



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:25 AM UTC

PDB ID : 1UD0 / pdb_00001ud0
Title : CRYSTAL STRUCTURE OF THE C-TERMINAL 10-kDA SUBDOMAIN OF HSC70
Authors : Chou, C.C.; Forouhar, F.; Yeh, Y.H.; Wang, C.; Hsiao, C.D.
Deposited on : 2003-04-24
Resolution : 3.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

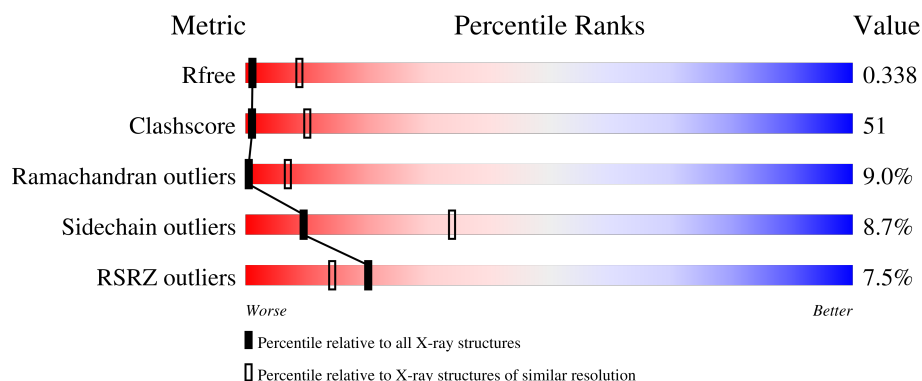
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	113	4% 24% 36% 11% • 26%
1	B	113	7% 18% 35% 18% • 27%
1	C	113	6% 23% 44% 9% • 22%
1	D	113	4% 20% 40% 9% 31%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2705 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 70 kDa heat-shock-like protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	84	Total	C	N	O	S	Se	0	0	0
			672	417	114	136	2	3			
1	B	82	Total	C	N	O	S	Se	0	0	0
			664	413	112	134	2	3			
1	C	88	Total	C	N	O	S	Se	0	0	0
			702	438	118	140	2	4			
1	D	78	Total	C	N	O	S	Se	0	0	0
			641	399	108	130	2	2			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	534	LEU	-	cloning artifact	UNP P63018
A	535	VAL	-	cloning artifact	UNP P63018
A	536	PRO	-	cloning artifact	UNP P63018
A	537	ARG	-	cloning artifact	UNP P63018
A	538	GLY	-	cloning artifact	UNP P63018
A	539	SER	-	cloning artifact	UNP P63018
A	540	HIS	-	cloning artifact	UNP P63018
A	541	MSE	-	cloning artifact	UNP P63018
A	549	MSE	MET	modified residue	UNP P63018
A	617	MSE	MET	modified residue	UNP P63018
A	621	MSE	MET	modified residue	UNP P63018
B	534	LEU	-	cloning artifact	UNP P63018
B	535	VAL	-	cloning artifact	UNP P63018
B	536	PRO	-	cloning artifact	UNP P63018
B	537	ARG	-	cloning artifact	UNP P63018
B	538	GLY	-	cloning artifact	UNP P63018
B	539	SER	-	cloning artifact	UNP P63018
B	540	HIS	-	cloning artifact	UNP P63018
B	541	MSE	-	cloning artifact	UNP P63018
B	549	MSE	MET	modified residue	UNP P63018
B	617	MSE	MET	modified residue	UNP P63018

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Chain	Residue	Modelled	Actual	Comment	Reference
B	621	MSE	MET	modified residue	UNP P63018
C	534	LEU	-	cloning artifact	UNP P63018
C	535	VAL	-	cloning artifact	UNP P63018
C	536	PRO	-	cloning artifact	UNP P63018
C	537	ARG	-	cloning artifact	UNP P63018
C	538	GLY	-	cloning artifact	UNP P63018
C	539	SER	-	cloning artifact	UNP P63018
C	540	HIS	-	cloning artifact	UNP P63018
C	541	MSE	-	cloning artifact	UNP P63018
C	549	MSE	MET	modified residue	UNP P63018
C	617	MSE	MET	modified residue	UNP P63018
C	621	MSE	MET	modified residue	UNP P63018
D	534	LEU	-	cloning artifact	UNP P63018
D	535	VAL	-	cloning artifact	UNP P63018
D	536	PRO	-	cloning artifact	UNP P63018
D	537	ARG	-	cloning artifact	UNP P63018
D	538	GLY	-	cloning artifact	UNP P63018
D	539	SER	-	cloning artifact	UNP P63018
D	540	HIS	-	cloning artifact	UNP P63018
D	541	MSE	-	cloning artifact	UNP P63018
D	549	MSE	MET	modified residue	UNP P63018
D	617	MSE	MET	modified residue	UNP P63018
D	621	MSE	MET	modified residue	UNP P63018

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Na 1 1	0	0
2	D	2	Total Na 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total O 8 8	0	0
3	B	7	Total O 7 7	0	0
3	C	5	Total O 5 5	0	0

