WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 09:20 AM EDT

PDB ID	:	3CQX
Title	:	Chaperone Complex
Authors	:	Xu, Z.; Nix, J.C.; Misra, S.
Deposited on	:	2008-04-03
Resolution	:	2.30 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
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)	:	2.35

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 2.30 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.
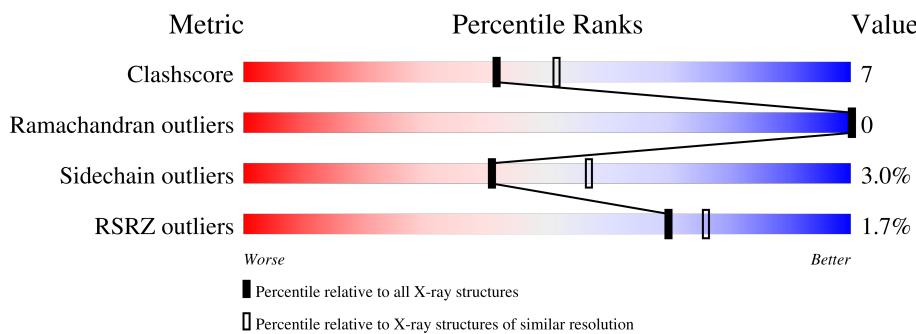
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	386	2% — 79% — 17% ··
1	B	386	% — 84% — 12% ··
2	C	88	2% — 82% — 9% · 8%
2	D	88	2% — 75% — 20% 5%
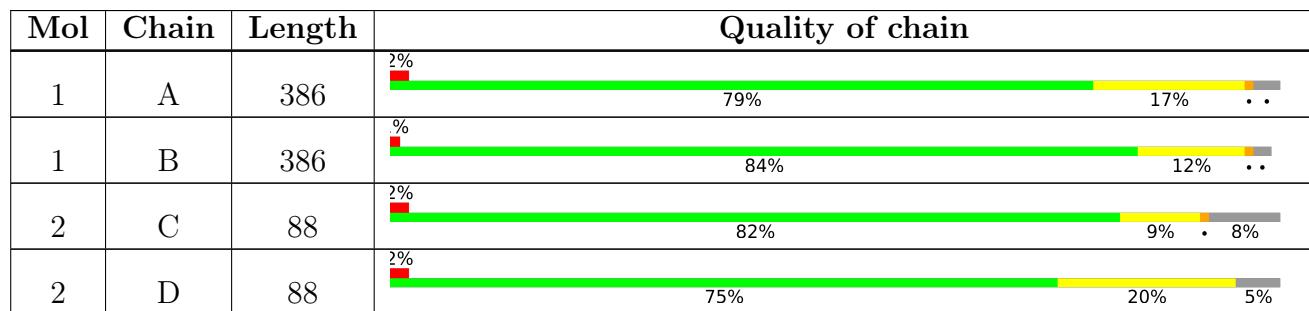
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SCN	A	404	-	-	X	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 7385 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 Heat shock cognate 71 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total 2918	C 1832	N 512	O 566	S 8	0	0	0
1	B	377	Total 2925	C 1837	N 513	O 567	S 8	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P63017
A	-3	ALA	-	expression tag	UNP P63017
A	-2	MET	-	expression tag	UNP P63017
A	-1	GLY	-	expression tag	UNP P63017
A	0	SER	-	expression tag	UNP P63017
B	-4	GLY	-	expression tag	UNP P63017
B	-3	ALA	-	expression tag	UNP P63017
B	-2	MET	-	expression tag	UNP P63017
B	-1	GLY	-	expression tag	UNP P63017
B	0	SER	-	expression tag	UNP P63017

