	C 17	O 4	0	0

3 Residue-property plots ⓘ

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.
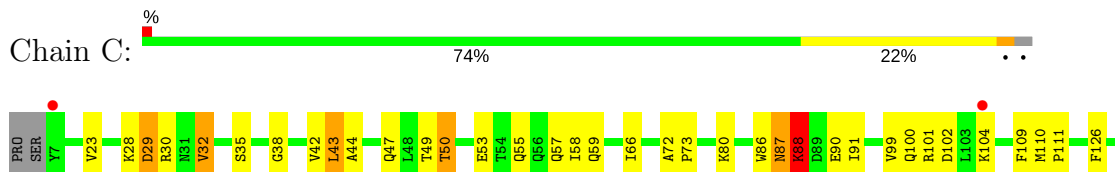
• Molecule 1: Plasminogen activator inhibitor 1

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V129 V140 I148 L152 L157 V157 L165 V166 N167 A168 L169 Q174 S183 T184 H185 R186 R187 L188 F189 H190 A203 E212 L224 P240 K243 E244 V245 S248 T251 Q257 W262 N265 M266 R271 L272 L273 V284 K288 P289 N292

T296 D297 M298 F299 R300 Q303 S310 D311 Q312 E313 P314 L315 Q322 N329 E330 S331 G332 T333 V334 ALA SER SER SER THR A340 V341 I342 V343 R346 P349 E350 P357 H364 T367 Q375 P379

• Molecule 1: Plasminogen activator inhibitor 1

Chain D:

%

69% 23% • •

P5 S6 Y7 V8 L11 G16 Q21 Q25 V32 V33 F34 S35 P36 Y37 G38 V39 V42 L43 A44 M45 L46 Q47 L48 I58 D67 D68 K69 A74 L78 L82 N87 E90 I91 R101 D102 V106 F109 L116 F117 F126 S127

V140 I148 S149 H150 L151 L152 G153 T154 V157 D158 Q159 L165 V166 N167 A168 L169 Y170 F171 N172 D181 R186 T196 V197 Q204 T205 N206 K207 F208 N209 Y210 T211 Y221 D222 I223 L224 H229 G230 D231 T232 L233 S234 M235 F236 I237 A238 K243 E244 L247

L250 Q257 S260 K263 F278 T282 E283 V284 R287 E291 M298 F299 R300 T307 S308 L309 S310 D311 Q312 E313 P314 L321 Q322 K323 V324 K325 I326 E327 V328 G332 THR VAL ALA SER SER SER THR ALA VAL ILE VAL SER ALA ARG MET A348 I352

L359 F360 V361 V362 R363 H364 Q375 P379

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	65.25Å 74.95Å 103.78Å 90.89° 93.33° 115.72°	Depositor
Resolution (Å)	58.69 – 2.42 57.72 – 2.42	Depositor EDS
% Data completeness (in resolution range)	96.6 (58.69-2.42) 95.0 (57.72-2.42)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.202 , 0.245 0.206 , 0.244	Depositor DCC
R_{free} test set	3288 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	34.5	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 34.5	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -h,h+k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11638	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: EMJ

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	0.75	1/2998 (0.0%)	0.86	5/4063 (0.1%)
1	B	0.73	0/2948	0.85	3/3995 (0.1%)
1	C	0.74	0/3005	0.83	2/4073 (0.0%)
1	D	0.72	0/2948	0.83	2/3995 (0.1%)
All	All	0.74	1/11899 (0.0%)	0.84	12/16126 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	283	GLU	CD-OE1	5.01	1.31	1.25

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	169	LEU	CA-CB-CG	7.55	132.66	115.30
1	A	169	LEU	CA-CB-CG	7.11	131.65	115.30
1	A	18	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	187	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	D	321	LEU	CA-CB-CG	6.03	129.17	115.30
1	D	169	LEU	CA-CB-CG	5.81	128.67	115.30
1	A	235	MET	CG-SD-CE	-5.77	90.97	100.20
1	B	321	LEU	CA-CB-CG	5.63	128.25	115.30
1	C	43	LEU	CA-CB-CG	-5.59	102.45	115.30
1	B	169	LEU	CA-CB-CG	5.37	127.66	115.30
1	A	288	LYS	CD-CE-NZ	5.18	123.61	111.70
1	B	162	ARG	NE-CZ-NH1	5.07	122.84	120.30

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	2928	0	2925	75	0
1	B	2877	0	2865	80	0
1	C	2935	0	2934	65	0
1	D	2877	0	2865	67	0
2	B	21	0	25	7	0
All	All	11638	0	11614	281	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 12.