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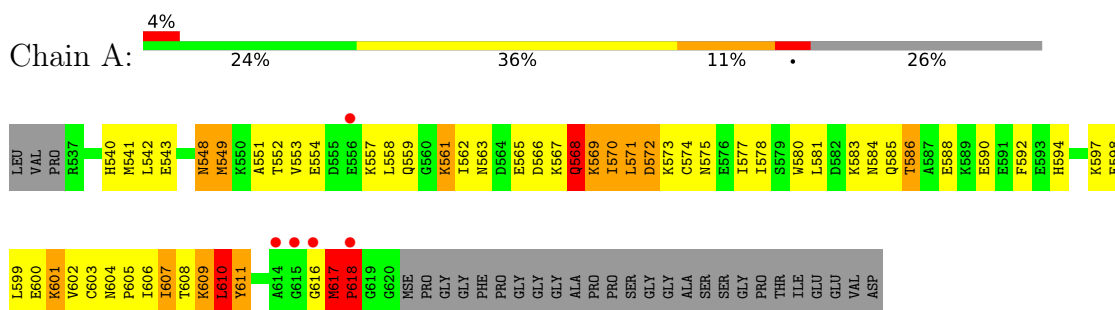
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	3	Total	O	0	0
			3	3		

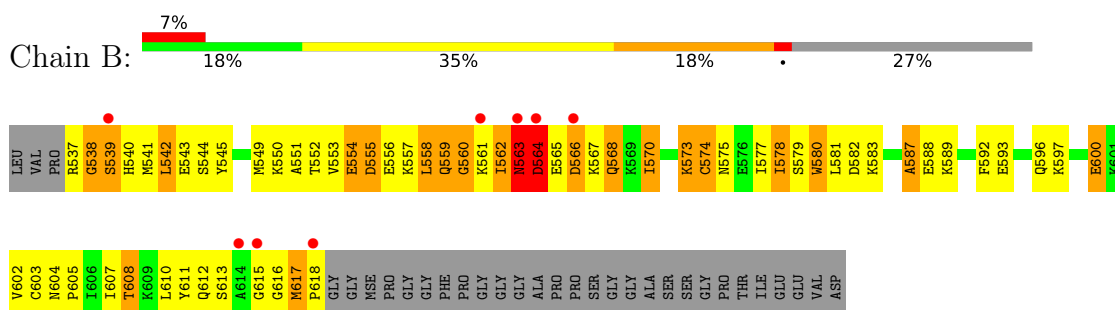
3 Residue-property plots [i](#)

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.

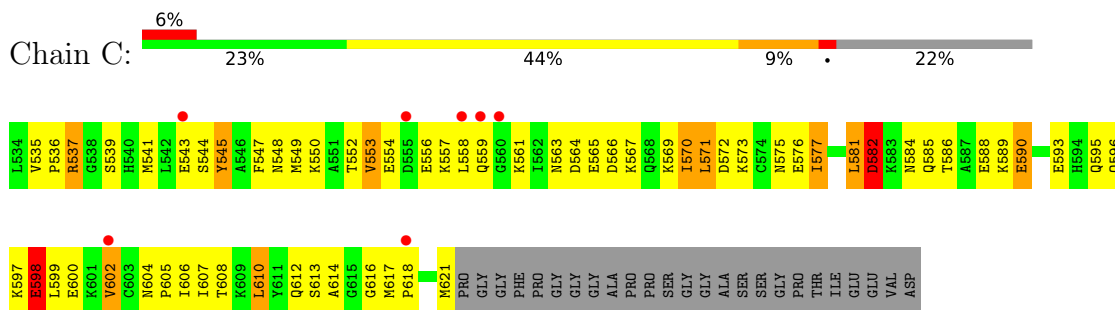
- Molecule 1: 70 kDa heat-shock-like protein



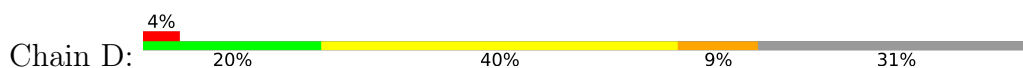
- Molecule 1: 70 kDa heat-shock-like protein

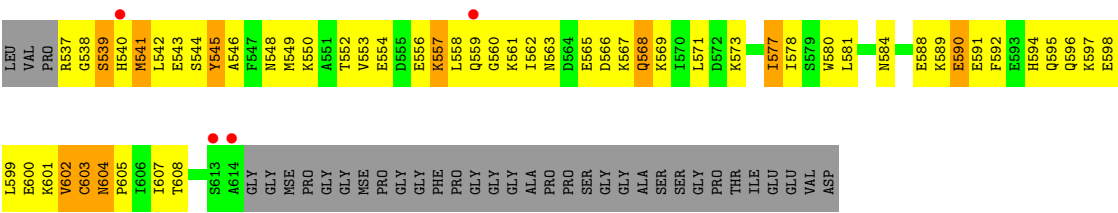


- Molecule 1: 70 kDa heat-shock-like protein



- Molecule 1: 70 kDa heat-shock-like protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	117.48Å 117.48Å 163.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.93 – 3.45 14.93 – 3.45	Depositor EDS
% Data completeness (in resolution range)	90.3 (14.93-3.45) 97.4 (14.93-3.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.30 (at 3.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.309 0.296 , 0.338	Depositor DCC
R_{free} test set	804 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	63.0	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 20.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	2705	wwPDB-VP
Average B, all atoms (Å ²)	43.0	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.*

