



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:56 PM UTC

PDB ID : 4Z42 / pdb_00004z42
Title : Crystal structure of urease from Yersinia enterocolitica
Authors : Studer, G.; Jakob, R.P.; Mahi, M.A.; Wiesand, U.; Schwede, T.; Maier, T.
Deposited on : 2015-04-01
Resolution : 3.01 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:

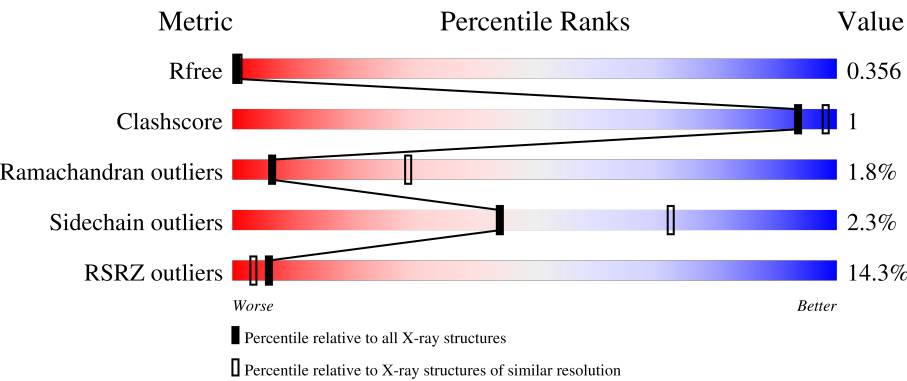
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.01 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	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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	100	9% 98% ..
1	D	100	4% 97% ..
1	G	100	11% 97% ..
1	J	100	7% 98% ..
2	B	164	12% 60% 7% .. 30%

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Mol	Chain	Length	Quality of chain
2	E	164	13%62%7%30%
2	H	164	23%61%5%30%
2	K	164	12%66%30%
3	C	572	19%94%6%
3	F	572	10%94%6%
3	I	572	15%94%6%
3	L	572	12%93%6%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 47288 atoms, of which 23471 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 Urease subunit gamma.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	99	Total	C	H	N	O	S	0	0	0
			1555	480	793	128	149	5			
1	D	99	Total	C	H	N	O	S	0	0	0
			1555	480	793	128	149	5			
1	G	99	Total	C	H	N	O	S	0	0	0
			1555	480	793	128	149	5			
1	J	99	Total	C	H	N	O	S	0	0	0
			1555	480	793	128	149	5			

- Molecule 2 is a protein called Urease subunit beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	114	Total	C	H	N	O	S	0	0	0
			1745	560	859	156	169	1			
2	E	114	Total	C	H	N	O	S	0	0	0
			1745	560	859	156	169	1			
2	H	114	Total	C	H	N	O	S	0	0	0
			1744	560	858	156	169	1			
2	K	114	Total	C	H	N	O	S	0	0	0
			1745	560	859	156	169	1			

- Molecule 3 is a protein called Urease subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	571	Total	C	H	N	O	S	0	0	0
			8493	2671	4216	759	822	25			
3	F	571	Total	C	H	N	O	S	0	0	0
			8493	2671	4216	759	822	25			
3	I	571	Total	C	H	N	O	S	0	0	0
			8493	2671	4216	759	822	25			
3	L	571	Total	C	H	N	O	S	0	0	0
			8493	2671	4216	759	822	25			

- Molecule 4 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total 2	Ni 2	0	0
4	F	2	Total 2	Ni 2	0	0
4	I	2	Total 2	Ni 2	0	0
4	L	2	Total 2	Ni 2	0	0

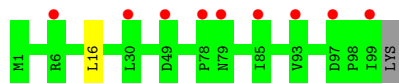
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	8	Total 8	O 8	0	0
5	C	15	Total 15	O 15	0	0
5	D	1	Total 1	O 1	0	0
5	E	8	Total 8	O 8	0	0
5	F	31	Total 31	O 31	0	0
5	I	17	Total 17	O 17	0	0
5	K	4	Total 4	O 4	0	0
5	L	25	Total 25	O 25	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: Urease subunit gamma



