Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2024 – 09:34 AM EDT

PDB ID	:	4EOZ
Title	:	Crystal structure of the SPOP BTB domain complexed with the Cul3 N-terminal domain
Authors	:	Prive, G.G.; Errington, W.J.
Deposited on	:	2012-04-16
Resolution	:	2.40 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:

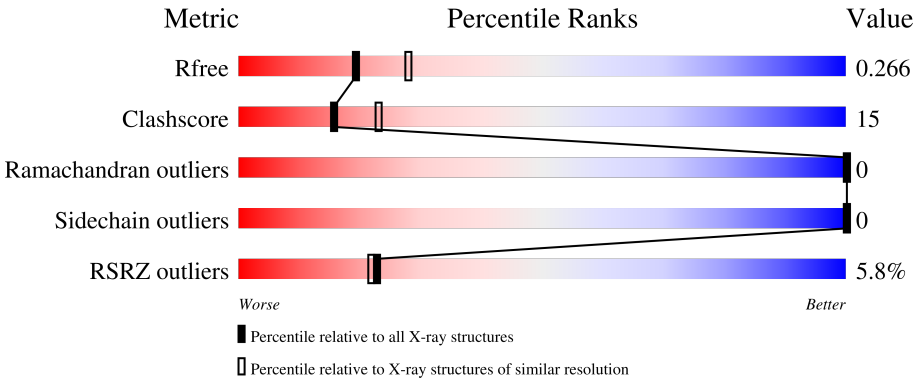
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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 <=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	145	% 71% 8% 21%
1	C	145	5% 66% 14% 20%
2	B	364	5% 64% 19% 17%
2	D	364	5% 60% 23% 17%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6785 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 Speckle-type POZ protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	114	Total	C	N	O	S	0	0	0
			896	563	149	172	12			
1	C	116	Total	C	N	O	S	0	0	0
			909	570	151	175	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	175	GLY	-	EXPRESSION TAG	UNP O43791
A	176	SER	-	EXPRESSION TAG	UNP O43791
C	175	GLY	-	EXPRESSION TAG	UNP O43791
C	176	SER	-	EXPRESSION TAG	UNP O43791

- Molecule 2 is a protein called Cullin-3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	302	Total	C	N	O	S	Se	0	0	0
			2469	1547	433	465	6	18			
2	D	301	Total	C	N	O	S	Se	0	0	0
			2465	1545	432	464	6	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	18	GLY	-	EXPRESSION TAG	UNP Q13618
B	19	SER	-	EXPRESSION TAG	UNP Q13618
B	342	ARG	ILE	ENGINEERED MUTATION	UNP Q13618
B	346	ASP	LEU	ENGINEERED MUTATION	UNP Q13618
D	18	GLY	-	EXPRESSION TAG	UNP Q13618
D	19	SER	-	EXPRESSION TAG	UNP Q13618
D	342	ARG	ILE	ENGINEERED MUTATION	UNP Q13618
D	346	ASP	LEU	ENGINEERED MUTATION	UNP Q13618

- Molecule 3 is water.

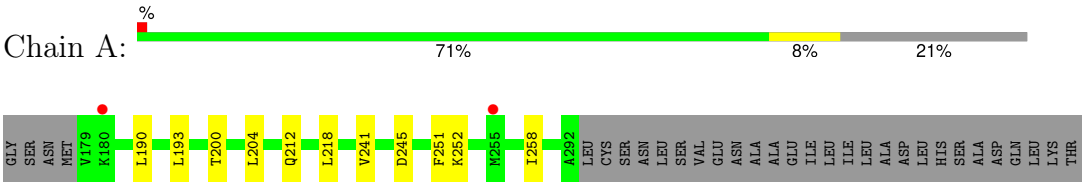
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total O 5 5	0	0
3	C	5	Total O 5 5	0	0
3	B	26	Total O 26 26	0	0
3	D	10	Total O 10 10	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