All (281) 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:42:VAL:HG21	1:C:167:ASN:HB2	1.52	0.90
1:C:35:SER:H	1:C:322:GLN:HE22	1.21	0.89
1:A:35:SER:H	1:A:322:GLN:HE22	1.19	0.88
1:A:191:LYS:HD3	1:A:378:GLU:OE1	1.73	0.88
1:A:42:VAL:HG21	1:A:167:ASN:HB2	1.59	0.83
1:C:87:ASN:O	1:C:88:LYS:HB3	1.79	0.80
1:C:174:GLN:HG2	1:C:332:GLY:HA3	1.65	0.79
1:D:243:LYS:O	1:D:244:GLU:HB2	1.85	0.76
1:B:221:TYR:CE1	1:B:223:ILE:HD11	2.22	0.74
1:B:247:LEU:HD11	1:B:359:LEU:HD12	1.68	0.74
1:A:17:VAL:HG22	1:A:373:MET:CE	2.17	0.74
1:C:329:ASN:ND2	1:C:331:SER:O	2.24	0.71
1:C:87:ASN:O	1:C:88:LYS:CB	2.37	0.70
1:C:243:LYS:O	1:C:244:GLU:HB2	1.92	0.70
1:A:58:ILE:HD11	1:A:298:MET:HE2	1.74	0.69
1:B:364:HIS:HD2	1:B:367:THR:OG1	1.76	0.69
1:C:87:ASN:O	1:C:90:GLU:OE2	2.14	0.65
1:A:17:VAL:HG22	1:A:373:MET:HE3	1.79	0.65
1:D:78:LEU:O	1:D:82:LEU:HG	1.97	0.65
1:B:251:THR:HG23	1:B:359:LEU:HD11	1.78	0.64
1:C:50:THR:HG23	1:C:55:GLN:HB2	1.81	0.63
1:A:185:HIS:HE1	1:A:187:ARG:HE	1.45	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:MET:CE	1:D:237:ILE:HD11	2.30	0.62
1:C:47:GLN:O	1:C:50:THR:HG22	1.99	0.62
1:A:183:SER:HB3	1:A:203:ALA:HB3	1.80	0.62
1:D:90:GLU:O	1:D:171:PHE:HA	2.00	0.62
1:B:90:GLU:O	1:B:171:PHE:HA	1.99	0.61
1:A:251:THR:HG22	1:A:359:LEU:HD21	1.81	0.61
1:A:87:ASN:O	1:A:90:GLU:OE2	2.19	0.61
1:D:35:SER:H	1:D:322:GLN:HE22	1.46	0.61
1:A:17:VAL:HG22	1:A:373:MET:HE1	1.81	0.60
1:A:259:ILE:HD13	1:A:361:VAL:HG11	1.83	0.60
1:D:154:THR:O	1:D:157:VAL:CG1	2.50	0.60
1:B:165:LEU:C	1:B:165:LEU:HD23	2.22	0.60
1:D:243:LYS:O	1:D:244:GLU:CB	2.48	0.60
1:A:100:GLN:HE22	1:A:126:PHE:H	1.49	0.60
1:B:235:MET:HE2	1:B:237:ILE:HD11	1.84	0.60
1:A:186:ARG:HB2	1:A:186:ARG:HH11	1.67	0.60
1:D:33:VAL:HG11	1:D:326:ILE:HG22	1.84	0.59
1:B:235:MET:CE	1:B:237:ILE:HD11	2.32	0.59
1:A:187:ARG:HG2	1:A:188:LEU:H	1.68	0.58
1:A:257:GLN:HG2	1:B:150:HIS:CD2	2.37	0.58
1:B:363:ARG:NH1	1:B:365:ASN:HD22	2.00	0.58
1:D:154:THR:O	1:D:157:VAL:HG12	2.03	0.58
1:B:106:VAL:HG23	1:B:109:PHE:HB2	1.86	0.57
1:B:100:GLN:HE22	1:B:126:PHE:H	1.49	0.57
1:C:331:SER:C	1:C:333:THR:H	2.08	0.57
1:D:42:VAL:HG11	1:D:167:ASN:HB2	1.86	0.57
1:B:8:VAL:HG21	1:B:74:ALA:CB	2.35	0.57
1:B:93:THR:CB	1:B:169:LEU:HD13	2.34	0.57
1:D:58:ILE:HD11	1:D:298:MET:HE3	1.87	0.57
1:C:50:THR:HG23	1:C:55:GLN:CB	2.35	0.56
1:D:33:VAL:HG11	1:D:326:ILE:CG2	2.35	0.56
1:C:42:VAL:CG2	1:C:167:ASN:HB2	2.32	0.56
1:C:296:THR:HB	1:C:300:ARG:HH21	1.70	0.56
1:A:187:ARG:HG2	1:A:188:LEU:N	2.21	0.56