- Molecule 1: Urease subunit gamma



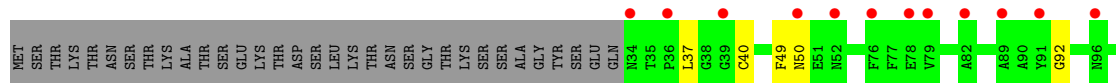
- Molecule 1: Urease subunit gamma

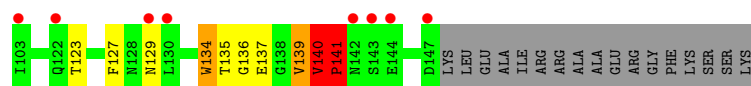


- Molecule 1: Urease subunit gamma

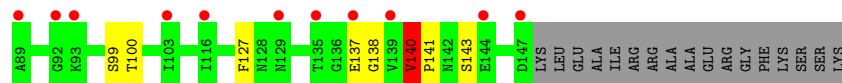
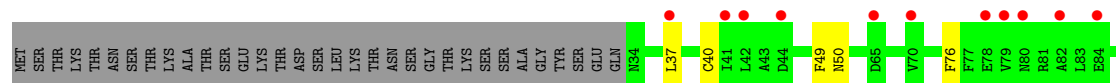


- Molecule 2: Urease subunit beta

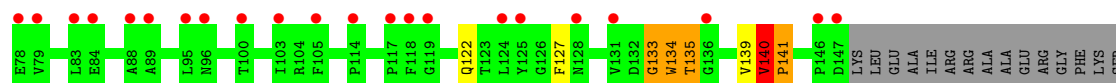
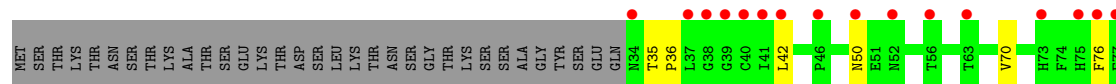




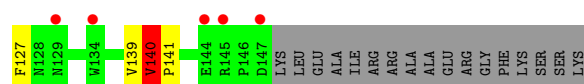
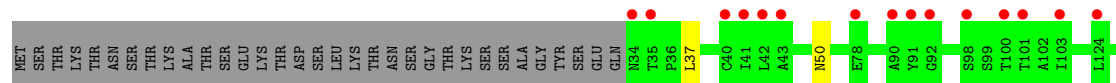
• Molecule 2: Urease subunit beta



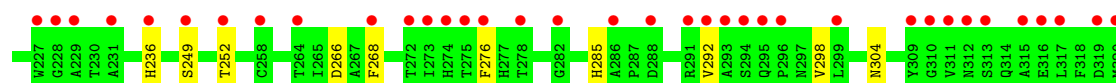
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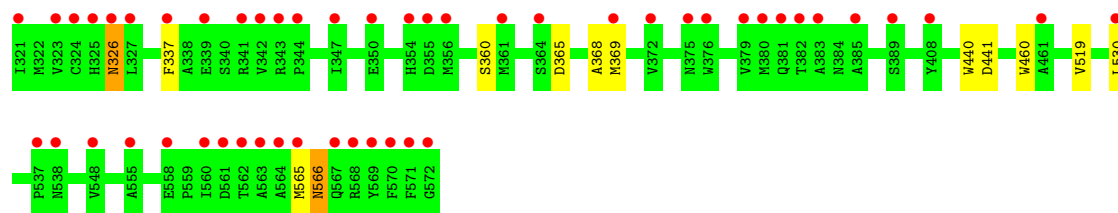