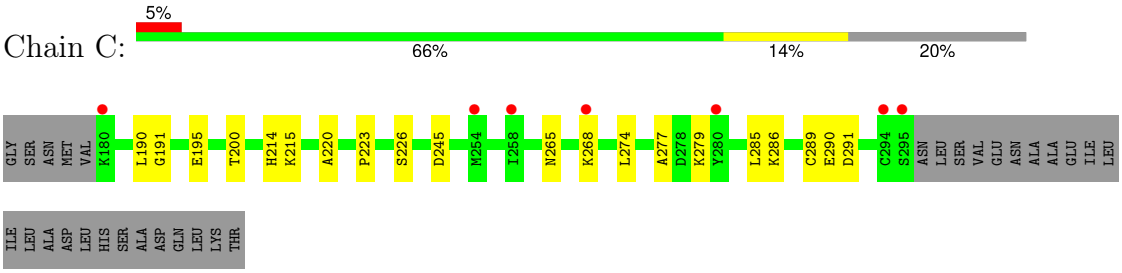
• Molecule 1: Speckle-type POZ protein

Chain A:



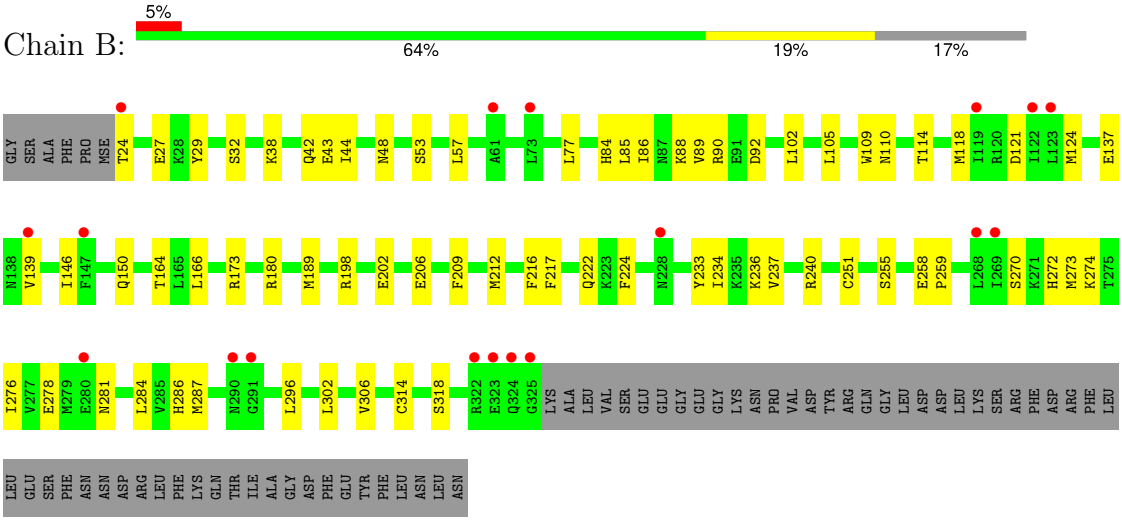
• Molecule 1: Speckle-type POZ protein

Chain C:



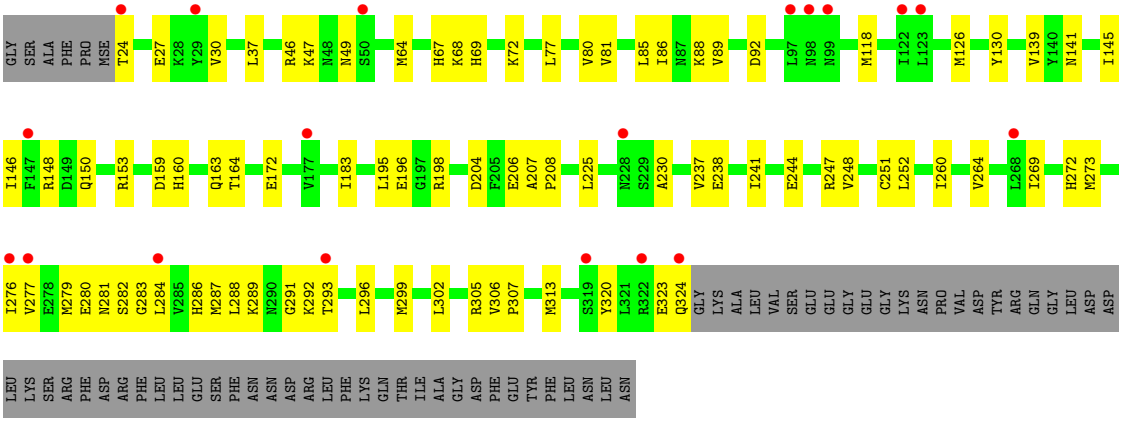
• Molecule 2: Cullin-3

Chain B:



• Molecule 2: Cullin-3

Chain D:


GLY SER ALA PHE PRO MSE T24 E27 K28 Y29 V30 L37 R46 K47 N48 N49 S50 M64 H67 K68 H69 K72 L77 V80 V81 L85 I86 N87 K88 V89 D92 L97 N98 N99 M118 I122 L123 M126 Y130 V139 Y140 N141 I145
I146 F147 R148 D149 Q150 R153 D159 H160 Q163 T164 E172 V177 I183 L195 E196 G197 R198 D204 F205 E206 A207 P208 L225 N228 S229 A230 V237 E238 I241 E244 R247 V248 C251 L252 I260 V264 L268 I269 H272 M273
I276 V277 E278 M279 E280 N281 S282 G283 L284 V285 H286 M287 L288 K289 N290 G291 K292 T293 L296 M299 L302 R305 V306 P307 M313 S319 Y320 L321 R322 E323 Q324 GLY LYS ALA LEU VAL SER GLU GLU GLY GLU GLY LYS ASN PRO VAL ASP TYR ARG GLN GLY LEU ASP ASP
LEU LYS SER ARG PHE ASP ARG PHE LEU LEU GLU SER PHE ASN ASN ASP ARG LEU PHE LYS GLN THR ILE ALA GLY ASP PHE GLU TYR PHE LEU ASN LEU ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	213.17Å 76.94Å 85.83Å 90.00° 108.34° 90.00°	Depositor
Resolution (Å)	19.61 – 2.40 19.61 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.6 (19.61-2.40) 95.6 (19.61-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.211 , 0.263 0.219 , 0.266	Depositor DCC
R_{free} test set	2513 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	70.7	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 59.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6785	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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	0.62	0/911	0.68	0/1224
1	C	0.62	0/924	0.70	0/1241
2	B	0.66	0/2486	0.70	1/3309 (0.0%)
2	D	0.52	0/2482	0.65	0/3304
All	All	0.60	0/6803	0.68	1/9078 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	105	LEU	CB-CG-CD2	-5.68	101.35	111.00

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	896	0	876	14	0
1	C	909	0	888	23	0
2	B	2469	0	2469	64	0
2	D	2465	0	2466	102	0
3	A	5	0	0	0	0
3	B	26	0	0	4	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6785	0	6699	198	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 15.