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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	0/678	1.09	6/900 (0.7%)
1	B	0.54	0/670	1.15	11/890 (1.2%)
1	C	0.57	0/708	1.04	5/940 (0.5%)
1	D	0.82	1/647 (0.2%)	1.11	8/861 (0.9%)
All	All	0.64	1/2703 (0.0%)	1.10	30/3591 (0.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	544	SER	C-N	14.27	1.51	1.33

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	607	ILE	N-CA-C	-8.65	102.39	110.53
1	D	541	MSE	N-CA-C	-8.29	103.31	113.50
1	B	558	LEU	N-CA-C	-8.15	103.84	113.21
1	D	540	HIS	N-CA-C	7.91	122.81	108.17
1	B	560	GLY	N-CA-C	-7.72	102.28	113.86
1	B	554	GLU	N-CA-C	-7.24	104.70	113.97
1	C	550	LYS	N-CA-C	-7.08	105.18	114.31
1	C	537	ARG	N-CA-C	-6.97	103.77	111.36
1	D	544	SER	O-C-N	-6.95	114.08	122.22
1	B	538	GLY	N-CA-C	-6.77	107.22	114.67
1	B	608	THR	N-CA-C	-6.58	103.60	111.69
1	D	544	SER	CA-C-N	6.33	130.39	120.89
1	D	544	SER	C-N-CA	6.33	130.39	120.89
1	B	539	SER	N-CA-C	-6.06	104.59	112.23
1	A	549	MSE	N-CA-C	-6.00	104.66	111.14
1	A	548	ASN	N-CA-C	6.00	118.78	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	602	VAL	N-CA-C	5.96	117.50	111.00
1	B	568	GLN	N-CA-C	-5.43	105.26	111.07
1	A	610	LEU	N-CA-C	-5.41	105.55	111.82
1	A	617	MSE	CA-C-N	5.39	126.58	119.84
1	A	617	MSE	C-N-CA	5.39	126.58	119.84
1	C	590	GLU	N-CA-C	-5.38	105.31	111.07
1	B	600	GLU	N-CA-C	-5.34	105.54	111.36
1	B	613	SER	N-CA-C	5.14	121.76	110.80
1	B	587	ALA	N-CA-C	-5.14	105.84	112.68
1	D	543	GLU	N-CA-C	-5.08	105.92	111.82
1	C	545	TYR	N-CA-C	-5.05	105.77	111.28
1	C	577	ILE	N-CA-C	5.05	116.38	110.62
1	D	545	TYR	O-C-N	5.01	128.03	122.11
1	B	542	LEU	N-CA-C	-5.00	105.52	110.97

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	672	0	659	73	0
1	B	664	0	653	95	0
1	C	702	0	695	64	0
1	D	641	0	631	74	1
2	B	1	0	0	0	0
2	D	2	0	0	0	0
3	A	8	0	0	0	0
3	B	7	0	0	0	0
3	C	5	0	0	0	0
3	D	3	0	0	0	0
All	All	2705	0	2638	270	1

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 51.

