



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:39 AM UTC

PDB ID : 1Q8A / pdb_00001q8a
Title : Cobalamin-dependent methionine synthase (1-566) from *Thermotoga maritima* (Cd²⁺:L-Hcy complex, Se-Met)
Authors : Evans, J.C.; Huddler, D.P.; Hilgers, M.T.; Romanchuk, G.; Matthews, R.G.; Ludwig, M.L.
Deposited on : 2003-08-20
Resolution : 1.70 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

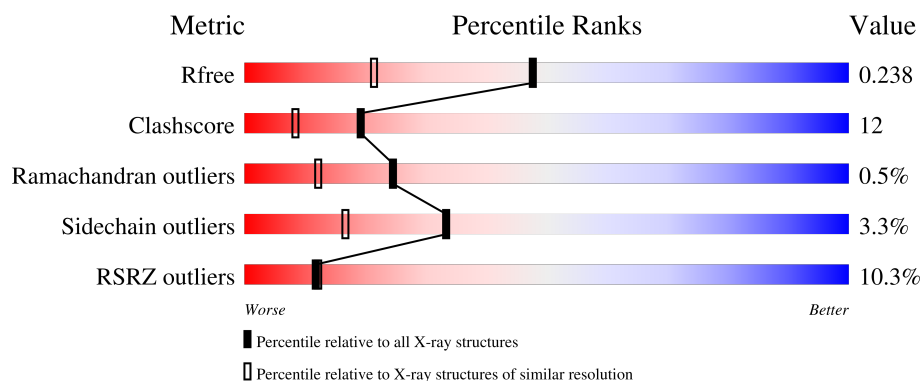
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	566	8% 74% 22% ..
1	B	566	11% 74% 20% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9007 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 5-methyltetrahydrofolate S-homocysteine methyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	559	Total	C	N	O	S	Se	0	0	0
			4423	2839	738	833	3	10			
1	B	547	Total	C	N	O	S	Se	0	0	0
			4333	2784	722	814	3	10			

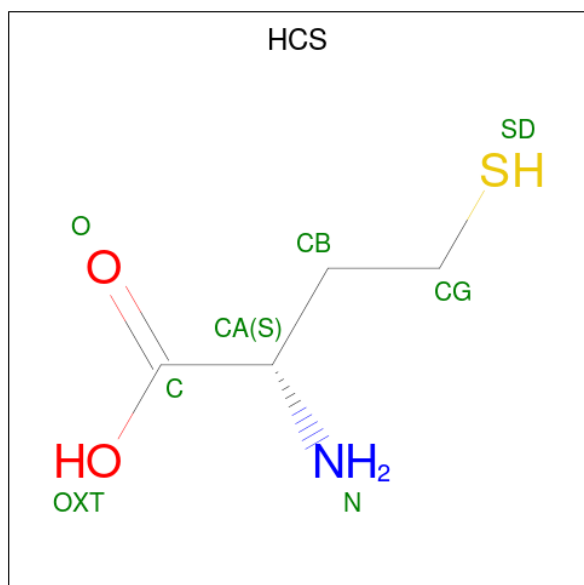
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q9WYA5
A	27	MSE	MET	modified residue	UNP Q9WYA5
A	71	MSE	MET	modified residue	UNP Q9WYA5
A	135	MSE	MET	modified residue	UNP Q9WYA5
A	174	MSE	MET	modified residue	UNP Q9WYA5
A	334	MSE	MET	modified residue	UNP Q9WYA5
A	422	MSE	MET	modified residue	UNP Q9WYA5
A	439	MSE	MET	modified residue	UNP Q9WYA5
A	537	MSE	MET	modified residue	UNP Q9WYA5
A	545	MSE	MET	modified residue	UNP Q9WYA5
B	1	MSE	MET	modified residue	UNP Q9WYA5
B	27	MSE	MET	modified residue	UNP Q9WYA5
B	71	MSE	MET	modified residue	UNP Q9WYA5
B	135	MSE	MET	modified residue	UNP Q9WYA5
B	174	MSE	MET	modified residue	UNP Q9WYA5
B	334	MSE	MET	modified residue	UNP Q9WYA5
B	422	MSE	MET	modified residue	UNP Q9WYA5
B	439	MSE	MET	modified residue	UNP Q9WYA5
B	537	MSE	MET	modified residue	UNP Q9WYA5
B	545	MSE	MET	modified residue	UNP Q9WYA5

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cd 1 1	0	0
2	B	1	Total Cd 1 1	0	0

- Molecule 3 is 2-AMINO-4-MERCAPTO-BUTYRIC ACID (CCD ID: HCS) (formula: $C_4H_9NO_2S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 8 4 1 2 1	0	0
3	B	1	Total C N O S 8 4 1 2 1	0	0