• Molecule 2: Urease subunit beta

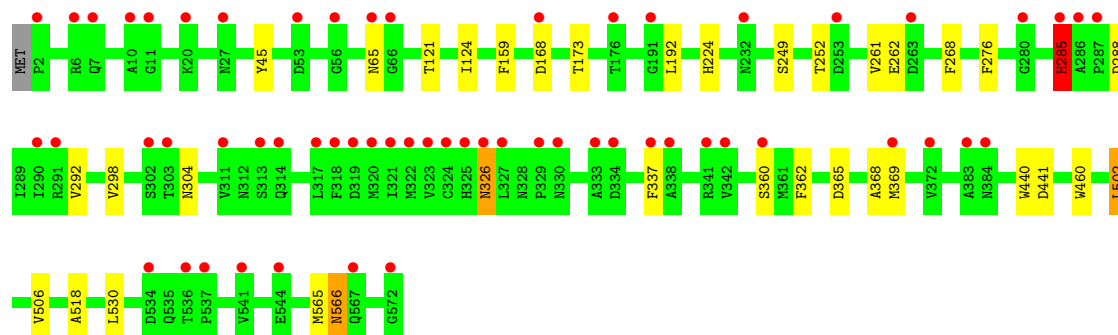


• Molecule 3: Urease subunit alpha

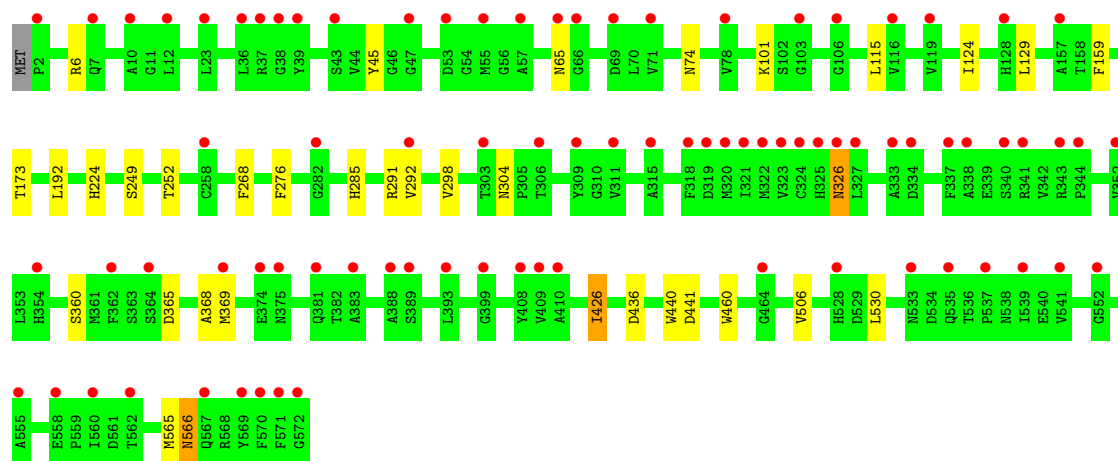
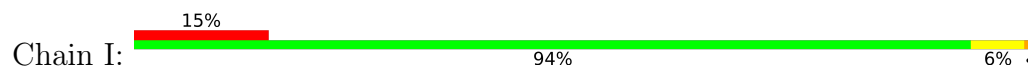




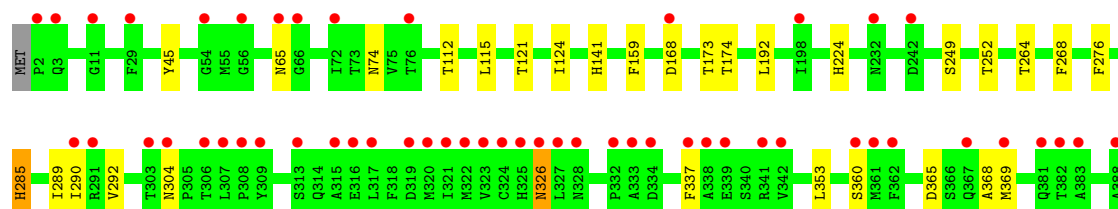
• Molecule 3: Urease subunit alpha

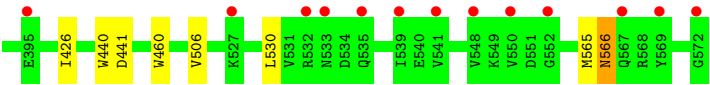


• Molecule 3: Urease subunit alpha



• Molecule 3: Urease subunit alpha





4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	157.20Å 157.20Å 774.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.71 – 3.01 29.71 – 3.01	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.71-3.01) 99.3 (29.71-3.01)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 3.00Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.277 , 0.298 0.331 , 0.356	Depositor DCC
R_{free} test set	3666 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	55.0	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	47288	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% 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:
NI