All (198) 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)
2:D:172:GLU:OE2	2:D:247:ARG:NH2	1.66	1.25
2:B:281:ASN:O	2:B:286:HIS:CD2	1.93	1.22
2:B:281:ASN:O	2:B:286:HIS:CG	1.96	1.18
2:B:284:LEU:CD1	2:B:296:LEU:HD11	1.74	1.16
2:B:166:LEU:HG	2:B:212:MSE:HE2	1.22	1.16
2:D:241:ILE:HD11	2:D:305:ARG:CZ	1.78	1.13
2:B:270:SER:HA	2:B:273:MSE:HE3	1.27	1.09
1:C:265:ASN:HB3	1:C:268:LYS:HE2	1.10	1.05
2:D:241:ILE:CD1	2:D:305:ARG:CZ	2.34	1.05
2:B:284:LEU:HD12	2:B:296:LEU:HD11	1.36	1.04
2:D:306:VAL:HG13	2:D:307:PRO:HD2	1.40	1.04
2:B:287:MSE:HE3	2:B:296:LEU:CD1	1.87	1.04
2:D:153:ARG:NH1	2:D:204:ASP:OD2	1.93	1.02
2:B:287:MSE:CE	2:B:296:LEU:HD12	1.90	1.01
1:A:190:LEU:HD21	1:C:190:LEU:HD21	1.42	1.00
2:B:284:LEU:HD12	2:B:296:LEU:CD1	1.92	0.98
2:D:241:ILE:HD11	2:D:305:ARG:NH1	1.78	0.97
2:B:287:MSE:HE3	2:B:296:LEU:HD12	1.43	0.97
1:A:190:LEU:CD2	1:C:190:LEU:HD21	1.97	0.95
2:D:145:ILE:HD11	2:D:195:LEU:HD11	1.50	0.94
1:A:204:LEU:HD13	1:A:251:PHE:HZ	1.31	0.92
1:C:265:ASN:HB3	1:C:268:LYS:CE	1.98	0.92
2:D:85:LEU:HD23	2:D:89:VAL:HG21	1.50	0.92
2:B:284:LEU:HD11	2:B:296:LEU:HD11	1.54	0.88
2:B:284:LEU:CD1	2:B:296:LEU:CD1	2.52	0.84
2:D:30:VAL:HG21	2:D:69:HIS:CD2	2.13	0.84
1:A:204:LEU:HD23	1:A:241:VAL:HB	1.59	0.83
2:B:273:MSE:HE1	2:B:306:VAL:HG21	1.60	0.83
1:C:245:ASP:OD1	1:C:279:LYS:HE3	1.78	0.83
2:D:284:LEU:HD23	2:D:284:LEU:O	1.79	0.82
2:B:284:LEU:HA	2:B:287:MSE:HE2	1.62	0.82
2:B:273:MSE:HE1	2:B:306:VAL:CG2	2.10	0.81
1:C:265:ASN:CB	1:C:268:LYS:HE2	2.03	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:85:LEU:HA	2:D:89:VAL:HB	1.61	0.80
2:D:284:LEU:HD21	2:D:288:LEU:CD1	2.11	0.80
2:D:172:GLU:CD	2:D:247:ARG:HH21	1.85	0.80
2:D:46:ARG:O	2:D:47:LYS:HB2	1.83	0.78
2:D:172:GLU:OE2	2:D:247:ARG:CZ	2.31	0.78
2:B:287:MSE:HE3	2:B:296:LEU:HD13	1.63	0.77
2:D:284:LEU:HD23	2:D:284:LEU:C	2.07	0.75
1:A:190:LEU:HD21	1:C:190:LEU:CD2	2.16	0.75
2:D:276:ILE:HA	2:D:279:MSE:HE3	1.67	0.75
2:D:284:LEU:HD21	2:D:288:LEU:HD11	1.66	0.75
2:D:306:VAL:HG13	2:D:307:PRO:CD	2.16	0.75
2:B:166:LEU:HG	2:B:212:MSE:CE	2.13	0.74
2:B:287:MSE:CE	2:B:296:LEU:CD1	2.58	0.73
2:D:141:ASN:O	2:D:145:ILE:HG12	1.89	0.72
2:D:238:GLU:HA	2:D:241:ILE:CG2	2.19	0.72