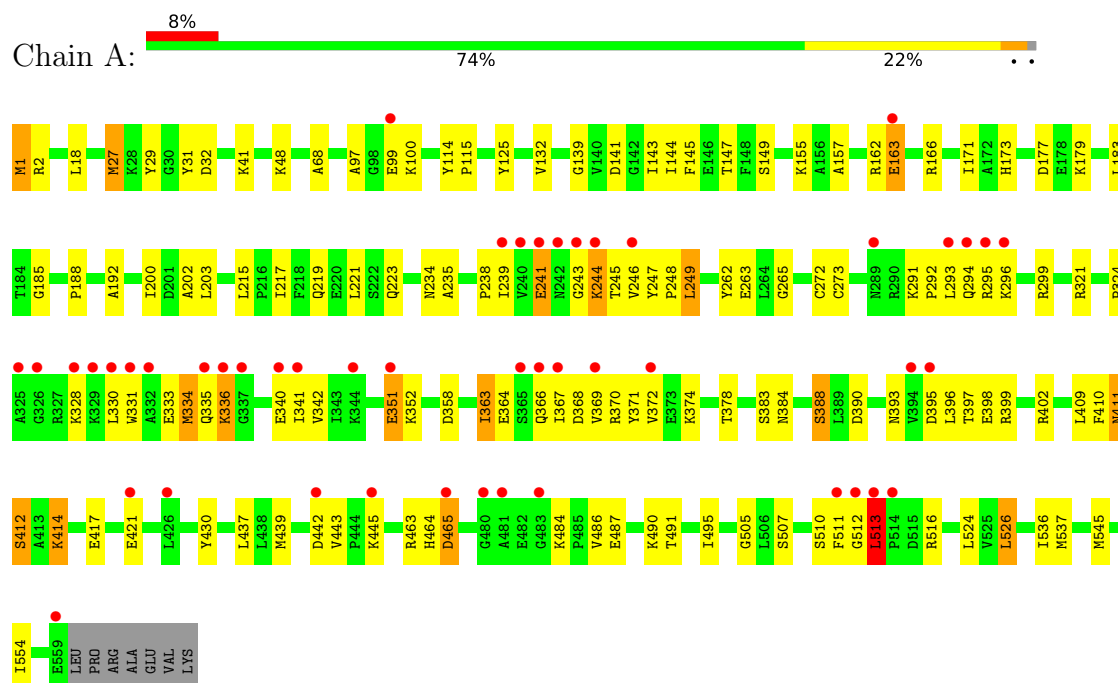
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	135	Total O 135 135	0	0
4	B	98	Total O 98 98	0	0

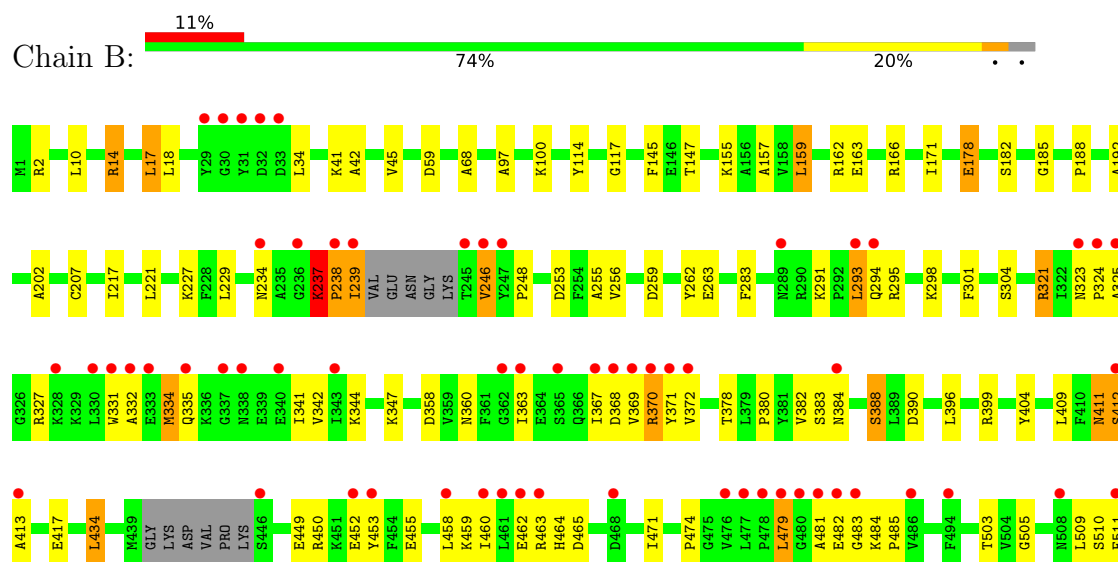
3 Residue-property plots [i](#)

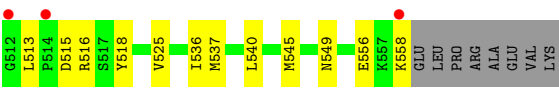
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 5-methyltetrahydrofolate S-homocysteine methyltransferase