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	0/770	0.96	0/1040
1	D	0.80	0/770	0.99	1/1040 (0.1%)
1	G	0.78	0/770	0.95	0/1040
1	J	0.78	0/770	0.98	0/1040
2	B	0.80	0/908	1.06	3/1235 (0.2%)
2	E	0.83	1/908 (0.1%)	1.05	1/1235 (0.1%)
2	H	0.82	1/908 (0.1%)	1.07	4/1235 (0.3%)
2	K	0.81	1/908 (0.1%)	1.04	0/1235
3	C	0.74	0/4362	1.04	5/5924 (0.1%)
3	F	0.74	0/4362	1.04	5/5924 (0.1%)
3	I	0.75	0/4362	1.04	3/5924 (0.1%)
3	L	0.75	0/4362	1.04	5/5924 (0.1%)
All	All	0.76	3/24160 (0.0%)	1.03	27/32796 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	140	VAL	CA-C	6.08	1.59	1.52
2	H	140	VAL	CA-C	5.10	1.58	1.52
2	K	140	VAL	CA-C	5.09	1.58	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	133	GLY	N-CA-C	7.50	120.68	112.29
3	C	268	PHE	CA-CB-CG	7.24	121.04	113.80
1	D	21	PHE	CA-CB-CG	7.16	120.96	113.80
3	I	268	PHE	CA-CB-CG	7.15	120.95	113.80
3	F	268	PHE	CA-CB-CG	7.04	120.84	113.80
3	L	268	PHE	CA-CB-CG	7.04	120.83	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	159	PHE	CA-CB-CG	6.94	120.74	113.80
3	I	159	PHE	CA-CB-CG	6.89	120.69	113.80
3	C	159	PHE	CA-CB-CG	6.86	120.66	113.80
2	H	140	VAL	N-CA-CB	6.82	120.76	111.21
3	F	337	PHE	CA-CB-CG	6.06	119.86	113.80
2	H	139	VAL	CA-C-N	5.86	132.97	122.13
2	H	139	VAL	C-N-CA	5.86	132.97	122.13
3	L	159	PHE	CA-CB-CG	5.84	119.64	113.80
3	C	168	ASP	CA-CB-CG	5.74	118.33	112.60
3	L	337	PHE	CA-CB-CG	5.61	119.41	113.80
2	B	49	PHE	CA-CB-CG	5.52	119.32	113.80
3	L	168	ASP	CA-CB-CG	5.48	118.08	112.60
3	C	337	PHE	CA-CB-CG	5.44	119.24	113.80
3	F	168	ASP	CA-CB-CG	5.43	118.03	112.60
2	B	141	PRO	CA-N-CD	-5.41	104.42	112.00
2	E	49	PHE	CA-CB-CG	5.27	119.07	113.80
2	B	137	GLU	N-CA-C	-5.26	98.44	108.17
3	L	326	ASN	CA-CB-CG	5.07	117.67	112.60
3	I	326	ASN	CA-CB-CG	5.07	117.67	112.60
3	C	326	ASN	CA-CB-CG	5.03	117.63	112.60
3	F	326	ASN	CA-CB-CG	5.01	117.61	112.60

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	762	793	793	0	0
1	D	762	793	793	0	0
1	G	762	793	793	0	0
1	J	762	793	793	0	0
2	B	886	859	859	14	7
2	E	886	859	859	4	0
2	H	886	858	858	11	2
2	K	886	859	859	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	4277	4216	4216	8	2
3	F	4277	4216	4216	10	0
3	I	4277	4216	4216	8	7
3	L	4277	4216	4216	11	0
4	C	2	0	0	0	0
4	F	2	0	0	0	0
4	I	2	0	0	0	0
4	L	2	0	0	0	0
5	B	8	0	0	0	0
5	C	15	0	0	0	0
5	D	1	0	0	0	0
5	E	8	0	0	0	0
5	F	31	0	0	0	0
5	I	17	0	0	0	0
5	K	4	0	0	0	0
5	L	25	0	0	0	0
All	All	23817	23471	23471	66	9

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 1.