2:D:195:LEU:O	2:D:196:GLU:HB3	1.88	0.72
2:D:153:ARG:NH1	2:D:204:ASP:CG	2.42	0.72
2:D:153:ARG:HH11	2:D:204:ASP:CG	1.94	0.71
2:D:269:ILE:O	2:D:273:MSE:HG3	1.91	0.70
2:D:292:LYS:O	2:D:296:LEU:HD12	1.92	0.70
2:B:43:GLU:OE1	2:B:48:ASN:ND2	2.24	0.69
2:B:209:PHE:HA	2:B:212:MSE:HE3	1.75	0.68
2:D:238:GLU:O	2:D:241:ILE:HG23	1.94	0.68
1:A:204:LEU:HD13	1:A:251:PHE:CZ	2.23	0.67
2:B:273:MSE:CE	2:B:306:VAL:HG21	2.24	0.67
2:B:281:ASN:O	2:B:286:HIS:CB	2.42	0.67
1:C:191:GLY:O	1:C:195:GLU:HG3	1.95	0.66
2:D:148:ARG:O	2:D:153:ARG:HG2	1.94	0.66
1:C:265:ASN:O	1:C:268:LYS:HG2	1.96	0.66
1:C:274:LEU:C	1:C:274:LEU:HD23	2.16	0.66
2:D:49:ASN:HD22	2:D:118:MSE:HE1	1.60	0.65
2:D:207:ALA:HB3	2:D:208:PRO:HD3	1.78	0.65
2:D:77:LEU:HD21	2:D:139:VAL:HG13	1.79	0.64
2:D:67:HIS:O	2:D:68:LYS:HB2	1.95	0.64
2:D:284:LEU:CD2	2:D:288:LEU:CD1	2.75	0.64
2:D:306:VAL:CG1	2:D:307:PRO:N	2.60	0.64
2:D:306:VAL:CG1	2:D:307:PRO:HD2	2.24	0.64
2:B:85:LEU:HD23	2:B:89:VAL:HG21	1.80	0.63
2:D:241:ILE:HD13	2:D:305:ARG:CZ	2.29	0.63
2:B:287:MSE:HE1	2:B:296:LEU:HD12	1.78	0.62
2:B:217:PHE:CE1	2:B:240:ARG:HD2	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:230:ALA:N	2:D:282:SER:OG	2.26	0.62
2:D:306:VAL:HG12	2:D:307:PRO:N	2.13	0.62
2:D:85:LEU:HD12	2:D:146:ILE:HG22	1.82	0.62
2:D:241:ILE:HD11	2:D:305:ARG:NH2	2.15	0.61
1:C:200:THR:HG22	1:C:214:HIS:CE1	2.35	0.61
1:A:193:LEU:HD21	1:C:220:ALA:HB2	1.83	0.61
2:D:237:VAL:O	2:D:241:ILE:HG22	2.01	0.61
2:D:159:ASP:O	2:D:163:GLN:HG3	2.00	0.60
2:D:238:GLU:O	2:D:241:ILE:CG2	2.49	0.60
2:B:88:LYS:NZ	2:B:92:ASP:OD2	2.23	0.60
2:D:284:LEU:CD2	2:D:288:LEU:HD12	2.32	0.59
2:D:230:ALA:CB	2:D:282:SER:OG	2.51	0.59
2:D:299:MSE:HE2	2:D:313:MSE:HE3	1.83	0.59
2:D:306:VAL:CG1	2:D:307:PRO:CD	2.81	0.58
2:B:274:LYS:O	2:B:278:GLU:HG2	2.04	0.58
2:B:110:ASN:O	2:B:114:THR:HG23	2.04	0.58
1:C:291:ASP:OD2	1:C:291:ASP:C	2.43	0.57
2:D:183:ILE:HB	2:D:251:CYS:SG	2.44	0.57
2:D:241:ILE:CD1	2:D:305:ARG:NH2	2.68	0.57
2:D:241:ILE:CD1	2:D:305:ARG:NH1	2.59	0.57
2:D:85:LEU:HA	2:D:89:VAL:CB	2.35	0.57
2:B:173:ARG:HD2	3:B:420:HOH:O	2.04	0.56
2:D:238:GLU:HA	2:D:241:ILE:HG22	1.86	0.56
2:D:64:MSE:HE1	2:D:72:LYS:HE2	1.88	0.55