- Molecule 2 is a protein called BAG family molecular chaperone regulator 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	81	Total 631	C 394	N 111	O 123	S 3	0	0	0
2	D	84	Total 652	C 406	N 115	O 128	S 3	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	102	GLY	-	expression tag	UNP Q91YN9
C	103	ALA	-	expression tag	UNP Q91YN9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	104	MET	-	expression tag	UNP Q91YN9
C	105	GLY	-	expression tag	UNP Q91YN9
C	106	SER	-	expression tag	UNP Q91YN9
C	189	LYS	-	expression tag	UNP Q91YN9
D	102	GLY	-	expression tag	UNP Q91YN9
D	103	ALA	-	expression tag	UNP Q91YN9
D	104	MET	-	expression tag	UNP Q91YN9
D	105	GLY	-	expression tag	UNP Q91YN9
D	106	SER	-	expression tag	UNP Q91YN9
D	189	LYS	-	expression tag	UNP Q91YN9

- Molecule 3 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).
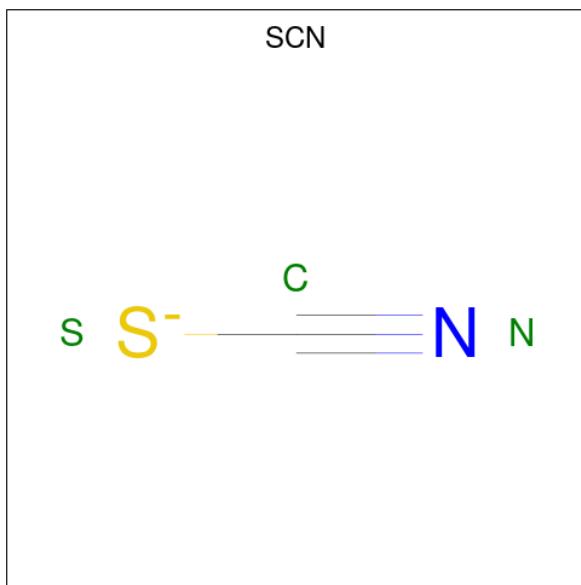
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total C N S 3 1 1 1			0	0
3	A	1	Total C N S 3 1 1 1			0	0
3	A	1	Total C N S 3 1 1 1			0	0
3	A	1	Total C N S 3 1 1 1			0	0
3	B	1	Total C N S 3 1 1 1			0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total 3	Na 3	0	0
4	D	1	Total 1	Na 1	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	75	Total 75	O 75	0	0
5	B	145	Total 145	O 145	0	0
5	C	15	Total 15	O 15	0	0
5	D	5	Total 5	O 5	0	0