1:A:296:THR:HB	1:A:300:ARG:HH21	1.71	0.55
1:C:30:ARG:HH11	1:C:30:ARG:HG3	1.72	0.55
1:D:39:VAL:O	1:D:43:LEU:HD23	2.06	0.55
1:C:53:GLU:O	1:C:57:GLN:HG3	2.07	0.55
1:D:35:SER:H	1:D:322:GLN:NE2	2.05	0.55
1:D:165:LEU:C	1:D:165:LEU:HD23	2.28	0.54
1:A:44:ALA:O	1:A:47:GLN:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:SER:O	1:C:185:HIS:HD2	1.91	0.54
1:C:240:PRO:HB3	1:C:245:VAL:HB	1.90	0.54
1:C:44:ALA:O	1:C:47:GLN:HB2	2.07	0.54
1:A:262:TRP:O	1:A:266:MET:HG3	2.07	0.54
1:A:243:LYS:O	1:A:244:GLU:HB2	2.07	0.54
1:A:240:PRO:HB3	1:A:245:VAL:HB	1.89	0.54
1:C:58:ILE:HD11	1:C:298:MET:CE	2.38	0.54
1:D:5:PRO:O	1:D:7:TYR:N	2.40	0.54
1:A:53:GLU:O	1:A:57:GLN:HG3	2.08	0.53
1:D:221:TYR:CE2	1:D:223:ILE:HD11	2.43	0.53
1:A:307:THR:HB	1:A:311:ASP:HB3	1.91	0.53
1:D:7:TYR:CZ	1:D:11:LEU:HD11	2.44	0.53
1:D:221:TYR:CE2	1:D:250:LEU:HD11	2.43	0.53
1:C:35:SER:H	1:C:322:GLN:NE2	1.99	0.53
1:D:235:MET:HE3	1:D:237:ILE:HD11	1.89	0.53
1:A:33:VAL:HG11	1:A:326:ILE:CG2	2.39	0.53
1:B:254:LEU:HD21	1:B:359:LEU:CD2	2.39	0.53
1:C:104:LYS:HE2	1:C:312:GLN:HB2	1.90	0.52
1:D:44:ALA:O	1:D:47:GLN:HB2	2.10	0.52
1:B:42:VAL:HG12	1:B:95:ASP:HB3	1.90	0.52
1:B:87:ASN:HD21	1:B:91:ILE:HG23	1.73	0.52
1:C:183:SER:HB3	1:C:203:ALA:HB3	1.90	0.52
1:D:87:ASN:HD21	1:D:91:ILE:CG2	2.22	0.52
1:A:92:SER:O	1:A:169:LEU:HA	2.09	0.52
1:B:291:GLU:OE2	1:B:300:ARG:NH1	2.42	0.52
1:B:313:GLU:HG2	1:B:314:PRO:HD2	1.92	0.52
1:B:330:GLU:O	1:B:331:SER:HB3	2.10	0.52
1:B:281:GLU:OE2	1:B:325:LYS:NZ	2.35	0.51
1:A:35:SER:H	1:A:322:GLN:NE2	2.00	0.51
1:D:42:VAL:HG23	1:D:43:LEU:HD22	1.92	0.51
1:B:248:SER:HA	1:B:251:THR:OG1	2.10	0.51
1:C:58:ILE:HD11	1:C:298:MET:HE2	1.91	0.51
1:A:101:ARG:HH11	1:A:101:ARG:HG3	1.76	0.51
1:C:243:LYS:O	1:C:244:GLU:CB	2.54	0.51
1:A:137:ASN:ND2	1:A:151:LEU:H	2.08	0.51
1:B:154:THR:O	1:B:157:VAL:HG13	2.10	0.51
1:C:257:GLN:HG2	1:D:150:HIS:CE1	2.46	0.51
1:D:260:SER:HB3	1:D:363:ARG:NH2	2.26	0.51
1:C:288:LYS:HB2	1:C:289:PRO:HD3	1.93	0.51
1:C:313:GLU:HG3	1:C:314:PRO:HD2	1.93	0.51
1:C:32:VAL:HG13	1:C:375:GLN:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:LEU:CD1	1:B:359:LEU:HD12	2.40	0.50
1:A:185:HIS:CG	1:C:152:LEU:HD12	2.46	0.50
1:D:236:PHE:O	1:D:360:PHE:HA	2.11	0.50
1:B:148:ILE:CG2	1:B:323:LYS:HD3	2.41	0.50
1:B:168:ALA:C	1:B:169:LEU:HD22	2.30	0.50
1:C:248:SER:HA	1:C:251:THR:OG1	2.12	0.49
1:C:87:ASN:HD21	1:C:91:ILE:HG23	1.77	0.49
1:B:42:VAL:HG11	1:B:167:ASN:HB2	1.95	0.49
1:A:185:HIS:CE1	1:A:187:ARG:HE	2.27	0.49
1:B:101:ARG:HB2	1:B:123:GLN:HB3	1.95	0.49