2:D:172:GLU:OE2	2:D:247:ARG:NE	2.40	0.54
2:D:284:LEU:C	2:D:284:LEU:CD2	2.75	0.54
2:D:77:LEU:O	2:D:80:VAL:HG12	2.06	0.54
2:B:258:GLU:HB3	2:B:259:PRO:HD3	1.89	0.54
2:D:280:GLU:O	2:D:281:ASN:HB2	2.06	0.54
2:B:198:ARG:NH1	2:B:255:SER:OG	2.40	0.54
2:D:248:VAL:O	2:D:252:LEU:O	2.25	0.53
2:D:195:LEU:O	2:D:196:GLU:CB	2.56	0.53
2:B:85:LEU:HD23	2:B:89:VAL:CG2	2.39	0.53
2:B:222:GLN:NE2	3:B:407:HOH:O	2.35	0.53
2:D:85:LEU:HD23	2:D:89:VAL:CG2	2.32	0.52
2:B:233:TYR:O	2:B:237:VAL:HG23	2.10	0.52
1:A:190:LEU:CD2	1:C:190:LEU:CD2	2.79	0.52
1:C:286:LYS:O	1:C:290:GLU:HG3	2.09	0.52
2:D:148:ARG:O	2:D:153:ARG:CG	2.57	0.51
2:D:252:LEU:CD1	2:D:252:LEU:N	2.72	0.51
2:D:30:VAL:HG21	2:D:69:HIS:CG	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:172:GLU:CD	2:D:247:ARG:NH2	2.54	0.51
2:D:289:LYS:HG2	2:D:320:TYR:OH	2.11	0.51
2:D:283:GLY:O	2:D:286:HIS:N	2.44	0.51
2:D:238:GLU:CA	2:D:241:ILE:HG22	2.40	0.50
2:D:230:ALA:HB3	2:D:282:SER:OG	2.12	0.50
2:B:198:ARG:HH22	2:B:206:GLU:CD	2.15	0.50
2:B:273:MSE:HE1	2:B:306:VAL:HG23	1.90	0.50
2:D:85:LEU:CD2	2:D:89:VAL:HG21	2.32	0.50
1:A:245:ASP:OD2	1:A:245:ASP:O	2.30	0.50
2:D:289:LYS:HG2	2:D:320:TYR:CZ	2.47	0.50
2:B:272:HIS:O	2:B:276:ILE:HG12	2.12	0.49
2:D:30:VAL:HG13	2:D:72:LYS:NZ	2.27	0.49
2:D:196:GLU:HG2	2:D:196:GLU:O	2.12	0.49
2:D:248:VAL:HA	2:D:252:LEU:HB2	1.93	0.49
2:D:291:GLY:O	2:D:293:THR:HG23	2.12	0.49
2:B:24:THR:HB	2:B:27:GLU:HG3	1.93	0.49
1:C:291:ASP:OD2	1:C:291:ASP:O	2.30	0.49
2:D:160:HIS:O	2:D:164:THR:HG23	2.12	0.49
2:D:284:LEU:HB2	2:D:299:MSE:HE1	1.94	0.49
2:B:85:LEU:HD12	2:B:146:ILE:HG22	1.96	0.48
1:C:274:LEU:HB2	1:C:289:CYS:HB3	1.95	0.48
2:B:85:LEU:CD2	2:B:89:VAL:HG21	2.43	0.48
2:D:283:GLY:O	2:D:284:LEU:C	2.52	0.48
2:D:272:HIS:O	2:D:276:ILE:HG12	2.13	0.47
2:D:24:THR:HB	2:D:27:GLU:HB2	1.97	0.47
2:D:49:ASN:ND2	2:D:118:MSE:HE1	2.28	0.46
2:D:291:GLY:O	2:D:292:LYS:C	2.54	0.46
1:C:274:LEU:HD23	1:C:274:LEU:O	2.15	0.46
2:B:224:PHE:CE2	2:B:236:LYS:HB3	2.50	0.46
1:A:218:LEU:HD23	1:A:258:ILE:HG21	1.98	0.46
1:C:277:ALA:HB2	1:C:285:LEU:HD23	1.98	0.45
1:C:245:ASP:OD1	1:C:279:LYS:CE	2.58	0.45
2:B:38:LYS:O	2:B:42:GLN:HG3	2.17	0.45
2:B:77:LEU:HD21	2:B:139:VAL:HG13	1.99	0.45