3 Residue-property plots ⓘ

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: Heat shock cognate 71 kDa protein
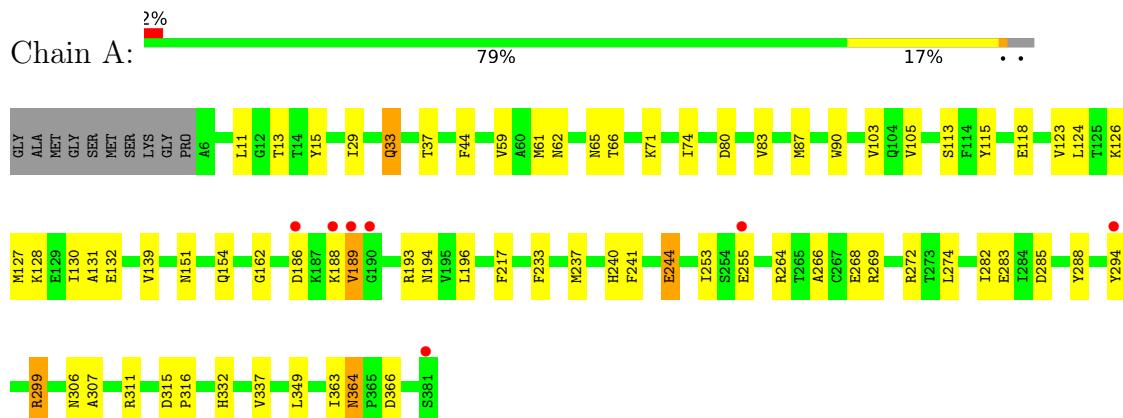
• Molecule 1: Heat shock cognate 71 kDa protein
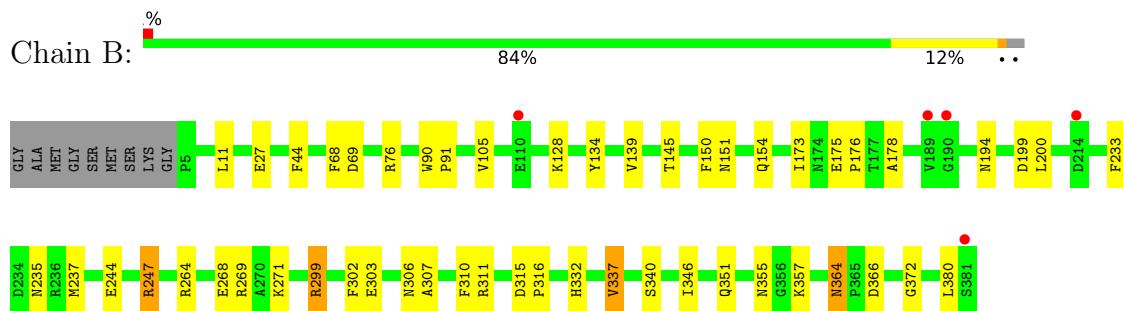
• Molecule 2: BAG family molecular chaperone regulator 2
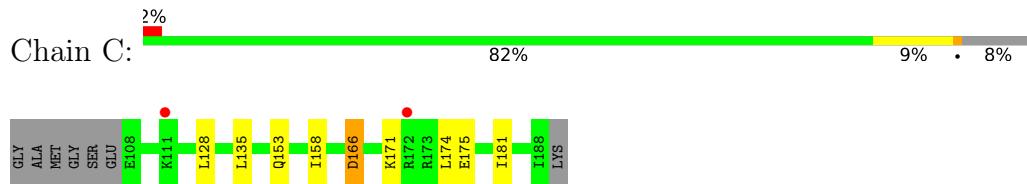
• Molecule 2: BAG family molecular chaperone regulator 2
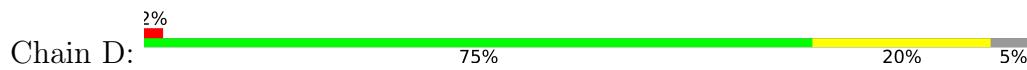
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	52.85Å 105.81Å 210.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.13 – 2.30	Depositor
	43.13 – 2.30	EDS
% Data completeness	98.8 (43.13-2.30)	Depositor
(in resolution range)	98.9 (43.13-2.30)	EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	8.28 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.256	Depositor
	0.214 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	33.2	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 38.7	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7385	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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: NA, SCN

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	0.34	0/2963	0.56	0/4000
1	B	0.38	0/2971	0.60	0/4011
2	C	0.32	0/638	0.53	0/857
2	D	0.31	0/659	0.49	0/883
All	All	0.35	0/7231	0.57	0/9751

There are no bond length outliers.

There are no bond angle outliers.

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	2918	0	2923	53	0
1	B	2925	0	2931	33	0
2	C	631	0	650	5	0
2	D	652	0	670	12	0
3	A	12	0	0	3	0
3	B	3	0	0	0	0
4	A	3	0	0	0	0
4	D	1	0	0	0	0
5	A	75	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	145	0	0	0	0
5	C	15	0	0	0	0
5	D	5	0	0	0	0
All	All	7385	0	7174	100	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 7.