All (66) 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:H:122:GLN:HB3	2:H:135:THR:CG2	1.98	0.94
2:H:122:GLN:HB3	2:H:135:THR:HG21	1.61	0.81
2:B:139:VAL:C	2:B:140:VAL:HG13	2.13	0.73
2:B:134:TRP:CZ2	2:B:136:GLY:HA2	2.23	0.72
2:H:134:TRP:CD1	2:H:135:THR:H	2.12	0.67
2:B:92:GLY:HA3	2:B:135:THR:HG21	1.77	0.66
2:B:139:VAL:O	2:B:140:VAL:HG22	1.95	0.66
2:B:92:GLY:CA	2:B:135:THR:HG21	2.26	0.66
2:B:139:VAL:O	2:B:140:VAL:HG13	1.96	0.64
3:F:261:VAL:HG22	3:F:285:HIS:ND1	2.17	0.59
3:F:261:VAL:HG21	3:F:288:ASP:O	2.05	0.57
2:B:123:THR:HB	2:B:134:TRP:HB2	1.88	0.56
2:B:134:TRP:CZ2	2:B:136:GLY:CA	2.89	0.55
2:E:137:GLU:OE2	2:E:143:SER:O	2.27	0.53
2:B:123:THR:HA	2:B:134:TRP:HA	1.90	0.52
2:B:134:TRP:CE2	2:B:136:GLY:HA2	2.44	0.52
3:C:292:VAL:HG12	3:C:298:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:173:THR:HG22	3:L:224:HIS:CD2	2.45	0.52
3:I:173:THR:HG22	3:I:224:HIS:CD2	2.46	0.51
3:C:173:THR:HG22	3:C:224:HIS:CD2	2.46	0.50
3:F:173:THR:HG22	3:F:224:HIS:CD2	2.47	0.50
3:F:292:VAL:HG12	3:F:298:VAL:HG21	1.94	0.49
2:E:137:GLU:HG3	2:E:138:GLY:N	2.27	0.49
3:L:289:ILE:O	3:L:292:VAL:HG22	2.13	0.48
2:B:139:VAL:C	2:B:141:PRO:HD3	2.38	0.48
3:C:219:VAL:CG2	3:C:519:VAL:HG11	2.43	0.48
3:F:502:LEU:HD13	3:F:518:ALA:HB2	1.94	0.48
3:L:360:SER:CB	3:L:530:LEU:HD13	2.44	0.47
2:B:139:VAL:C	2:B:140:VAL:CG1	2.86	0.47
3:C:360:SER:CB	3:C:530:LEU:HD13	2.45	0.47
3:F:360:SER:CB	3:F:530:LEU:HD13	2.44	0.47
3:I:360:SER:CB	3:I:530:LEU:HD13	2.44	0.47
3:F:261:VAL:HG22	3:F:285:HIS:CE1	2.48	0.47
2:H:133:GLY:O	2:H:134:TRP:HB3	2.16	0.46
2:H:122:GLN:O	2:H:135:THR:HG23	2.16	0.45
3:L:173:THR:HG22	3:L:224:HIS:CG	2.51	0.45
3:C:173:THR:HG22	3:C:224:HIS:CG	2.52	0.45
2:H:35:THR:HG23	2:H:36:PRO:HD2	1.99	0.45
3:F:262:GLU:CG	2:K:139:VAL:HG21	2.47	0.45
3:I:173:THR:HG22	3:I:224:HIS:CG	2.52	0.44
2:B:134:TRP:O	2:B:134:TRP:CE3	2.70	0.44
3:L:112:THR:CG2	3:L:115:LEU:HD13	2.48	0.44
2:H:133:GLY:O	2:H:134:TRP:CB	2.66	0.44
3:L:112:THR:HG22	3:L:115:LEU:HD13	2.00	0.44
3:F:249:SER:HB3	3:F:276:PHE:CE2	2.53	0.43
2:B:123:THR:CB	2:B:134:TRP:HB2	2.48	0.43
3:C:249:SER:HB3	3:C:276:PHE:CE2	2.53	0.43
3:I:249:SER:HB3	3:I:276:PHE:CE2	2.53	0.43
3:I:426:ILE:HD13	3:I:436:ASP:HB2	2.01	0.43
2:H:140:VAL:HG22	2:H:141:PRO:HD3	2.00	0.43
3:L:249:SER:HB3	3:L:276:PHE:CE2	2.54	0.43
2:H:42:LEU:HD11	3:I:6:ARG:HB3	2.01	0.43
2:E:140:VAL:HB	2:E:141:PRO:HD3	2.00	0.42
2:H:134:TRP:CG	2:H:135:THR:H	2.37	0.42
2:H:70:VAL:HG11	2:H:76:PHE:CE1	2.55	0.42
3:C:82:LEU:O	3:C:82:LEU:HD12	2.19	0.42
3:I:292:VAL:HG12	3:I:298:VAL:HG21	2.01	0.42
2:E:99:SER:O	2:E:100:THR:HB	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:115:LEU:HD12	3:L:115:LEU:N	2.35	0.42
3:F:173:THR:HG22	3:F:224:HIS:CG	2.55	0.41
3:L:141:HIS:CE1	3:L:174:THR:HG23	2.56	0.41
3:L:264:THR:HG21	3:L:285:HIS:CE1	2.56	0.41
3:L:290:ILE:HD11	3:L:353:LEU:CD1	2.51	0.41
3:C:163:GLY:HA3	3:C:170:THR:HG23	2.03	0.40
3:I:101:LYS:C	3:I:115:LEU:HD23	2.46	0.40
2:K:140:VAL:HB	2:K:141:PRO:HD3	2.04	0.40