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.12Å 86.19Å 126.08Å 90.00° 99.99° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 20.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.70) 92.0 (20.00-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 1.65Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.242 0.210 , 0.238	Depositor DCC
R_{free} test set	13568 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 50.2	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	0.95	EDS
Total number of atoms	9007	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.78	1/4496 (0.0%)	1.12	21/6056 (0.3%)
1	B	0.64	0/4403	1.07	29/5929 (0.5%)
All	All	0.71	1/8899 (0.0%)	1.10	50/11985 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	334	MSE	SE-CE	-10.61	1.63	1.95

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	SER	N-CA-C	11.56	135.42	110.80
1	A	321	ARG	N-CA-C	10.84	124.17	111.71
1	B	321	ARG	N-CA-C	10.54	125.24	112.38
1	A	378	THR	N-CA-C	9.64	123.16	111.40
1	B	412	SER	N-CA-C	8.56	129.03	110.80
1	A	411	ASN	CA-C-N	8.13	137.07	121.54
1	A	411	ASN	C-N-CA	8.13	137.07	121.54
1	A	244	LYS	N-CA-C	7.24	118.72	108.74
1	A	248	PRO	N-CA-C	7.06	123.99	114.18
1	B	68	ALA	N-CA-C	6.89	119.96	109.62
1	B	97	ALA	N-CA-C	6.61	119.49	111.82
1	B	378	THR	N-CA-C	6.57	119.42	111.40
1	A	245	THR	N-CA-C	6.49	120.03	110.30
1	B	298	LYS	N-CA-C	-6.46	101.39	110.50
1	B	536	ILE	N-CA-C	-6.43	98.39	108.23
1	A	536	ILE	N-CA-C	-6.42	98.41	108.23
1	A	234	ASN	N-CA-C	-6.42	102.51	110.41
1	B	248	PRO	N-CA-C	6.41	121.99	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	GLY	N-CA-C	6.33	124.88	115.64
1	B	117	GLY	N-CA-C	-6.14	102.66	111.20
1	A	241	GLU	CB-CA-C	-6.13	107.52	116.53
1	B	388	SER	N-CA-C	-6.10	97.78	108.20
1	B	237	LYS	CA-C-N	6.09	127.45	119.84
1	B	237	LYS	C-N-CA	6.09	127.45	119.84
1	A	364	GLU	N-CA-C	6.08	119.53	111.75
1	A	409	LEU	N-CA-C	-6.06	99.32	109.07
1	B	505	GLY	N-CA-C	-6.06	98.83	113.18
1	B	304	SER	N-CA-C	6.04	117.96	108.96
1	B	182	SER	N-CA-C	-5.94	102.87	110.53
1	B	14	ARG	N-CA-C	5.93	118.13	108.76
1	A	411	ASN	O-C-N	5.92	130.19	122.68
1	A	505	GLY	N-CA-C	-5.86	99.30	113.18
1	B	34	LEU	N-CA-C	-5.84	102.41	109.83
1	A	185	GLY	N-CA-C	5.83	124.15	115.64
1	A	414	LYS	N-CA-C	-5.69	103.19	110.53
1	B	41	LYS	N-CA-C	5.68	119.39	112.23
1	B	409	LEU	N-CA-C	-5.62	100.02	109.07
1	B	434	LEU	N-CA-C	5.61	118.24	108.76
1	B	411	ASN	CA-C-N	5.41	131.88	121.54
1	B	411	ASN	C-N-CA	5.41	131.88	121.54
1	A	388	SER	N-CA-C	-5.38	98.46	107.99
1	B	334	MSE	N-CA-C	-5.37	106.56	113.01
1	B	411	ASN	N-CA-C	5.35	116.96	108.67
1	A	97	ALA	N-CA-C	5.35	118.03	111.82
1	A	68	ALA	N-CA-C	5.32	118.07	110.68
1	B	59	ASP	N-CA-C	-5.21	107.09	113.50
1	B	291	LYS	N-CA-C	-5.20	103.22	109.72
1	B	255	ALA	N-CA-C	5.16	117.65	111.71
1	B	114	TYR	N-CA-C	-5.08	103.38	109.83
1	A	513	LEU	N-CA-C	5.01	114.06	108.25