All (100) 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:349:LEU:HD11	3:A:404:SCN:N	1.53	1.21
1:A:13:THR:HG22	1:A:71:LYS:HD3	1.52	0.91
1:B:151:ASN:H	1:B:154:GLN:HE21	1.18	0.87
1:A:194:ASN:H	1:A:332:HIS:HD2	1.23	0.86
1:A:151:ASN:H	1:A:154:GLN:HE21	1.22	0.86
1:B:194:ASN:H	1:B:332:HIS:HD2	1.23	0.82
1:A:194:ASN:H	1:A:332:HIS:CD2	2.04	0.75
1:A:186:ASP:HB3	1:A:217:PHE:CZ	2.25	0.70
1:B:264:ARG:O	1:B:268:GLU:HG3	1.91	0.70
1:A:151:ASN:H	1:A:154:GLN:NE2	1.90	0.69
1:A:233:PHE:HA	1:A:306:ASN:HD21	1.57	0.69
2:D:155:PHE:O	2:D:159:VAL:HG23	1.93	0.69
1:B:364:ASN:C	1:B:364:ASN:HD22	1.96	0.68
1:A:349:LEU:CD1	3:A:404:SCN:N	2.44	0.68
1:A:33:GLN:NE2	1:A:33:GLN:H	1.91	0.68
1:B:315:ASP:HB2	1:B:316:PRO:HD3	1.75	0.67
1:B:237:MET:HE1	1:B:271:LYS:HB2	1.76	0.67
1:B:269:ARG:HH21	2:C:158:ILE:HA	1.60	0.66
1:B:364:ASN:ND2	1:B:366:ASP:H	1.94	0.65
1:A:364:ASN:HD22	1:A:366:ASP:H	1.46	0.63
1:A:62:ASN:HD21	1:A:65:ASN:HB2	1.64	0.62
1:A:268:GLU:O	1:A:272:ARG:HD3	1.99	0.62
2:D:188:ILE:O	2:D:188:ILE:HG22	2.00	0.62
1:B:194:ASN:H	1:B:332:HIS:CD2	2.12	0.61
1:A:315:ASP:HB2	1:A:316:PRO:HD3	1.83	0.60
1:A:59:VAL:HG22	1:A:66:THR:HG21	1.84	0.60
1:B:364:ASN:HD22	1:B:366:ASP:H	1.48	0.60
1:A:115:TYR:HB2	1:A:118:GLU:HG3	1.84	0.60
1:A:364:ASN:ND2	1:A:366:ASP:H	2.00	0.59
1:A:364:ASN:HD22	1:A:364:ASN:C	2.05	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:LYS:CG	1:A:189:VAL:H	2.15	0.59
1:A:264:ARG:O	1:A:268:GLU:HG3	2.03	0.58
2:C:128:LEU:HD22	2:C:181:ILE:HG23	1.86	0.58
1:A:233:PHE:HA	1:A:306:ASN:ND2	2.18	0.58
1:B:151:ASN:H	1:B:154:GLN:NE2	1.96	0.57
2:C:135:LEU:HD12	2:C:181:ILE:HD12	1.85	0.57
1:B:145:THR:HG22	1:B:173:ILE:HG13	1.86	0.56
2:C:166:ASP:OD2	2:D:110:LEU:HG	2.05	0.56
1:B:310:PHE:CD1	1:B:346:ILE:HD11	2.42	0.55
1:A:188:LYS:HG2	1:A:189:VAL:H	1.72	0.55
2:D:171:LYS:O	2:D:175:GLU:HG3	2.07	0.55
1:A:62:ASN:ND2	1:A:65:ASN:HB2	2.22	0.53
1:A:266:ALA:HB1	1:A:282:ILE:HG23	1.91	0.53
1:A:188:LYS:HG2	1:A:189:VAL:N	2.23	0.53
2:D:115:ARG:O	2:D:119:GLU:HG3	2.08	0.53
2:C:171:LYS:O	2:C:175:GLU:HG3	2.08	0.53
1:A:188:LYS:CG	1:A:189:VAL:N	2.71	0.53
1:A:128:LYS:O	1:A:132:GLU:HG3	2.10	0.52
1:B:178:ALA:O	1:B:372:GLY:HA3	2.10	0.50
1:B:299:ARG:O	1:B:303:GLU:HG3	2.12	0.50
1:B:128:LYS:HE3	1:B:139:VAL:O	2.12	0.50
1:B:233:PHE:HA	1:B:306:ASN:HD21	1.77	0.50
2:D:111:LYS:HD3	2:D:111:LYS:C	2.33	0.49
1:A:283:GLU:HG2	1:A:294:TYR:CD2	2.48	0.48
1:B:233:PHE:HA	1:B:306:ASN:ND2	2.29	0.48