All (270) 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:D:537:ARG:HG2	1:D:538:GLY:H	1.15	1.08
1:B:617:MSE:H	1:B:618:PRO:HD2	1.18	1.05
1:B:562:ILE:HB	1:B:566:ASP:HB3	1.48	0.93
1:B:561:LYS:C	1:B:563:ASN:H	1.71	0.92
1:A:558:LEU:HD23	1:A:562:ILE:HB	1.53	0.91
1:A:549:MSE:HA	1:A:549:MSE:HE3	1.54	0.89
1:B:617:MSE:H	1:B:618:PRO:CD	1.87	0.87
1:C:536:PRO:HD3	1:D:537:ARG:HD3	1.55	0.86
1:D:549:MSE:HE3	1:D:549:MSE:HA	1.63	0.81
1:C:556:GLU:HG3	1:C:557:LYS:H	1.45	0.79
1:D:563:ASN:HD21	1:D:565:GLU:HB3	1.47	0.79
1:B:537:ARG:HD2	1:B:539:SER:HB3	1.65	0.78
1:D:563:ASN:HB3	1:D:566:ASP:OD2	1.83	0.77
1:B:559:GLN:HG2	1:B:563:ASN:ND2	1.99	0.77
1:C:596:GLN:O	1:C:600:GLU:HG2	1.84	0.77
1:B:565:GLU:C	1:B:567:LYS:H	1.91	0.77
1:B:562:ILE:O	1:B:564:ASP:N	2.19	0.76
1:D:577:ILE:HG22	1:D:581:LEU:HD21	1.68	0.74
1:C:565:GLU:O	1:C:569:LYS:HB2	1.89	0.73
1:C:553:VAL:HG12	1:C:567:LYS:HG3	1.70	0.73
1:B:567:LYS:HA	1:B:570:ILE:HD13	1.72	0.72
1:C:610:LEU:HD22	1:C:616:GLY:HA2	1.72	0.71
1:C:536:PRO:HA	1:C:539:SER:HB2	1.72	0.71
1:D:577:ILE:HG22	1:D:581:LEU:CD2	2.20	0.71
1:A:599:LEU:HD12	1:B:545:TYR:CE1	2.26	0.71
1:B:559:GLN:HA	1:B:563:ASN:OD1	1.91	0.70
1:C:536:PRO:CD	1:D:537:ARG:HD3	2.22	0.69
1:A:561:LYS:O	1:A:561:LYS:HD3	1.92	0.69
1:C:608:THR:O	1:C:612:GLN:HG3	1.93	0.68
1:B:561:LYS:C	1:B:563:ASN:N	2.45	0.68
1:B:567:LYS:CA	1:B:570:ILE:HD13	2.24	0.67
1:B:593:GLU:O	1:B:597:LYS:HG3	1.93	0.67
1:D:580:TRP:CZ3	1:D:581:LEU:HD13	2.29	0.67
1:B:549:MSE:HA	1:B:552:THR:HG22	1.78	0.66
1:B:562:ILE:CB	1:B:566:ASP:HB3	2.24	0.66
1:A:617:MSE:H	1:A:618:PRO:HD2	1.59	0.66
1:D:559:GLN:HG3	1:D:560:GLY:H	1.60	0.65
1:D:537:ARG:CG	1:D:538:GLY:H	1.98	0.65
1:A:607:ILE:O	1:A:611:TYR:HB2	1.96	0.65
1:A:597:LYS:O	1:A:601:LYS:HB2	1.96	0.65
1:B:537:ARG:HD2	1:B:539:SER:CB	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:553:VAL:HG12	1:C:553:VAL:O	1.97	0.65
1:D:537:ARG:HG2	1:D:538:GLY:N	1.98	0.64
1:B:549:MSE:HE3	1:B:549:MSE:O	1.97	0.64
1:D:580:TRP:HZ3	1:D:581:LEU:HD13	1.62	0.64
1:B:617:MSE:N	1:B:618:PRO:HD2	2.03	0.64
1:B:570:ILE:HD12	1:B:570:ILE:N	2.13	0.64
1:B:559:GLN:HA	1:B:563:ASN:CG	2.22	0.64
1:D:578:ILE:HA	1:D:581:LEU:HD23	1.79	0.64
1:B:557:LYS:C	1:B:559:GLN:H	2.07	0.63
1:A:592:PHE:CE2	1:B:537:ARG:HD3	2.34	0.63
1:D:563:ASN:ND2	1:D:565:GLU:HB3	2.12	0.63
1:A:606:ILE:HG22	1:B:561:LYS:NZ	2.14	0.63
1:A:574:CYS:O	1:A:578:ILE:HG12	2.00	0.62
1:A:599:LEU:HD12	1:B:545:TYR:CD1	2.34	0.62
1:C:536:PRO:HD3	1:D:537:ARG:CD	2.28	0.62
1:A:570:ILE:O	1:A:571:LEU:C	2.41	0.62
1:C:598:GLU:O	1:C:602:VAL:HG13	1.98	0.62
1:A:548:ASN:O	1:A:551:ALA:HB3	2.00	0.62
1:C:563:ASN:O	1:C:566:ASP:HB2	1.99	0.62
1:A:563:ASN:HD21	1:A:565:GLU:HB3	1.65	0.61
1:C:552:THR:C	1:C:554:GLU:H	2.09	0.61
1:A:563:ASN:ND2	1:A:565:GLU:HB3	2.16	0.61
1:C:557:LYS:O	1:C:561:LYS:HD2	2.01	0.60
1:C:548:ASN:O	1:C:552:THR:HG23	2.01	0.60
1:B:565:GLU:O	1:B:567:LYS:N	2.30	0.60
1:A:549:MSE:HA	1:A:549:MSE:CE	2.30	0.60
1:B:558:LEU:HD23	1:B:558:LEU:O	2.00	0.60
1:A:617:MSE:N	1:A:618:PRO:HD2	2.17	0.60
1:D:573:LYS:O	1:D:577:ILE:HG12	2.02	0.59
1:A:558:LEU:N	1:A:558:LEU:HD12	2.17	0.59
1:A:592:PHE:HE2	1:B:537:ARG:HD3	1.65	0.59
1:D:577:ILE:CG2	1:D:581:LEU:HD21	2.33	0.59
1:A:570:ILE:HG22	1:A:571:LEU:N	2.18	0.59
1:B:537:ARG:O	1:B:540:HIS:HB2	2.03	0.59
1:B:561:LYS:HG3	1:B:562:ILE:N	2.17	0.59
1:A:606:ILE:HG22	1:B:561:LYS:HZ2	1.67	0.58
1:A:580:TRP:CZ3	1:A:581:LEU:HD23	2.38	0.58
1:D:556:GLU:O	1:D:559:GLN:N	2.36	0.58
1:B:604:ASN:N	1:B:605:PRO:HD2	2.18	0.58
1:C:543:GLU:HB2	1:C:581:LEU:CD1	2.33	0.58
1:A:608:THR:HG22	1:A:608:THR:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:538:GLY:O	1:D:539:SER:C	2.46	0.57
1:C:570:ILE:O	1:C:571:LEU:C	2.45	0.57
1:C:543:GLU:O	1:C:547:PHE:HB2	2.04	0.57
1:D:560:GLY:C	1:D:562:ILE:H	2.11	0.57
1:C:599:LEU:HD13	1:D:573:LYS:HG3	1.87	0.57
1:D:538:GLY:O	1:D:539:SER:O	2.22	0.57