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	4423	0	4510	122	0
1	B	4333	0	4416	88	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	8	0	7	0	0
3	B	8	0	7	0	0
4	A	135	0	0	5	0
4	B	98	0	0	0	0
All	All	9007	0	8940	207	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 (207) 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:B:372:VAL:HG21	1:B:396:LEU:HD11	1.20	1.15
1:A:241:GLU:HG2	1:A:246:VAL:HG11	1.40	1.02
1:A:331:TRP:CH2	1:A:367:ILE:HD11	2.11	0.86
1:A:27:MSE:HE3	1:A:32:ASP:N	1.94	0.81
1:A:241:GLU:HG2	1:A:246:VAL:CG1	2.10	0.79
1:A:330:LEU:O	1:A:334:MSE:HG3	1.83	0.79
1:B:321:ARG:NE	1:B:540:LEU:HD22	1.97	0.78
1:B:449:GLU:O	1:B:452:GLU:HG2	1.83	0.77
1:A:328:LYS:N	1:A:328:LYS:HE2	1.99	0.77
1:A:369:VAL:CG2	1:A:399:ARG:HD3	2.14	0.77
1:B:458:LEU:O	1:B:462:GLU:HG2	1.84	0.76
1:A:241:GLU:CG	1:A:246:VAL:HG11	2.16	0.75
1:A:331:TRP:HH2	1:A:367:ILE:HD11	1.50	0.75
1:A:484:LYS:HG2	1:A:487:GLU:HG2	1.69	0.74
1:A:369:VAL:HG21	1:A:399:ARG:HD3	1.67	0.74
1:A:486:VAL:HG12	1:A:490:LYS:HE3	1.71	0.71
1:A:484:LYS:HD2	1:B:556:GLU:OE2	1.90	0.71
1:B:239:ILE:C	1:B:239:ILE:HD13	2.15	0.71
1:A:336:LYS:HB3	1:A:336:LYS:NZ	2.06	0.71
1:A:363:ILE:H	1:A:363:ILE:HD12	1.57	0.70
1:A:333:GLU:OE2	1:A:336:LYS:HE2	1.92	0.70
1:A:367:ILE:HD12	1:A:367:ILE:N	2.06	0.70
1:A:336:LYS:HB3	1:A:336:LYS:HZ3	1.57	0.69
1:A:363:ILE:HD12	1:A:363:ILE:N	2.08	0.69
1:A:340:GLU:HB2	4:A:828:HOH:O	1.93	0.68
1:B:372:VAL:HG21	1:B:396:LEU:CD1	2.13	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:ASP:HA	1:B:411:ASN:HB3	1.73	0.68
1:A:100:LYS:HE3	4:A:836:HOH:O	1.93	0.67
1:B:331:TRP:O	1:B:335:GLN:HG2	1.96	0.65
1:B:324:PRO:HG3	1:B:334:MSE:SE	2.46	0.65
1:A:484:LYS:CG	1:A:487:GLU:HG2	2.27	0.65
1:A:369:VAL:HG21	1:A:399:ARG:CD	2.28	0.64
1:B:227:LYS:O	1:B:295:ARG:NH2	2.29	0.64
1:B:369:VAL:O	1:B:372:VAL:HG22	1.98	0.64
1:B:159:LEU:O	1:B:163:GLU:HG3	1.97	0.64
1:A:1:MSE:SE	1:A:139:GLY:O	2.66	0.64
1:A:192:ALA:HB2	1:A:221:LEU:HD12	1.80	0.64
1:A:510:SER:HA	1:A:513:LEU:HD21	1.78	0.64
1:B:341:ILE:O	1:B:344:LYS:HB3	1.98	0.64
1:B:363:ILE:H	1:B:363:ILE:HD12	1.63	0.63
1:B:259:ASP:O	1:B:263:GLU:HG2	1.98	0.63
1:A:299:ARG:HH21	1:A:299:ARG:HG2	1.63	0.62
1:A:238:PRO:HG3	1:A:247:TYR:HE1	1.65	0.62
1:B:347:LYS:HE3	1:B:382:VAL:HG22	1.82	0.62
1:A:366:GLN:C	1:A:367:ILE:HD12	2.25	0.62
1:B:331:TRP:CH2	1:B:367:ILE:HD11	2.34	0.61