1:B:53:GLU:O	1:B:57:GLN:HG3	2.13	0.49
1:C:99:VAL:HG22	1:C:100:GLN:N	2.28	0.49
1:C:224:LEU:HD11	1:C:273:LEU:HD13	1.94	0.49
1:C:44:ALA:HB1	1:C:66:ILE:HD13	1.94	0.49
1:A:137:ASN:HD21	1:A:151:LEU:H	1.60	0.49
1:B:191:LYS:NZ	1:B:378:GLU:OE2	2.42	0.49
1:A:296:THR:HB	1:A:300:ARG:NH2	2.28	0.48
1:C:185:HIS:HE1	1:C:187:ARG:HE	1.61	0.48
1:D:45:MET:HA	1:D:117:PHE:CZ	2.48	0.48
1:D:69:LYS:HA	1:D:69:LYS:HE3	1.94	0.48
1:B:93:THR:HB	1:B:169:LEU:HD13	1.93	0.48
1:C:300:ARG:HB3	1:C:303:GLN:HB2	1.95	0.48
1:B:95:ASP:HB2	2:B:401:EMJ:O10	2.13	0.48
1:B:210:TYR:CG	1:B:211:THR:N	2.81	0.48
1:B:8:VAL:HG21	1:B:74:ALA:HB3	1.95	0.48
1:D:247:LEU:HD21	1:D:359:LEU:HD22	1.96	0.48
1:D:263:LYS:HD3	1:D:263:LYS:O	2.13	0.48
1:B:235:MET:HA	1:B:361:VAL:O	2.13	0.48
1:C:87:ASN:ND2	1:C:91:ILE:HG23	2.28	0.48
1:B:282:THR:HG22	1:B:284:VAL:HG13	1.95	0.48
1:B:271:ARG:HD3	1:B:350:GLU:HB2	1.95	0.48
1:B:8:VAL:HG21	1:B:74:ALA:HB1	1.96	0.48
1:C:110:MET:HB2	1:C:111:PRO:HD3	1.95	0.47
1:D:16:GLY:HA3	1:D:36:PRO:HB3	1.96	0.47
1:C:55:GLN:O	1:C:59:GLN:HG3	2.13	0.47
1:C:38:GLY:O	1:C:42:VAL:HG23	2.15	0.47
1:A:258:LEU:HD13	1:B:152:LEU:HG	1.97	0.47
1:A:33:VAL:HG11	1:A:326:ILE:HG22	1.95	0.47
1:B:137:ASN:ND2	1:B:151:LEU:H	2.11	0.47
1:D:235:MET:HE2	1:D:237:ILE:HD11	1.96	0.47
1:C:364:HIS:HD2	1:C:367:THR:OG1	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:THR:HG22	1:C:109:PHE:HZ	1.80	0.47
1:D:307:THR:HA	1:D:310:SER:O	2.14	0.47
1:D:87:ASN:HD21	1:D:91:ILE:HG23	1.80	0.47
1:D:106:VAL:CG2	1:D:109:PHE:HB2	2.45	0.47
1:A:104:LYS:HE2	1:A:312:GLN:HB2	1.96	0.47
1:B:87:ASN:HD21	1:B:91:ILE:CG2	2.28	0.47
1:A:179:PHE:O	1:A:180:PRO:C	2.52	0.46
1:A:221:TYR:CZ	1:A:250:LEU:HB2	2.50	0.46
1:B:282:THR:O	1:B:323:LYS:HA	2.16	0.46
1:A:28:LYS:O	1:A:29:ASP:HB2	2.15	0.46
1:A:8:VAL:HG21	1:A:74:ALA:CB	2.45	0.46
1:B:35:SER:H	1:B:322:GLN:HE22	1.61	0.46
1:A:50:THR:HG23	1:A:55:GLN:HB2	1.97	0.46
1:A:329:ASN:HD22	1:A:331:SER:H	1.64	0.46
1:B:284:VAL:HG23	1:B:284:VAL:O	2.15	0.46
1:B:221:TYR:CD1	1:B:223:ILE:HD11	2.51	0.46
1:C:88:LYS:HB2	1:C:88:LYS:NZ	2.31	0.46
1:D:287:ARG:O	1:D:291:GLU:HG3	2.15	0.46
1:A:101:ARG:N	1:A:124:VAL:O	2.47	0.46
1:A:32:VAL:HG13	1:A:375:GLN:HG2	1.97	0.46
1:B:110:MET:HB2	1:B:111:PRO:HD3	1.98	0.46
1:B:223:ILE:HA	1:B:237:ILE:O	2.15	0.46
1:B:243:LYS:HE3	1:B:356:ARG:HB3	1.98	0.46
1:D:210:TYR:CG	1:D:211:THR:N	2.84	0.45
2:B:401:EMJ:H5	2:B:401:EMJ:O9	2.16	0.45
1:D:87:ASN:O	1:D:90:GLU:HG3	2.16	0.45
1:A:168:ALA:C	1:A:169:LEU:HD23	2.37	0.45