1:A:583:LYS:O	1:A:586:THR:HG22	2.06	0.56
1:B:583:LYS:O	1:B:587:ALA:HB2	2.05	0.56
1:C:535:VAL:HG13	1:D:588:GLU:HG3	1.87	0.56
1:B:579:SER:O	1:B:582:ASP:N	2.39	0.56
1:D:580:TRP:O	1:D:581:LEU:C	2.49	0.55
1:C:553:VAL:CG1	1:C:567:LYS:HG3	2.36	0.55
1:B:558:LEU:O	1:B:560:GLY:N	2.37	0.55
1:C:544:SER:HA	1:C:547:PHE:HB2	1.89	0.55
1:D:566:ASP:O	1:D:567:LYS:C	2.48	0.55
1:B:588:GLU:O	1:B:589:LYS:C	2.49	0.55
1:D:557:LYS:C	1:D:558:LEU:HD12	2.32	0.55
1:A:566:ASP:O	1:A:567:LYS:C	2.50	0.55
1:B:607:ILE:HD12	1:B:608:THR:N	2.22	0.54
1:A:603:CYS:C	1:A:605:PRO:HD2	2.33	0.54
1:A:600:GLU:C	1:A:602:VAL:H	2.16	0.54
1:A:599:LEU:HD22	1:B:573:LYS:HG2	1.90	0.53
1:B:559:GLN:HG2	1:B:563:ASN:CG	2.32	0.53
1:C:537:ARG:O	1:C:541:MSE:HG3	2.08	0.53
1:B:558:LEU:C	1:B:560:GLY:H	2.16	0.53
1:B:575:ASN:HA	1:B:578:ILE:HB	1.90	0.53
1:B:602:VAL:HG12	1:B:602:VAL:O	2.08	0.53
1:A:549:MSE:HG2	1:B:603:CYS:SG	2.48	0.53
1:A:542:LEU:HD23	1:A:581:LEU:HD21	1.90	0.53
1:C:604:ASN:N	1:C:605:PRO:HD2	2.24	0.53
1:D:594:HIS:O	1:D:597:LYS:HB3	2.09	0.53
1:D:539:SER:O	1:D:541:MSE:HG3	2.09	0.52
1:A:597:LYS:C	1:A:599:LEU:H	2.17	0.52
1:C:600:GLU:HB2	1:C:604:ASN:HD21	1.74	0.52
1:A:558:LEU:HB3	1:A:562:ILE:HG22	1.92	0.52
1:C:549:MSE:HG3	1:C:549:MSE:O	2.09	0.52
1:D:558:LEU:HD12	1:D:558:LEU:N	2.25	0.52
1:A:604:ASN:N	1:A:605:PRO:HD2	2.24	0.51
1:A:557:LYS:HB3	1:A:558:LEU:HD12	1.93	0.51
1:A:606:ILE:CG2	1:B:561:LYS:HZ2	2.24	0.51
1:D:556:GLU:O	1:D:558:LEU:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:616:GLY:C	1:C:618:PRO:HD2	2.36	0.51
1:C:553:VAL:HG21	1:C:570:ILE:HD12	1.93	0.51
1:B:556:GLU:C	1:B:558:LEU:H	2.19	0.50
1:D:597:LYS:O	1:D:598:GLU:C	2.54	0.50
1:B:542:LEU:HD23	1:B:581:LEU:HD21	1.94	0.50
1:B:570:ILE:O	1:B:574:CYS:HB2	2.12	0.50
1:C:553:VAL:HG21	1:C:570:ILE:CD1	2.42	0.50
1:D:605:PRO:O	1:D:608:THR:N	2.45	0.50
1:A:602:VAL:HG21	1:B:573:LYS:HD2	1.94	0.49
1:C:621:MSE:HE2	1:D:557:LYS:HD2	1.94	0.49
1:C:577:ILE:HG13	1:D:595:GLN:NE2	2.26	0.49
1:A:543:GLU:HB2	1:A:581:LEU:CD1	2.43	0.49
1:D:563:ASN:O	1:D:566:ASP:HB2	2.12	0.49
1:C:599:LEU:CD1	1:D:573:LYS:HG3	2.43	0.49
1:D:588:GLU:HB3	1:D:592:PHE:CE2	2.48	0.49
1:A:606:ILE:CG2	1:B:561:LYS:NZ	2.75	0.49
1:D:559:GLN:HG3	1:D:560:GLY:N	2.27	0.49
1:B:565:GLU:C	1:B:567:LYS:N	2.60	0.48
1:C:535:VAL:N	1:C:536:PRO:HD2	2.27	0.48
1:A:552:THR:O	1:A:554:GLU:N	2.46	0.48
1:B:553:VAL:O	1:B:553:VAL:HG22	2.12	0.48
1:C:575:ASN:O	1:C:576:GLU:C	2.55	0.48
1:B:543:GLU:O	1:B:544:SER:C	2.56	0.48
1:B:579:SER:O	1:B:580:TRP:C	2.56	0.48
1:C:545:TYR:CE1	1:D:599:LEU:HG	2.49	0.48
1:B:551:ALA:C	1:B:553:VAL:H	2.22	0.48
1:C:589:LYS:O	1:C:593:GLU:HG3	2.13	0.48
1:D:589:LYS:O	1:D:590:GLU:C	2.55	0.48
1:A:600:GLU:C	1:A:602:VAL:N	2.71	0.47
1:B:565:GLU:O	1:B:568:GLN:N	2.47	0.47
1:B:615:GLY:HA3	1:B:618:PRO:CG	2.44	0.47
1:C:539:SER:O	1:C:581:LEU:HD11	2.14	0.47
1:C:606:ILE:HD12	1:D:566:ASP:OD1	2.14	0.47
1:D:577:ILE:O	1:D:580:TRP:N	2.46	0.47
1:A:542:LEU:HA	1:B:596:GLN:OE1	2.14	0.47
1:B:549:MSE:CA	1:B:552:THR:HG22	2.45	0.47
1:D:588:GLU:HA	1:D:588:GLU:OE1	2.15	0.47
1:A:542:LEU:HD13	1:B:596:GLN:HB2	1.97	0.47
1:D:548:ASN:O	1:D:549:MSE:C	2.58	0.47
1:B:562:ILE:O	1:B:562:ILE:HG22	2.15	0.47
1:B:602:VAL:O	1:B:602:VAL:CG1	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:MSE:HG2	1:B:558:LEU:HD12	1.97	0.46
1:B:589:LYS:O	1:B:592:PHE:HB2	2.15	0.46
1:D:542:LEU:HD23	1:D:581:LEU:HD11	1.97	0.46
1:B:549:MSE:HA	1:B:552:THR:CG2	2.43	0.46
1:A:563:ASN:HB3	1:A:566:ASP:HB2	1.98	0.46
1:A:580:TRP:CD2	1:A:580:TRP:O	2.68	0.46
1:C:535:VAL:H	1:C:536:PRO:HD2	1.80	0.46
1:A:600:GLU:HB2	1:A:604:ASN:ND2	2.30	0.46
1:A:602:VAL:O	1:A:606:ILE:HD13	2.16	0.46
1:A:603:CYS:SG	1:B:549:MSE:HG2	2.56	0.46
1:B:570:ILE:N	1:B:570:ILE:CD1	2.79	0.46
1:C:595:GLN:HA	1:C:595:GLN:OE1	2.15	0.46
1:D:549:MSE:HA	1:D:549:MSE:CE	2.41	0.46
1:D:580:TRP:CE3	1:D:581:LEU:HA	2.51	0.45