1:A:166:ARG:N	1:A:166:ARG:HD2	2.15	0.61
1:A:114:TYR:CZ	1:A:374:LYS:HE2	2.36	0.60
1:B:479:LEU:C	1:B:481:ALA:H	2.08	0.60
1:A:1:MSE:SE	1:A:1:MSE:N	2.85	0.60
1:A:397:THR:HG23	1:A:410:PHE:CE1	2.37	0.60
1:B:331:TRP:CZ3	1:B:367:ILE:HD11	2.38	0.59
1:B:481:ALA:O	1:B:482:GLU:HB2	2.01	0.59
1:A:513:LEU:HD23	1:A:513:LEU:N	2.18	0.59
1:B:332:ALA:O	1:B:335:GLN:HB2	2.03	0.58
1:B:178:GLU:H	1:B:178:GLU:CD	2.11	0.58
1:A:1:MSE:SE	1:A:1:MSE:H1	2.37	0.58
1:A:238:PRO:HG3	1:A:247:TYR:CE1	2.38	0.58
1:A:200:ILE:HD11	1:A:203:LEU:HD21	1.84	0.58
1:A:414:LYS:NZ	1:A:439:MSE:SE	2.86	0.58
1:B:325:ALA:O	1:B:327:ARG:HG3	2.04	0.57
1:A:328:LYS:HE2	1:A:328:LYS:CA	2.34	0.57
1:A:486:VAL:O	1:A:490:LYS:HG3	2.04	0.57
1:A:200:ILE:CD1	1:A:203:LEU:HD21	2.35	0.56
1:A:239:ILE:HG13	1:A:246:VAL:HG13	1.85	0.56
1:A:484:LYS:HG2	1:A:487:GLU:CG	2.35	0.56
1:B:166:ARG:HH11	1:B:166:ARG:HG3	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:LEU:HD11	1:B:14:ARG:NH1	2.21	0.56
1:A:390:ASP:HA	1:A:411:ASN:HB3	1.89	0.55
1:A:166:ARG:HD3	4:A:767:HOH:O	2.07	0.55
1:B:549:ASN:OD1	1:B:558:LYS:NZ	2.36	0.55
1:A:188:PRO:HG3	1:A:217:ILE:HG23	1.89	0.54
1:B:42:ALA:O	1:B:45:VAL:HG12	2.07	0.54
1:A:331:TRP:CZ3	1:A:367:ILE:HD11	2.41	0.54
1:A:443:VAL:CG2	1:A:445:LYS:HE2	2.38	0.54
1:B:229:LEU:HG	1:B:295:ARG:NH2	2.22	0.54
1:B:367:ILE:HD12	1:B:367:ILE:N	2.22	0.54
1:A:27:MSE:HE3	1:A:31:TYR:C	2.32	0.54
1:A:294:GLN:HA	1:A:294:GLN:OE1	2.06	0.54
1:A:27:MSE:HE3	1:A:32:ASP:HB3	1.90	0.54
1:B:207:CYS:HA	1:B:234:ASN:OD1	2.08	0.54
1:B:460:ILE:HA	1:B:463:ARG:HH11	1.73	0.53
1:B:510:SER:OG	1:B:516:ARG:HB2	2.09	0.53
1:A:99:GLU:OE1	1:A:99:GLU:N	2.32	0.53
1:B:321:ARG:CZ	1:B:540:LEU:HD22	2.39	0.53
1:A:239:ILE:O	1:A:246:VAL:HG12	2.09	0.52
1:A:331:TRP:CZ2	1:A:363:ILE:HD13	2.44	0.52
1:A:336:LYS:NZ	1:A:336:LYS:CB	2.68	0.52
1:A:27:MSE:HE3	1:A:32:ASP:CB	2.40	0.52
1:B:358:ASP:HA	1:B:388:SER:HB3	1.92	0.52
1:A:200:ILE:CD1	1:A:203:LEU:CD2	2.89	0.51
1:A:398:GLU:O	1:A:402:ARG:HG2	2.11	0.51
1:B:239:ILE:C	1:B:239:ILE:CD1	2.83	0.51
1:A:177:ASP:OD1	1:A:179:LYS:HG3	2.10	0.51
1:B:341:ILE:HG23	1:B:342:VAL:N	2.24	0.51
1:B:515:ASP:HB3	1:B:518:TYR:HD1	1.76	0.51
1:B:479:LEU:HD21	1:B:513:LEU:CD1	2.40	0.51
1:B:238:PRO:O	1:B:246:VAL:O	2.29	0.50
1:A:155:LYS:HE2	1:A:402:ARG:O	2.11	0.50
1:B:479:LEU:HD23	1:B:479:LEU:N	2.27	0.50
1:B:331:TRP:CZ2	1:B:363:ILE:HD13	2.47	0.49
1:A:27:MSE:SE	1:A:32:ASP:HB3	2.61	0.49