2:B:234:ILE:HG23	2:B:302:LEU:HD22	1.99	0.45
2:B:86:ILE:HD11	2:B:150:GLN:OE1	2.17	0.45
2:B:212:MSE:HE3	2:B:212:MSE:HB3	1.92	0.45
2:B:53:SER:O	2:B:57:LEU:HG	2.17	0.44
2:B:173:ARG:HD3	2:B:216:PHE:CE2	2.51	0.44
2:D:85:LEU:HA	2:D:89:VAL:CG2	2.48	0.44
2:D:88:LYS:O	2:D:88:LYS:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:80:VAL:HG13	2:D:81:VAL:N	2.32	0.44
2:D:145:ILE:CD1	2:D:195:LEU:HD11	2.33	0.44
2:D:277:VAL:HG12	2:D:299:MSE:HE3	1.99	0.43
2:D:126:MSE:HG3	2:D:130:TYR:HB3	2.00	0.43
1:A:200:THR:HG21	1:A:212:GLN:CB	2.49	0.43
2:B:217:PHE:HE1	2:B:240:ARG:HD2	1.81	0.43
1:A:200:THR:HG21	1:A:212:GLN:HB2	2.01	0.43
2:B:198:ARG:NH2	2:B:206:GLU:OE2	2.49	0.43
2:D:72:LYS:HE2	2:D:72:LYS:HB3	1.62	0.43
2:B:102:LEU:HD13	2:B:164:THR:HG21	2.00	0.43
2:D:86:ILE:HD11	2:D:150:GLN:OE1	2.19	0.43
1:A:204:LEU:HD23	1:A:241:VAL:CB	2.41	0.42
2:D:225:LEU:HD22	2:D:279:MSE:HE1	2.01	0.42
2:D:244:GLU:HG3	2:D:264:VAL:HG11	2.02	0.42
2:B:84:HIS:HE1	3:B:421:HOH:O	2.02	0.42
2:B:137:GLU:OE1	3:B:425:HOH:O	2.22	0.42
2:D:288:LEU:HD23	2:D:288:LEU:HA	1.67	0.42
2:B:121:ASP:O	2:B:124:MSE:HE3	2.19	0.42
2:D:238:GLU:HA	2:D:241:ILE:HG21	2.00	0.42
2:D:237:VAL:HG12	2:D:302:LEU:HD11	2.01	0.42
2:B:86:ILE:HD12	2:B:90:ARG:NH2	2.35	0.42
2:D:323:GLU:HB2	2:D:324:GLN:OE1	2.20	0.42
2:B:86:ILE:HD11	2:B:150:GLN:CD	2.40	0.42
2:B:44:ILE:HG23	2:B:118:MSE:HE3	2.02	0.41
2:D:37:LEU:HD23	2:D:37:LEU:HA	1.91	0.41
1:C:215:LYS:HB2	1:C:215:LYS:HE2	1.85	0.41
2:D:241:ILE:CD1	2:D:305:ARG:NE	2.80	0.41
1:A:252:LYS:HE3	1:A:252:LYS:HB2	1.85	0.41
2:B:314:CYS:O	2:B:318:SER:HB2	2.20	0.41
2:D:198:ARG:NH2	2:D:206:GLU:OE2	2.40	0.41
2:D:88:LYS:NZ	2:D:92:ASP:OD2	2.31	0.41
2:B:109:TRP:CE2	2:B:189:MSE:HG3	2.56	0.41
2:B:284:LEU:HD12	2:B:287:MSE:CE	2.51	0.41
2:D:287:MSE:O	2:D:291:GLY:N	2.53	0.41
1:C:223:PRO:HA	1:C:226:SER:HB3	2.03	0.40
2:B:180:ARG:HG2	2:B:251:CYS:SG	2.60	0.40
2:B:29:TYR:O	2:B:32:SER:HB3	2.21	0.40
2:B:209:PHE:HA	2:B:212:MSE:CE	2.48	0.40
1:C:274:LEU:C	1:C:274:LEU:CD2	2.88	0.40
2:B:202:GLU:HA	2:B:206:GLU:HB3	2.03	0.40
2:D:252:LEU:N	2:D:252:LEU:HD12	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:260:ILE:HD12	2:D:260:ILE:HA	1.88	0.40