1:B:542:LEU:O	1:B:543:GLU:C	2.60	0.45
1:D:566:ASP:O	1:D:569:LYS:N	2.50	0.45
1:D:577:ILE:O	1:D:580:TRP:HB3	2.17	0.45
1:A:549:MSE:O	1:A:552:THR:N	2.46	0.45
1:B:554:GLU:O	1:B:555:ASP:C	2.59	0.45
1:A:568:GLN:O	1:A:569:LYS:C	2.60	0.45
1:C:573:LYS:O	1:C:576:GLU:HB3	2.17	0.45
1:B:561:LYS:HG2	1:B:567:LYS:HB2	1.98	0.44
1:D:550:LYS:O	1:D:553:VAL:HG22	2.18	0.44
1:A:585:GLN:O	1:A:588:GLU:HB2	2.17	0.44
1:A:606:ILE:O	1:A:609:LYS:HB3	2.16	0.44
1:D:565:GLU:O	1:D:569:LYS:HG3	2.17	0.44
1:A:571:LEU:O	1:A:572:ASP:C	2.60	0.44
1:A:577:ILE:O	1:A:578:ILE:C	2.61	0.44
1:C:617:MSE:N	1:C:618:PRO:CD	2.81	0.44
1:C:570:ILE:HG22	1:C:571:LEU:N	2.33	0.44
1:D:603:CYS:O	1:D:607:ILE:HG12	2.17	0.44
1:A:540:HIS:O	1:A:541:MSE:C	2.60	0.44
1:B:611:TYR:O	1:B:612:GLN:HG3	2.17	0.44
1:C:573:LYS:HD2	1:C:576:GLU:OE1	2.18	0.44
1:A:597:LYS:C	1:A:599:LEU:N	2.76	0.44
1:D:558:LEU:O	1:D:562:ILE:HG22	2.16	0.44
1:D:560:GLY:C	1:D:562:ILE:N	2.76	0.44
1:D:562:ILE:O	1:D:562:ILE:HG23	2.17	0.43
1:A:542:LEU:CD1	1:B:596:GLN:HA	2.49	0.43
1:B:617:MSE:N	1:B:618:PRO:CD	2.62	0.43
1:C:621:MSE:SE	1:D:552:THR:HG23	2.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:HIS:O	1:B:543:GLU:N	2.51	0.43
1:C:552:THR:C	1:C:554:GLU:N	2.73	0.43
1:A:542:LEU:HD13	1:B:596:GLN:CA	2.49	0.43
1:A:552:THR:C	1:A:554:GLU:N	2.77	0.43
1:A:599:LEU:HD21	1:B:574:CYS:HA	2.00	0.43
1:C:571:LEU:O	1:C:572:ASP:C	2.62	0.43
1:B:596:GLN:O	1:B:600:GLU:HG3	2.19	0.43
1:A:541:MSE:O	1:A:542:LEU:C	2.62	0.43
1:B:615:GLY:HA3	1:B:618:PRO:HG2	2.00	0.43
1:D:591:GLU:O	1:D:592:PHE:C	2.61	0.43
1:A:610:LEU:HD13	1:B:561:LYS:HE2	2.02	0.42
1:D:568:GLN:O	1:D:569:LYS:C	2.61	0.42
1:A:558:LEU:O	1:A:559:GLN:C	2.62	0.42
1:A:575:ASN:HA	1:A:578:ILE:HG12	2.00	0.42
1:B:600:GLU:C	1:B:602:VAL:N	2.76	0.42
1:C:600:GLU:HB2	1:C:604:ASN:ND2	2.34	0.42
1:C:557:LYS:C	1:C:558:LEU:HD12	2.45	0.42
1:D:600:GLU:O	1:D:604:ASN:HB2	2.19	0.42
1:B:538:GLY:HA2	1:B:541:MSE:HG3	2.02	0.42
1:B:570:ILE:O	1:B:570:ILE:HG22	2.18	0.42
1:B:579:SER:O	1:B:581:LEU:N	2.53	0.42
1:C:556:GLU:HG3	1:C:557:LYS:N	2.23	0.42
1:C:559:GLN:OE1	1:C:559:GLN:N	2.51	0.42
1:D:577:ILE:O	1:D:578:ILE:C	2.62	0.42
1:A:590:GLU:O	1:A:594:HIS:N	2.53	0.42
1:B:557:LYS:C	1:B:559:GLN:N	2.75	0.42
1:C:582:ASP:HA	1:C:585:GLN:OE1	2.20	0.42
1:B:616:GLY:N	1:B:618:PRO:HD2	2.35	0.42
1:C:535:VAL:N	1:C:536:PRO:CD	2.82	0.42
1:D:580:TRP:CE3	1:D:581:LEU:N	2.88	0.42
1:C:535:VAL:HB	1:C:536:PRO:HD3	2.02	0.42
1:D:545:TYR:O	1:D:546:ALA:C	2.63	0.42
1:C:581:LEU:O	1:C:584:ASN:HB3	2.19	0.42
1:B:577:ILE:O	1:B:578:ILE:C	2.63	0.42
1:A:570:ILE:O	1:A:573:LYS:N	2.53	0.41
1:D:568:GLN:HA	1:D:571:LEU:HB2	2.01	0.41
1:B:561:LYS:O	1:B:563:ASN:N	2.48	0.41
1:D:558:LEU:O	1:D:559:GLN:C	2.63	0.41
1:D:580:TRP:HE3	1:D:581:LEU:HD22	1.84	0.41
1:D:550:LYS:HG3	1:D:571:LEU:HD23	2.01	0.41
1:A:548:ASN:HA	1:A:551:ALA:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:ASN:HA	1:A:551:ALA:CB	2.50	0.41
1:A:558:LEU:HD21	1:B:610:LEU:HD22	2.01	0.41
1:A:561:LYS:HD2	1:B:610:LEU:HD13	2.02	0.41
1:B:577:ILE:N	1:B:577:ILE:HD12	2.36	0.41
1:C:544:SER:HA	1:C:547:PHE:CB	2.50	0.41
1:C:553:VAL:O	1:C:553:VAL:CG1	2.68	0.41
1:C:588:GLU:OE2	1:D:584:ASN:OD1	2.39	0.41
1:C:613:SER:OG	1:C:614:ALA:N	2.52	0.41
1:D:549:MSE:O	1:D:552:THR:HB	2.20	0.41
1:B:579:SER:C	1:B:581:LEU:N	2.79	0.41
1:C:564:ASP:C	1:C:566:ASP:N	2.77	0.41
1:C:573:LYS:HG2	1:D:602:VAL:HG21	2.02	0.41
1:B:561:LYS:HE2	1:B:561:LYS:HB2	1.88	0.41
1:C:549:MSE:HG2	1:D:603:CYS:SG	2.61	0.41
1:D:556:GLU:C	1:D:558:LEU:H	2.29	0.41
1:B:600:GLU:C	1:B:602:VAL:H	2.29	0.40
1:D:600:GLU:O	1:D:601:LYS:C	2.64	0.40
1:A:542:LEU:HD13	1:B:596:GLN:HA	2.02	0.40
1:B:550:LYS:O	1:B:553:VAL:HG12	2.21	0.40
1:B:581:LEU:HD23	1:B:581:LEU:HA	1.92	0.40
1:C:573:LYS:HD2	1:C:573:LYS:HA	1.85	0.40
1:A:558:LEU:CD2	1:A:562:ILE:HB	2.36	0.40
1:A:562:ILE:O	1:A:562:ILE:HG23	2.20	0.40
1:D:596:GLN:O	1:D:600:GLU:HG3	2.21	0.40