All (9) 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)
2:B:139:VAL:HG12	3:I:291:ARG:NH2[3_545]	0.59	1.01
2:B:139:VAL:HG12	3:I:291:ARG:HH22[3_545]	0.67	0.93
2:B:139:VAL:CG1	3:I:291:ARG:NH2[3_545]	1.31	0.89
2:B:139:VAL:HG12	3:I:291:ARG:HH21[3_545]	0.94	0.66
2:B:139:VAL:CG1	3:I:291:ARG:HH22[3_545]	1.30	0.30
3:C:266:ASP:OD1	2:H:134:TRP:HZ2[3_545]	1.42	0.18
2:B:139:VAL:CG1	3:I:291:ARG:CZ[3_545]	2.10	0.10
3:C:266:ASP:CG	2:H:134:TRP:HZ2[3_545]	1.54	0.06
2:B:139:VAL:HG11	3:I:291:ARG:NH2[3_545]	1.59	0.01

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	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
1	D	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
1	G	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
1	J	97/100 (97%)	94 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	112/164 (68%)	95 (85%)	12 (11%)	5 (4%)	2	11
2	E	112/164 (68%)	96 (86%)	13 (12%)	3 (3%)	4	20
2	H	112/164 (68%)	96 (86%)	11 (10%)	5 (4%)	2	11
2	K	112/164 (68%)	99 (88%)	10 (9%)	3 (3%)	4	20
3	C	569/572 (100%)	512 (90%)	47 (8%)	10 (2%)	6	29
3	F	569/572 (100%)	510 (90%)	50 (9%)	9 (2%)	7	32
3	I	569/572 (100%)	510 (90%)	49 (9%)	10 (2%)	6	29
3	L	569/572 (100%)	511 (90%)	48 (8%)	10 (2%)	6	29
All	All	3112/3344 (93%)	2805 (90%)	252 (8%)	55 (2%)	6	29

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	50	ASN
2	B	140	VAL
2	E	50	ASN
2	E	140	VAL
2	H	140	VAL
3	I	74	ASN
2	K	140	VAL
3	L	285	HIS
2	B	141	PRO
3	C	285	HIS
3	C	365	ASP
3	F	365	ASP
2	H	134	TRP
3	I	285	HIS
3	I	365	ASP
3	C	369	MET
3	F	285	HIS
3	F	369	MET
3	I	369	MET
2	K	50	ASN
3	L	65	ASN
3	L	365	ASP
3	L	369	MET
2	B	127	PHE
3	C	65	ASN
3	C	326	ASN