1:B:48:LEU:HD11	1:B:112:HIS:CE1	2.51	0.45
1:B:365:ASN:N	1:B:366:PRO:CD	2.79	0.45
1:D:247:LEU:HD11	1:D:359:LEU:CD2	2.47	0.45
1:D:21:GLN:O	1:D:25:GLN:HG3	2.16	0.45
1:B:239:ALA:HB1	1:B:356:ARG:HD2	1.98	0.45
1:B:35:SER:H	1:B:322:GLN:NE2	2.15	0.45
1:C:49:THR:HG22	1:C:109:PHE:CZ	2.52	0.45
1:A:140:VAL:HG12	1:A:148:ILE:O	2.16	0.45
1:A:52:GLY:O	1:A:56:GLN:HG2	2.17	0.45
1:D:313:GLU:HG2	1:D:314:PRO:N	2.31	0.45
1:B:287:ARG:O	1:B:291:GLU:HG3	2.17	0.45
1:C:262:TRP:O	1:C:266:MET:HG3	2.16	0.45
1:D:32:VAL:HG13	1:D:375:GLN:HG2	1.99	0.45
1:B:106:VAL:CG2	1:B:109:PHE:HB2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:LEU:HD23	1:C:165:LEU:C	2.37	0.44
1:C:28:LYS:HG2	1:C:29:ASP:OD1	2.17	0.44
1:A:281:GLU:HB2	1:A:325:LYS:HG2	1.99	0.44
1:C:271:ARG:HE	1:C:350:GLU:HB2	1.83	0.44
1:D:206:ASN:OD1	1:D:207:LYS:N	2.43	0.44
1:A:185:HIS:CE1	1:A:187:ARG:HH21	2.35	0.44
1:A:18:ARG:NH2	1:B:130:GLU:OE1	2.51	0.44
1:A:185:HIS:CD2	1:C:152:LEU:HD12	2.53	0.44
1:D:167:ASN:O	1:D:322:GLN:HA	2.17	0.44
1:A:243:LYS:O	1:A:244:GLU:CB	2.65	0.44
1:A:45:MET:HA	1:A:117:PHE:CZ	2.52	0.44
1:C:167:ASN:O	1:C:322:GLN:HA	2.17	0.44
1:D:196:THR:O	1:D:197:VAL:HG13	2.18	0.44
1:A:305:ASP:OD1	1:A:305:ASP:C	2.55	0.44
1:B:202:MET:HG3	1:B:277:LYS:HG2	2.00	0.44
1:D:221:TYR:CE2	1:D:223:ILE:CD1	3.01	0.44
1:A:185:HIS:HE1	1:A:187:ARG:NE	2.14	0.44
1:C:140:VAL:HG12	1:C:148:ILE:O	2.18	0.44
1:D:233:LEU:HD23	1:D:364:HIS:HA	2.00	0.44
1:A:257:GLN:HG2	1:B:150:HIS:NE2	2.32	0.44
1:D:106:VAL:HG23	1:D:109:PHE:HB2	2.00	0.44
1:A:300:ARG:HG2	1:A:303:GLN:NE2	2.33	0.43
1:A:364:HIS:HD2	1:A:367:THR:OG1	2.01	0.43
1:B:87:ASN:O	1:B:90:GLU:OE2	2.36	0.43
1:C:342:ILE:HG22	1:C:343:VAL:N	2.33	0.43
1:A:363:ARG:HH11	1:A:365:ASN:HD22	1.64	0.43
1:B:7:TYR:CZ	1:B:11:LEU:HD11	2.54	0.43
1:B:251:THR:HG22	1:B:359:LEU:HD21	2.00	0.43
1:D:38:GLY:HA3	1:D:167:ASN:HD21	1.83	0.43
1:D:8:VAL:HG21	1:D:74:ALA:HB3	1.99	0.43
1:A:110:MET:HB2	1:A:111:PRO:HD3	2.00	0.43
2:B:401:EMJ:C13	2:B:401:EMJ:O9	2.66	0.43
1:A:254:LEU:HD13	1:A:258:LEU:HD23	2.01	0.43
1:B:236:PHE:O	1:B:360:PHE:HA	2.19	0.43
1:B:5:PRO:N	1:B:8:VAL:HG23	2.34	0.43
1:D:58:ILE:HD11	1:D:298:MET:CE	2.49	0.43
1:B:222:ASP:O	1:B:238:ALA:HA	2.19	0.42
1:B:8:VAL:HG11	1:B:75:LEU:HG	2.01	0.42
1:A:258:LEU:O	1:A:261:HIS:HB3	2.19	0.42
1:C:190:HIS:O	1:C:357:PRO:HD3	2.19	0.42
1:A:72:ALA:N	1:A:73:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ASN:HD21	1:B:332:GLY:N	2.17	0.42
1:B:363:ARG:HH11	1:B:365:ASN:HD22	1.63	0.42
1:D:46:LEU:HD23	1:D:298:MET:HE1	2.00	0.42