1:A:363:ILE:H	1:A:363:ILE:CD1	2.24	0.49
1:A:486:VAL:CG1	1:A:490:LYS:HE3	2.39	0.49
1:B:166:ARG:HG3	1:B:166:ARG:NH1	2.27	0.49
1:B:537:MSE:HE2	1:B:545:MSE:SE	2.62	0.49
1:A:299:ARG:HG2	1:A:299:ARG:NH2	2.26	0.49
1:A:351:GLU:OE2	1:A:352:LYS:HD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:PRO:HA	1:A:330:LEU:HD23	1.94	0.49
1:A:1:MSE:HG2	1:A:141:ASP:OD2	2.12	0.49
1:B:479:LEU:HD22	1:B:509:LEU:O	2.12	0.49
1:B:145:PHE:CE2	1:B:157:ALA:HB1	2.48	0.49
1:B:479:LEU:H	1:B:479:LEU:CD2	2.25	0.49
1:A:235:ALA:C	1:A:249:LEU:HB2	2.39	0.48
1:A:328:LYS:HE2	1:A:328:LYS:HA	1.95	0.48
1:B:363:ILE:HD12	1:B:363:ILE:N	2.29	0.48
1:A:188:PRO:CG	1:A:217:ILE:HG23	2.43	0.48
1:B:450:ARG:NH2	1:B:474:PRO:O	2.47	0.48
1:A:383:SER:O	1:A:384:ASN:HB2	2.14	0.48
1:B:207:CYS:SG	1:B:234:ASN:OD1	2.72	0.48
1:B:479:LEU:HD21	1:B:513:LEU:HD11	1.96	0.48
1:A:437:LEU:HG	1:A:439:MSE:HG2	1.96	0.47
1:B:253:ASP:O	1:B:256:VAL:HG22	2.14	0.47
1:B:332:ALA:HA	1:B:335:GLN:HG3	1.96	0.47
1:B:474:PRO:HD2	1:B:503:THR:O	2.14	0.47
1:B:301:PHE:CE1	1:B:471:ILE:HD11	2.49	0.47
1:A:219:GLN:O	1:A:223:GLN:HG3	2.14	0.47
1:A:507:SER:HB3	1:A:511:PHE:CE1	2.50	0.47
1:A:29:TYR:HE2	1:A:48:LYS:HE3	1.79	0.47
1:A:443:VAL:HG21	1:A:445:LYS:HE2	1.96	0.47
1:B:2:ARG:N	1:B:2:ARG:HD3	2.30	0.47
1:B:155:LYS:HE3	1:B:404:TYR:O	2.14	0.47
1:B:301:PHE:CZ	1:B:471:ILE:HG13	2.50	0.47
1:B:479:LEU:CD2	1:B:509:LEU:O	2.63	0.47
1:A:333:GLU:HA	1:A:336:LYS:HG2	1.96	0.47
1:B:178:GLU:CD	1:B:178:GLU:N	2.72	0.47
1:A:27:MSE:HA	1:A:27:MSE:HE2	1.97	0.47
1:A:265:GLY:HA3	1:A:295:ARG:HD3	1.96	0.47
1:B:188:PRO:HG2	1:B:217:ILE:HG23	1.97	0.47
1:A:239:ILE:CG1	1:A:246:VAL:HG13	2.45	0.47
1:A:491:THR:O	1:A:495:ILE:HG12	2.15	0.46
1:A:372:VAL:HG21	1:A:396:LEU:HD21	1.97	0.46
1:A:125:TYR:OH	1:A:163:GLU:HG3	2.15	0.46
1:A:341:ILE:HG23	1:A:342:VAL:N	2.30	0.46
1:B:188:PRO:CG	1:B:217:ILE:HG23	2.45	0.46
1:A:145:PHE:CE2	1:A:157:ALA:HB1	2.51	0.46
1:B:368:ASP:OD1	1:B:370:ARG:HG2	2.16	0.46
1:A:464:HIS:O	1:A:465:ASP:C	2.59	0.45
1:A:244:LYS:HA	1:A:244:LYS:HD3	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:ILE:HG23	1:B:485:PRO:HB2	1.98	0.45
1:A:27:MSE:HE3	1:A:32:ASP:CA	2.46	0.45
1:B:479:LEU:C	1:B:481:ALA:N	2.74	0.45
1:A:291:LYS:HG3	1:A:292:PRO:HD2	1.97	0.45
1:A:166:ARG:CD	4:A:767:HOH:O	2.65	0.45
1:A:367:ILE:N	1:A:367:ILE:CD1	2.77	0.45
1:B:171:ILE:HG12	1:B:202:ALA:HB3	1.98	0.45