All (1) 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:D:554:GLU:OE2	1:D:554:GLU:OE2[7_556]	1.50	0.70

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	82/113 (73%)	54 (66%)	17 (21%)	11 (13%)	0	3
1	B	80/113 (71%)	49 (61%)	23 (29%)	8 (10%)	0	6
1	C	86/113 (76%)	61 (71%)	20 (23%)	5 (6%)	1	13
1	D	76/113 (67%)	51 (67%)	20 (26%)	5 (7%)	1	11
All	All	324/452 (72%)	215 (66%)	80 (25%)	29 (9%)	0	7

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	618	PRO
1	B	559	GLN
1	B	563	ASN
1	B	617	MSE
1	D	539	SER
1	D	557	LYS
1	A	553	VAL
1	A	571	LEU
1	A	616	GLY
1	B	555	ASP
1	B	566	ASP
1	C	598	GLU
1	A	568	GLN
1	A	569	LYS
1	A	598	GLU
1	C	597	LYS
1	D	561	LYS
1	A	572	ASP
1	A	617	MSE
1	B	562	ILE
1	B	580	TRP
1	D	590	GLU
1	A	609	LYS
1	B	564	ASP
1	C	571	LEU
1	C	553	VAL
1	C	582	ASP
1	A	570	ILE
1	D	577	ILE