1:C:157:VAL:HG23	1:C:157:VAL:O	2.19	0.42
1:A:165:LEU:HD23	1:A:165:LEU:C	2.40	0.42
1:A:43:LEU:HA	1:A:43:LEU:HD13	1.84	0.42
1:A:93:THR:O	1:A:94:THR:HB	2.20	0.42
1:D:278:PHE:CZ	1:D:328:VAL:HG21	2.55	0.42
1:D:224:LEU:HD11	1:D:352:ILE:HG21	2.01	0.42
1:A:311:ASP:N	1:A:311:ASP:OD1	2.51	0.42
1:A:87:ASN:HD21	1:A:91:ILE:HG23	1.84	0.42
1:C:72:ALA:N	1:C:73:PRO:CD	2.83	0.42
1:D:48:LEU:HD21	1:D:116:LEU:HD22	2.02	0.42
1:B:307:THR:HA	1:B:310:SER:O	2.20	0.42
1:C:187:ARG:CG	1:C:188:LEU:N	2.83	0.42
1:A:50:THR:HG23	1:A:55:GLN:CB	2.50	0.41
1:B:148:ILE:HG23	1:B:323:LYS:HD3	2.02	0.41
1:D:109:PHE:CD1	1:D:109:PHE:C	2.93	0.41
1:A:288:LYS:HB2	1:A:289:PRO:HD3	2.03	0.41
1:D:282:THR:O	1:D:323:LYS:HA	2.19	0.41
1:B:207:LYS:HA	1:B:269:LEU:O	2.20	0.41
1:A:140:VAL:HG11	1:A:148:ILE:HG22	2.02	0.41
1:C:185:HIS:HE1	1:C:187:ARG:NE	2.19	0.41
1:C:331:SER:C	1:C:333:THR:N	2.73	0.41
1:D:140:VAL:HG12	1:D:148:ILE:O	2.20	0.41
1:A:215:THR:HG22	1:A:253:ILE:CD1	2.51	0.41
1:B:16:GLY:HA3	1:B:36:PRO:HB3	2.02	0.41
1:B:191:LYS:NZ	1:B:378:GLU:CD	2.73	0.41
1:C:292:ASN:O	1:D:159:GLN:NE2	2.54	0.41
1:B:247:LEU:HD11	1:B:359:LEU:CD1	2.45	0.41
1:C:86:TRP:CE3	1:C:87:ASN:HA	2.56	0.41
1:D:204:GLN:HG3	1:D:208:PHE:HZ	1.86	0.41
1:D:238:ALA:HB1	1:D:250:LEU:HD21	2.03	0.41
1:D:33:VAL:HG12	1:D:360:PHE:HZ	1.85	0.41
1:B:122:LYS:NZ	2:B:401:EMJ:H11	2.35	0.41
1:D:229:HIS:O	1:D:229:HIS:CG	2.73	0.41
1:B:44:ALA:O	1:B:47:GLN:HB2	2.21	0.41
1:D:235:MET:HA	1:D:361:VAL:O	2.21	0.41
1:B:167:ASN:O	1:B:322:GLN:HA	2.21	0.41
1:B:139:TRP:HZ2	2:B:401:EMJ:H5	1.86	0.41
1:B:119:SER:HB3	2:B:401:EMJ:H6	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:THR:O	1:D:157:VAL:HG13	2.20	0.41
1:D:126:PHE:O	1:D:159:GLN:HA	2.21	0.41
1:B:119:SER:OG	2:B:401:EMJ:H4	2.21	0.40
1:B:201:MET:HA	1:B:276:PRO:HA	2.03	0.40
1:A:90:GLU:O	1:A:171:PHE:HA	2.21	0.40
1:C:100:GLN:HE22	1:C:126:PHE:H	1.69	0.40
1:C:310:SER:HB3	1:C:315:LEU:HD12	2.03	0.40
1:A:35:SER:N	1:A:322:GLN:HE22	2.01	0.40
1:C:329:ASN:HD22	1:C:329:ASN:C	2.24	0.40
1:A:162:ARG:HD2	1:A:313:GLU:OE1	2.22	0.40
1:B:33:VAL:HG21	1:B:280:LEU:HB2	2.03	0.40
1:C:224:LEU:CD1	1:C:273:LEU:HD13	2.52	0.40
1:D:87:ASN:ND2	1:D:91:ILE:HG22	2.36	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	363/375 (97%)	340 (94%)	16 (4%)	7 (2%)	9	11
1	B	356/375 (95%)	340 (96%)	12 (3%)	4 (1%)	17	23
1	C	364/375 (97%)	344 (94%)	12 (3%)	8 (2%)	8	8
1	D	356/375 (95%)	338 (95%)	14 (4%)	4 (1%)	17	23
All	All	1439/1500 (96%)	1362 (95%)	54 (4%)	23 (2%)	11	14