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Mol	Chain	Res	Type
2	E	127	PHE
3	F	65	ASN
3	F	326	ASN
2	H	127	PHE
3	I	65	ASN
3	I	326	ASN
3	I	566	ASN
2	K	127	PHE
3	L	326	ASN
3	C	565	MET
3	C	566	ASN
3	F	368	ALA
3	F	565	MET
3	F	566	ASN
2	H	50	ASN
3	I	368	ALA
3	I	565	MET
3	L	74	ASN
3	L	368	ALA
3	L	565	MET
3	L	566	ASN
3	C	368	ALA
2	H	141	PRO
2	B	139	VAL
3	C	217	GLY
3	C	304	ASN
3	F	304	ASN
3	I	304	ASN
3	L	304	ASN

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	86/87 (99%)	85 (99%)	1 (1%)	63	81
1	D	86/87 (99%)	85 (99%)	1 (1%)	63	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	86/87 (99%)	84 (98%)	2 (2%)	44	72
1	J	86/87 (99%)	85 (99%)	1 (1%)	63	81
2	B	96/138 (70%)	90 (94%)	6 (6%)	16	46
2	E	96/138 (70%)	93 (97%)	3 (3%)	35	67
2	H	96/138 (70%)	95 (99%)	1 (1%)	68	83
2	K	96/138 (70%)	94 (98%)	2 (2%)	47	74
3	C	457/458 (100%)	449 (98%)	8 (2%)	51	76
3	F	457/458 (100%)	444 (97%)	13 (3%)	38	69
3	I	457/458 (100%)	446 (98%)	11 (2%)	43	72
3	L	457/458 (100%)	446 (98%)	11 (2%)	43	72
All	All	2556/2732 (94%)	2496 (98%)	60 (2%)	44	72

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
2	B	37	LEU
2	B	40	CYS
2	B	129	ASN
2	B	134	TRP
2	B	140	VAL
2	B	141	PRO
3	C	45	TYR
3	C	124	ILE
3	C	236	HIS
3	C	252	THR
3	C	440	TRP
3	C	441	ASP
3	C	460	TRP
3	C	566	ASN
1	D	16	LEU
2	E	37	LEU
2	E	40	CYS
2	E	76	PHE
3	F	45	TYR
3	F	121	THR
3	F	124	ILE
3	F	192	LEU

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Mol	Chain	Res	Type
3	F	252	THR
3	F	285	HIS
3	F	362	PHE
3	F	440	TRP
3	F	441	ASP
3	F	460	TRP
3	F	502	LEU
3	F	506	VAL
3	F	566	ASN
1	G	16	LEU
1	G	21	PHE
2	H	135	THR
3	I	45	TYR
3	I	124	ILE
3	I	129	LEU
3	I	192	LEU
3	I	252	THR
3	I	426	ILE
3	I	440	TRP
3	I	441	ASP
3	I	460	TRP
3	I	506	VAL
3	I	566	ASN
1	J	16	LEU
2	K	37	LEU
2	K	140	VAL
3	L	45	TYR
3	L	121	THR
3	L	124	ILE
3	L	192	LEU
3	L	252	THR
3	L	426	ILE
3	L	440	TRP
3	L	441	ASP
3	L	460	TRP
3	L	506	VAL
3	L	566	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN

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Mol	Chain	Res	Type
2	B	52	ASN
2	B	129	ASN
3	C	181	ASN
3	C	420	GLN
3	C	528	HIS
3	C	554	HIS
1	D	2	GLN
1	D	96	HIS
2	E	52	ASN
2	E	69	GLN
2	E	129	ASN
3	F	181	ASN
3	F	247	GLN
3	F	328	ASN
3	F	330	ASN
3	F	420	GLN
3	F	528	HIS
3	F	554	HIS
1	G	2	GLN
2	H	52	ASN
2	H	129	ASN
3	I	74	ASN
3	I	181	ASN
3	I	247	GLN
3	I	328	ASN
3	I	330	ASN
3	I	420	GLN
3	I	528	HIS
2	K	52	ASN
2	K	129	ASN
3	L	74	ASN
3	L	147	GLN
3	L	150	HIS
3	L	181	ASN
3	L	247	GLN
3	L	256	ASN
3	L	295	GLN
3	L	330	ASN
3	L	420	GLN
3	L	521	ASN
3	L	528	HIS
3	L	554	HIS