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	74/89 (83%)	66 (89%)	8 (11%)	6	27
1	B	74/89 (83%)	68 (92%)	6 (8%)	11	36
1	C	78/89 (88%)	69 (88%)	9 (12%)	5	25
1	D	72/89 (81%)	69 (96%)	3 (4%)	26	53
All	All	298/356 (84%)	272 (91%)	26 (9%)	9	34

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	561	LYS
1	A	568	GLN
1	A	584	ASN
1	A	586	THR
1	A	601	LYS
1	A	610	LEU
1	A	611	TYR
1	A	618	PRO
1	B	563	ASN
1	B	564	ASP
1	B	570	ILE
1	B	573	LYS
1	B	574	CYS
1	B	578	ILE
1	C	570	ILE
1	C	581	LEU
1	C	582	ASP
1	C	586	THR
1	C	590	GLU
1	C	598	GLU
1	C	602	VAL
1	C	607	ILE
1	C	610	LEU
1	D	568	GLN

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Mol	Chain	Res	Type
1	D	603	CYS
1	D	604	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	594	HIS
1	A	595	GLN
1	A	604	ASN
1	B	559	GLN
1	B	585	GLN
1	B	595	GLN
1	B	604	ASN
1	B	612	GLN
1	C	548	ASN
1	C	568	GLN
1	C	596	GLN
1	C	604	ASN
1	C	612	GLN
1	D	563	ASN
1	D	584	ASN
1	D	595	GLN
1	D	604	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	81/113 (71%)	0.79	5 (6%) 26 17	44, 44, 44, 44	0
1	B	79/113 (69%)	0.75	8 (10%) 12 9	44, 44, 44, 44	0
1	C	84/113 (74%)	0.64	7 (8%) 17 13	44, 44, 44, 44	0
1	D	76/113 (67%)	0.56	4 (5%) 32 20	44, 44, 44, 44	0
All	All	320/452 (70%)	0.68	24 (7%) 20 14	44, 44, 44, 44	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	618	PRO	5.4
1	A	616	GLY	5.4
1	A	615	GLY	4.6
1	C	560	GLY	4.2
1	B	614	ALA	4.0
1	C	555	ASP	3.7
1	A	618	PRO	3.6
1	B	561	LYS	3.2
1	A	556	GLU	2.9
1	A	614	ALA	2.9
1	B	563	ASN	2.8
1	C	558	LEU	2.8
1	B	539	SER	2.7
1	D	540	HIS	2.6
1	D	614	ALA	2.5
1	C	618	PRO	2.5
1	D	559	GLN	2.4
1	C	559	GLN	2.2
1	C	602	VAL	2.2
1	B	564	ASP	2.1
1	D	613	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	566	ASP	2.1
1	B	615	GLY	2.1
1	C	543	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NA	D	702	1/1	0.83	0.08	25,25,25,25	0
2	NA	B	701	1/1	0.87	0.14	34,34,34,34	1
2	NA	D	703	1/1	0.94	0.07	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.