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	ASP
1	B	87	ASN

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Mol	Chain	Res	Type
1	B	331	SER
1	A	87	ASN
1	A	129	VAL
1	B	88	LYS
1	C	101	ARG
1	D	6	SER
1	D	244	GLU
1	A	88	LYS
1	A	331	SER
1	B	244	GLU
1	C	87	ASN
1	C	88	LYS
1	C	333	THR
1	C	102	ASP
1	C	244	GLU
1	A	244	GLU
1	D	87	ASN
1	D	314	PRO
1	A	155	GLY
1	C	349	PRO
1	C	129	VAL

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	322/329 (98%)	300 (93%)	22 (7%)	18	28
1	B	317/329 (96%)	298 (94%)	19 (6%)	22	34
1	C	323/329 (98%)	310 (96%)	13 (4%)	36	54
1	D	317/329 (96%)	293 (92%)	24 (8%)	15	23
All	All	1279/1316 (97%)	1201 (94%)	78 (6%)	22	33

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

Mol	Chain	Res	Type
1	A	25	GLN
1	A	32	VAL
1	A	50	THR
1	A	53	GLU
1	A	102	ASP
1	A	130	GLU
1	A	149	SER
1	A	158	ASP
1	A	165	LEU
1	A	169	LEU
1	A	182	SER
1	A	186	ARG
1	A	215	THR
1	A	242	GLU
1	A	248	SER
1	A	254	LEU
1	A	255	SER
1	A	271	ARG
1	A	284	VAL
1	A	312	GLN
1	A	329	ASN
1	A	346	ARG
1	B	8	VAL
1	B	21	GLN
1	B	32	VAL
1	B	69	LYS
1	B	91	ILE
1	B	101	ARG
1	B	107	GLN
1	B	145	LYS
1	B	152	LEU
1	B	157	VAL
1	B	159	GLN
1	B	165	LEU
1	B	169	LEU
1	B	196	THR
1	B	254	LEU
1	B	257	GLN
1	B	321	LEU
1	B	329	ASN
1	B	356	ARG
1	C	23	VAL
1	C	29	ASP