1:A:41:LYS:HE3	1:A:41:LYS:HB2	1.84	0.44
1:B:262:TYR:CZ	1:B:293:LEU:HD13	2.52	0.44
1:B:417:GLU:HG2	1:B:460:ILE:CD1	2.47	0.44
1:A:537:MSE:HE2	1:A:545:MSE:SE	2.67	0.44
1:B:464:HIS:O	1:B:465:ASP:C	2.60	0.44
1:A:2:ARG:NH2	1:A:99:GLU:O	2.50	0.44
1:A:398:GLU:HG3	1:A:430:TYR:CE2	2.53	0.44
1:A:393:ASN:OD1	1:A:395:ASP:HB3	2.18	0.44
1:B:239:ILE:O	1:B:239:ILE:HG23	2.18	0.44
1:A:27:MSE:CE	1:A:31:TYR:C	2.90	0.43
1:A:369:VAL:HG13	1:A:370:ARG:N	2.33	0.43
1:B:479:LEU:N	1:B:479:LEU:CD2	2.80	0.43
1:A:331:TRP:O	1:A:335:GLN:HG3	2.18	0.43
1:B:192:ALA:HB2	1:B:221:LEU:HD12	1.99	0.43
1:A:27:MSE:HE2	1:A:31:TYR:N	2.34	0.43
1:A:239:ILE:HG13	1:A:246:VAL:CG1	2.48	0.43
1:A:368:ASP:O	1:A:371:TYR:N	2.50	0.43
1:B:479:LEU:HA	1:B:483:GLY:HA3	2.00	0.43
1:B:162:ARG:HA	1:B:162:ARG:HD3	1.69	0.42
1:B:484:LYS:N	1:B:485:PRO:HD3	2.34	0.42
1:A:144:ILE:HD11	1:A:173:HIS:CE1	2.55	0.42
1:A:417:GLU:OE1	1:A:463:ARG:NH1	2.48	0.42
1:A:262:TYR:CZ	1:A:293:LEU:HD13	2.55	0.42
1:A:510:SER:OG	1:A:516:ARG:HB2	2.20	0.42
1:B:323:ASN:HA	1:B:324:PRO:HD3	1.85	0.42
1:B:360:ASN:HB2	1:B:390:ASP:HB3	2.02	0.42
1:A:263:GLU:HA	1:A:293:LEU:CD2	2.50	0.42
1:A:272:CYS:O	1:A:273:CYS:C	2.62	0.42
1:A:507:SER:HB3	1:A:511:PHE:CZ	2.55	0.42
1:A:526:LEU:HD13	1:B:525:VAL:HG12	2.02	0.42
4:A:826:HOH:O	1:B:485:PRO:HD2	2.18	0.42
1:A:243:GLY:O	1:A:244:LYS:HG2	2.20	0.41
1:A:368:ASP:O	1:A:371:TYR:HB3	2.21	0.41
1:A:149:SER:HB3	1:A:183:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ASP:HA	1:A:388:SER:HB3	2.03	0.41
1:A:516:ARG:HG2	1:A:516:ARG:HH11	1.86	0.41
1:A:132:VAL:HG13	1:A:143:ILE:CD1	2.51	0.41
1:B:237:LYS:HG3	1:B:238:PRO:HD2	2.02	0.41
1:B:370:ARG:HG2	1:B:370:ARG:H	1.59	0.41
1:B:383:SER:O	1:B:384:ASN:HB2	2.21	0.41
1:B:413:ALA:HB2	1:B:434:LEU:HD11	2.02	0.41
1:A:162:ARG:HD3	1:A:162:ARG:HA	1.79	0.41
1:B:368:ASP:O	1:B:371:TYR:N	2.46	0.40
1:B:459:LYS:O	1:B:463:ARG:HG3	2.21	0.40
1:A:417:GLU:O	1:A:421:GLU:HG3	2.21	0.40
1:B:17:LEU:HD11	1:B:283:PHE:HB3	2.04	0.40
1:B:511:PHE:CD1	1:B:511:PHE:C	3.00	0.40
1:A:171:ILE:HG12	1:A:202:ALA:HB3	2.03	0.40
1:A:114:TYR:CE2	1:A:374:LYS:HE2	2.56	0.40
1:A:166:ARG:HD2	1:A:166:ARG:H	1.83	0.40
1:B:380:PRO:O	1:B:384:ASN:HA	2.21	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	557/566 (98%)	531 (95%)	23 (4%)	3 (0%)	24	12
1	B	541/566 (96%)	515 (95%)	24 (4%)	2 (0%)	30	16
All	All	1098/1132 (97%)	1046 (95%)	47 (4%)	5 (0%)	24	12