There are no symmetry-related clashes.

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	112/145 (77%)	112 (100%)	0	0	100	100
1	C	114/145 (79%)	114 (100%)	0	0	100	100
2	B	300/364 (82%)	294 (98%)	6 (2%)	0	100	100
2	D	299/364 (82%)	288 (96%)	11 (4%)	0	100	100
All	All	825/1018 (81%)	808 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	96/122 (79%)	96 (100%)	0	100	100
1	C	98/122 (80%)	98 (100%)	0	100	100
2	B	276/311 (89%)	276 (100%)	0	100	100
2	D	276/311 (89%)	276 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	746/866 (86%)	746 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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, 95^{th} 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	114/145 (78%)	-0.02	2 (1%)	68	66	57, 75, 111, 143	0
1	C	116/145 (80%)	0.10	7 (6%)	21	20	57, 76, 120, 144	0
2	B	284/364 (78%)	0.16	18 (6%)	20	18	52, 74, 118, 152	0
2	D	283/364 (77%)	0.33	19 (6%)	17	16	65, 94, 131, 156	0
All	All	797/1018 (78%)	0.19	46 (5%)	23	22	52, 81, 125, 156	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	180	LYS	5.1
2	D	322	ARG	4.4
1	C	295	SER	4.0
2	D	319	SER	3.5
1	C	254	MET	3.5
2	D	228	ASN	3.3
2	B	323	GLU	3.2
2	D	268	LEU	3.2
2	B	291	GLY	3.2
2	D	122	ILE	3.1
2	B	325	GLY	3.1
1	C	180	LYS	3.1
2	B	268	LEU	2.9
2	B	123	LEU	2.9
1	A	255	MET	2.8
2	D	276	ILE	2.8
2	D	29	TYR	2.7
2	B	228	ASN	2.7
1	C	268	LYS	2.6
2	D	277	VAL	2.6
2	B	139	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	98	ASN	2.6
2	D	123	LEU	2.5
2	B	322	ARG	2.5
2	D	50	SER	2.4
1	C	258	ILE	2.3
2	D	99	ASN	2.3
2	B	324	GLN	2.3
2	B	290	ASN	2.2
2	D	147	PHE	2.2
2	D	284	LEU	2.2
1	C	280	TYR	2.2
2	D	24	THR	2.2
2	D	324	GLN	2.2
2	B	122	ILE	2.2
2	B	24	THR	2.1
2	D	97	LEU	2.1
1	C	294	CYS	2.1
2	D	177	VAL	2.1
2	B	73	LEU	2.1
2	B	280	GLU	2.1
2	B	147	PHE	2.1
2	D	293	THR	2.0
2	B	119	ILE	2.0
2	B	269	ILE	2.0
2	B	61	ALA	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.