1:A:13:THR:CG2	1:A:71:LYS:HD3	2.34	0.48
1:A:126:LYS:O	1:A:130:ILE:HG13	2.14	0.48
1:B:307:ALA:HB1	1:B:311:ARG:NH1	2.29	0.48
1:B:351:GLN:HG3	1:B:357:LYS:O	2.14	0.48
1:A:123:VAL:O	1:A:127:MET:HG2	2.14	0.47
1:A:103:VAL:O	1:A:113:SER:HA	2.14	0.47
1:B:44:PHE:CD1	1:B:105:VAL:HG21	2.50	0.46
1:A:274:LEU:O	1:A:299:ARG:HD2	2.15	0.46
1:A:87:MET:HA	1:A:90:TRP:CE3	2.50	0.46
1:A:15:TYR:CD2	1:A:37:THR:HB	2.51	0.46
1:A:269:ARG:HB3	1:A:269:ARG:CZ	2.45	0.46
1:A:33:GLN:NE2	1:A:33:GLN:N	2.62	0.46
1:A:307:ALA:O	1:A:311:ARG:HG2	2.15	0.46
3:A:405:SCN:S	2:D:172:ARG:HG3	2.55	0.46
1:A:196:LEU:C	1:A:196:LEU:HD23	2.37	0.45
1:A:253:ILE:HG22	1:A:288:TYR:CG	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:ASP:HB2	1:B:337:VAL:HG13	1.98	0.45
1:A:237:MET:O	1:A:240:HIS:HB3	2.16	0.45
1:B:271:LYS:HG3	1:B:302:PHE:CZ	2.52	0.45
1:A:80:ASP:HB3	1:A:83:VAL:HG23	1.99	0.44
1:B:199:ASP:HA	1:B:337:VAL:O	2.17	0.44
1:B:244:GLU:OE1	1:B:247:ARG:NH1	2.50	0.44
2:D:176:THR:HG23	2:D:179:ARG:HH21	1.82	0.44
1:A:269:ARG:HB3	1:A:269:ARG:NH1	2.33	0.44
1:A:241:PHE:HA	1:A:244:GLU:HB2	2.00	0.44
1:A:61:MET:SD	2:D:149:GLY:HA2	2.58	0.43
1:B:307:ALA:HB1	1:B:311:ARG:HH12	1.83	0.43
1:B:364:ASN:C	1:B:364:ASN:ND2	2.68	0.43
2:D:111:LYS:HE3	2:D:115:ARG:NH1	2.33	0.43
1:B:27:GLU:HG2	1:B:134:TYR:OH	2.18	0.43
1:A:124:LEU:HD13	1:A:162:GLY:HA2	2.01	0.43
2:D:132:LYS:O	2:D:136:MET:HB2	2.19	0.43
1:A:186:ASP:OD1	1:A:186:ASP:N	2.52	0.42
1:A:363:ILE:O	1:A:364:ASN:C	2.57	0.42
1:A:128:LYS:NZ	1:A:139:VAL:O	2.49	0.42
1:A:29:ILE:HD13	1:A:131:ALA:HA	2.01	0.42
1:A:44:PHE:CD1	1:A:105:VAL:HG21	2.55	0.41
2:D:117:ILE:O	2:D:121:VAL:HG23	2.20	0.41
1:A:115:TYR:HD1	1:A:118:GLU:OE2	2.03	0.41
1:A:74:ILE:HG23	1:A:74:ILE:O	2.21	0.41
1:B:90:TRP:HA	1:B:91:PRO:HD3	1.91	0.41
1:B:68:PHE:O	1:B:69:ASP:HB2	2.21	0.41
1:B:150:PHE:HA	1:B:154:GLN:NE2	2.36	0.41
1:B:175:GLU:N	1:B:176:PRO:HD2	2.35	0.41
1:B:200:LEU:HG	1:B:340:SER:HB2	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	374/386 (97%)	363 (97%)	11 (3%)	0	100	100
1	B	375/386 (97%)	368 (98%)	7 (2%)	0	100	100
2	C	79/88 (90%)	77 (98%)	2 (2%)	0	100	100
2	D	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
All	All	910/948 (96%)	887 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	312/318 (98%)	302 (97%)	10 (3%)	39	54
1	B	313/318 (98%)	304 (97%)	9 (3%)	42	58
2	C	73/77 (95%)	70 (96%)	3 (4%)	30	43
2	D	75/77 (97%)	74 (99%)	1 (1%)	69	82
All	All	773/790 (98%)	750 (97%)	23 (3%)	41	57