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	412	SER

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Mol	Chain	Res	Type
1	A	512	GLY
1	B	238	PRO
1	B	412	SER
1	A	465	ASP

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	488/484 (101%)	472 (97%)	16 (3%)	33	17
1	B	478/484 (99%)	462 (97%)	16 (3%)	33	17
All	All	966/968 (100%)	934 (97%)	32 (3%)	33	17

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	18	LEU
1	A	27	MSE
1	A	115	PRO
1	A	147	THR
1	A	163	GLU
1	A	215	LEU
1	A	249	LEU
1	A	296	LYS
1	A	336	LYS
1	A	351	GLU
1	A	363	ILE
1	A	442	ASP
1	A	513	LEU
1	A	524	LEU
1	A	526	LEU
1	B	17	LEU
1	B	18	LEU
1	B	100	LYS

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Mol	Chain	Res	Type
1	B	147	THR
1	B	159	LEU
1	B	178	GLU
1	B	237	LYS
1	B	239	ILE
1	B	246	VAL
1	B	293	LEU
1	B	294	GLN
1	B	370	ARG
1	B	399	ARG
1	B	453	TYR
1	B	455	GLU
1	B	479	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	GLN
1	A	464	HIS
1	B	76	HIS
1	B	294	GLN

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	HCS	B	702	-	6,7,7	1.30	1 (16%)	5,8,8	0.56	0
3	HCS	A	701	-	6,7,7	1.39	1 (16%)	5,8,8	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HCS	B	702	-	-	0/7/7/7	-
3	HCS	A	701	-	-	0/7/7/7	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	HCS	CB-CG	2.72	1.56	1.52
3	B	702	HCS	CB-CG	2.19	1.55	1.52

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	549/566 (96%)	0.41	48 (8%)	16 17	14, 25, 46, 59	0
1	B	537/566 (94%)	0.69	64 (11%)	9 8	17, 31, 52, 58	0
All	All	1086/1132 (95%)	0.55	112 (10%)	12 12	14, 28, 50, 59	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	511	PHE	8.8
1	B	245	THR	7.5
1	B	239	ILE	6.1
1	A	240	VAL	6.0
1	B	363	ILE	5.8
1	A	243	GLY	5.4
1	A	512	GLY	5.3
1	B	238	PRO	5.0
1	B	446	SER	4.9
1	A	242	ASN	4.9
1	A	513	LEU	4.8
1	B	332	ALA	4.7
1	B	365	SER	4.5
1	B	367	ILE	4.3
1	B	369	VAL	4.2
1	A	293	LEU	3.9
1	A	241	GLU	3.9
1	A	367	ILE	3.8
1	B	372	VAL	3.7
1	B	331	TRP	3.7
1	A	341	ILE	3.7
1	A	480	GLY	3.6
1	B	476	VAL	3.5
1	B	29	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	336	LYS	3.4
1	B	324	PRO	3.3
1	A	337	GLY	3.3
1	B	412	SER	3.2
1	A	331	TRP	3.2
1	B	483	GLY	3.2
1	A	329	LYS	3.1
1	B	330	LEU	3.1
1	A	395	ASP	3.1
1	B	362	GLY	3.1
1	A	559	GLU	3.0
1	B	325	ALA	3.0
1	A	340	GLU	3.0
1	A	365	SER	2.9
1	A	328	LYS	2.9
1	B	481	ALA	2.9
1	A	163	GLU	2.9
1	B	478	PRO	2.9
1	B	234	ASN	2.9
1	A	483	GLY	2.9
1	A	330	LEU	2.9
1	A	99	GLU	2.9
1	A	332	ALA	2.8
1	A	296	LYS	2.8
1	B	384	ASN	2.8
1	A	325	ALA	2.7
1	B	294	GLN	2.7
1	B	462	GLU	2.7
1	A	372	VAL	2.6
1	B	486	VAL	2.6
1	B	511	PHE	2.6
1	A	246	VAL	2.6
1	B	453	TYR	2.6
1	B	337	GLY	2.6
1	A	465	ASP	2.6
1	B	31	TYR	2.6
1	A	244	LYS	2.6
1	A	514	PRO	2.6
1	B	480	GLY	2.5
1	B	479	LEU	2.5
1	A	394	VAL	2.5
1	B	340	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	514	PRO	2.5
1	A	421	GLU	2.5
1	A	369	VAL	2.5
1	B	413	ALA	2.5
1	B	371	TYR	2.5
1	B	370	ARG	2.5
1	B	335	GLN	2.4
1	B	293	LEU	2.4
1	A	326	GLY	2.4
1	B	246	VAL	2.4
1	B	368	ASP	2.4
1	B	338	ASN	2.4
1	B	508	ASN	2.4
1	B	460	ILE	2.4
1	B	512	GLY	2.4
1	A	481	ALA	2.4
1	A	295	ARG	2.3
1	B	32	ASP	2.3
1	B	463	ARG	2.3
1	B	343	ILE	2.3
1	A	335	GLN	2.3
1	B	458	LEU	2.3
1	A	239	ILE	2.3
1	B	477	LEU	2.2
1	A	344	LYS	2.2
1	A	351	GLU	2.2
1	A	442	ASP	2.2
1	B	247	TYR	2.2
1	B	468	ASP	2.1
1	B	289	ASN	2.1
1	B	494	PHE	2.1
1	A	366	GLN	2.1
1	B	333	GLU	2.1
1	B	482	GLU	2.1
1	A	426	LEU	2.1
1	B	461	LEU	2.1
1	B	558	LYS	2.1
1	A	294	GLN	2.1
1	B	236	GLY	2.0
1	A	289	ASN	2.0
1	B	323	ASN	2.0
1	B	452	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	328	LYS	2.0
1	B	30	GLY	2.0
1	B	33	ASP	2.0
1	A	445	LYS	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($\text{\AA}^2$)	Q<0.9
3	HCS	A	701	8/8	0.97	0.07	14,19,23,23	0
3	HCS	B	702	8/8	0.98	0.06	15,21,22,23	0
2	CD	A	601	1/1	0.99	0.04	21,21,21,21	0
2	CD	B	602	1/1	0.99	0.02	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.