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Mol	Chain	Res	Type
1	C	32	VAL
1	C	43	LEU
1	C	50	THR
1	C	80	LYS
1	C	88	LYS
1	C	169	LEU
1	C	212	GLU
1	C	265	ASN
1	C	284	VAL
1	C	329	ASN
1	C	346	ARG
1	D	8	VAL
1	D	32	VAL
1	D	67	ASP
1	D	69	LYS
1	D	101	ARG
1	D	127	SER
1	D	152	LEU
1	D	157	VAL
1	D	159	GLN
1	D	165	LEU
1	D	169	LEU
1	D	172	ASN
1	D	181	ASP
1	D	186	ARG
1	D	223	ILE
1	D	224	LEU
1	D	257	GLN
1	D	263	LYS
1	D	284	VAL
1	D	298	MET
1	D	300	ARG
1	D	308	SER
1	D	321	LEU
1	D	325	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	59	GLN
1	A	100	GLN

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Mol	Chain	Res	Type
1	A	137	ASN
1	A	167	ASN
1	A	172	ASN
1	A	185	HIS
1	A	190	HIS
1	A	292	ASN
1	A	301	GLN
1	A	303	GLN
1	A	312	GLN
1	A	322	GLN
1	A	329	ASN
1	A	364	HIS
1	A	365	ASN
1	B	21	GLN
1	B	59	GLN
1	B	100	GLN
1	B	107	GLN
1	B	112	HIS
1	B	137	ASN
1	B	143	HIS
1	B	167	ASN
1	B	292	ASN
1	B	322	GLN
1	B	329	ASN
1	B	364	HIS
1	B	365	ASN
1	C	21	GLN
1	C	25	GLN
1	C	100	GLN
1	C	112	HIS
1	C	137	ASN
1	C	159	GLN
1	C	167	ASN
1	C	172	ASN
1	C	185	HIS
1	C	204	GLN
1	C	265	ASN
1	C	292	ASN
1	C	322	GLN
1	C	329	ASN
1	C	364	HIS
1	C	365	ASN

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Mol	Chain	Res	Type
1	D	25	GLN
1	D	167	ASN
1	D	172	ASN
1	D	257	GLN
1	D	261	HIS
1	D	292	ASN
1	D	303	GLN
1	D	322	GLN
1	D	364	HIS
1	D	365	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 carbohydrates in this entry.

5.6   Ligand geometry ⓘ

1 ligand is 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	EMJ	B	401	-	21,21,21	1.38	2 (9%)	22,26,26	1.88	2 (9%)

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
2	EMJ	B	401	-	-	0/11/31/31	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	EMJ	C4-C5	-3.14	1.39	1.44
2	B	401	EMJ	C6-C7	3.23	1.40	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	EMJ	O9-C2-C7	-4.12	114.33	120.28
2	B	401	EMJ	C12-C3-C2	6.00	126.28	116.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	EMJ	7	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	367/375 (97%)	-0.29	1 (0%) 93	93	15, 31, 61, 97	0
1	B	360/375 (96%)	-0.18	5 (1%) 75	73	18, 34, 65, 102	0
1	C	368/375 (98%)	-0.26	3 (0%) 86	84	16, 31, 62, 95	0
1	D	360/375 (96%)	-0.14	5 (1%) 75	73	17, 35, 67, 98	0
All	All	1455/1500 (97%)	-0.22	14 (0%) 82	80	15, 33, 64, 102	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	7	TYR	3.9
1	C	334	VAL	3.8
1	B	312	GLN	3.2
1	C	104	LYS	3.0
1	D	312	GLN	2.6
1	B	88	LYS	2.6
1	D	102	ASP	2.5
1	B	313	GLU	2.4
1	D	231	ASP	2.4
1	D	87	ASN	2.3
1	B	87	ASN	2.3
1	A	333	THR	2.1
1	B	86	TRP	2.1
1	D	313	GLU	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 (i)

There are no carbohydrates 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. 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
2	EMJ	B	401	21/21	0.68	0.32	7.70	57,63,74,75	0

6.5 Other polymers (i)

There are no such residues in this entry.

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