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	33	GLN
1	A	189	VAL
1	A	193	ARG
1	A	244	GLU
1	A	255	GLU
1	A	285	ASP
1	A	299	ARG
1	A	337	VAL
1	A	364	ASN
1	B	11	LEU
1	B	76	ARG
1	B	235	ASN

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Mol	Chain	Res	Type
1	B	247	ARG
1	B	299	ARG
1	B	337	VAL
1	B	355	ASN
1	B	364	ASN
1	B	380	LEU
2	C	153	GLN
2	C	166	ASP
2	C	174	LEU
2	D	164	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	33	GLN
1	A	154	GLN
1	A	194	ASN
1	A	239	ASN
1	A	249	HIS
1	A	279	GLN
1	A	306	ASN
1	A	332	HIS
1	A	364	ASN
1	A	376	GLN
1	B	154	GLN
1	B	194	ASN
1	B	235	ASN
1	B	306	ASN
1	B	332	HIS
1	B	355	ASN
1	B	364	ASN
1	B	376	GLN
2	C	153	GLN
2	D	153	GLN
2	D	180	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	SCN	A	402	-	1,2,2	0.35	0	0,1,1	-	-
3	SCN	A	403	-	1,2,2	0.27	0	0,1,1	-	-
3	SCN	B	401	-	1,2,2	0.46	0	0,1,1	-	-
3	SCN	A	405	-	1,2,2	0.31	0	0,1,1	-	-
3	SCN	A	404	-	1,2,2	0.35	0	0,1,1	-	-

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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	405	SCN	1	0
3	A	404	SCN	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	376/386 (97%)	-0.07	7 (1%)	66	73	18, 33, 54, 67	0
1	B	377/386 (97%)	-0.32	5 (1%)	77	81	15, 26, 43, 64	0
2	C	81/88 (92%)	0.06	2 (2%)	57	64	23, 38, 59, 73	0
2	D	84/88 (95%)	0.16	2 (2%)	59	66	32, 46, 57, 70	0
All	All	918/948 (96%)	-0.14	16 (1%)	70	76	15, 31, 54, 73	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	189	VAL	12.6
1	A	188	LYS	8.0
1	A	190	GLY	5.3
1	B	189	VAL	4.7
1	A	381	SER	3.9
1	B	214	ASP	3.1
1	A	294	TYR	3.0
2	D	130	ASN	2.8
1	B	381	SER	2.7
2	C	172	ARG	2.5
1	A	186	ASP	2.3
2	D	189	LYS	2.2
2	C	111	LYS	2.2
1	A	255	GLU	2.2
1	B	110	GLU	2.2
1	B	190	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

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6.3 Carbohydrates (i)

There are no monosaccharides 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(Å^2)	Q<0.9
3	SCN	A	405	3/3	0.52	0.26	76,76,77,79	0
4	NA	A	503	1/1	0.76	0.14	66,66,66,66	0
3	SCN	A	402	3/3	0.77	0.20	45,45,47,52	0
4	NA	A	501	1/1	0.81	0.25	59,59,59,59	0
3	SCN	A	404	3/3	0.89	0.43	50,50,53,57	0
3	SCN	A	403	3/3	0.91	0.10	55,55,57,58	0
3	SCN	B	401	3/3	0.91	0.14	38,38,41,42	0
4	NA	A	502	1/1	0.95	0.40	49,49,49,49	0
4	NA	D	504	1/1	0.95	0.10	57,57,57,57	0

6.5 Other polymers (i)

There are no such residues in this entry.