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 8 ligands modelled in this entry, 8 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	99/100 (99%)	0.98	9 (9%) 15 8	79, 103, 127, 142	0
1	D	99/100 (99%)	1.16	4 (4%) 42 23	83, 111, 137, 152	0
1	G	99/100 (99%)	1.09	11 (11%) 10 6	90, 115, 137, 145	0
1	J	99/100 (99%)	1.04	7 (7%) 22 11	77, 101, 128, 137	0
2	B	114/164 (69%)	1.32	20 (17%) 4 2	24, 106, 143, 153	0
2	E	114/164 (69%)	1.48	22 (19%) 3 2	60, 105, 146, 165	0
2	H	114/164 (69%)	1.75	38 (33%) 1 1	24, 163, 195, 203	0
2	K	114/164 (69%)	1.26	20 (17%) 4 2	63, 102, 161, 164	0
3	C	571/572 (99%)	1.17	108 (18%) 3 2	27, 98, 201, 231	0
3	F	571/572 (99%)	0.85	59 (10%) 12 6	15, 80, 165, 225	0
3	I	571/572 (99%)	1.07	84 (14%) 6 3	16, 91, 176, 222	0
3	L	571/572 (99%)	0.83	66 (11%) 9 5	15, 82, 169, 201	0
All	All	3136/3344 (93%)	1.06	448 (14%) 6 3	15, 96, 176, 231	0

All (448) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	325	HIS	8.7
3	I	324	CYS	8.2
3	L	66	GLY	6.6
3	I	326	ASN	6.4
3	I	323	VAL	5.9
3	C	324	CYS	5.5
3	L	323	VAL	5.4
3	L	321	ILE	5.3
2	E	92	GLY	5.3
3	F	321	ILE	5.2
3	C	572	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
3	L	337	PHE	5.1
3	I	320	MET	5.1
3	F	326	ASN	5.1
3	L	324	CYS	5.1
3	C	383	ALA	5.0
3	F	324	CYS	5.0
3	I	321	ILE	4.8
3	I	572	GLY	4.8
3	F	320	MET	4.8
3	I	337	PHE	4.8
3	C	278	THR	4.6
3	I	282	GLY	4.6
3	F	65	ASN	4.5
3	C	66	GLY	4.5
3	L	326	ASN	4.5
3	L	65	ASN	4.4
3	F	360	SER	4.4
1	J	42	THR	4.4
3	L	325	HIS	4.4
3	L	320	MET	4.4
3	F	66	GLY	4.2
3	C	292	VAL	4.2
3	C	320	MET	4.2
3	F	325	HIS	4.2
2	B	129	ASN	4.1
3	I	362	PHE	4.1
2	B	79	VAL	4.0
2	E	147	ASP	4.0
3	F	541	VAL	3.9
3	L	541	VAL	3.9
3	L	362	PHE	3.9
2	E	144	GLU	3.9
3	C	326	ASN	3.9
2	E	44	ASP	3.8
3	C	341	ARG	3.8
3	F	317	LEU	3.8
2	H	77	PHE	3.8
1	A	85	ILE	3.8
3	L	572	GLY	3.8
2	H	100	THR	3.7
3	C	354	HIS	3.6
3	F	318	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
3	I	340	SER	3.6
3	I	383	ALA	3.6
3	C	325	HIS	3.6
3	L	383	ALA	3.6
3	C	385	ALA	3.6
2	H	34	ASN	3.6
3	L	334	ASP	3.6
3	C	337	PHE	3.5
3	C	372	VAL	3.5
3	C	157	ALA	3.5
2	H	147	ASP	3.5
3	I	541	VAL	3.5
2	K	147	ASP	3.5
3	L	319	ASP	3.5
3	F	27	ASN	3.4
3	C	223	VAL	3.4
3	I	552	GLY	3.4
2	H	103	ILE	3.4
2	B	143	SER	3.4
1	D	21	PHE	3.4
3	I	464	GLY	3.4
3	L	56	GLY	3.3
2	H	37	LEU	3.3
3	C	537	PRO	3.3
3	F	330	ASN	3.3
2	H	76	PHE	3.3
2	E	129	ASN	3.3
3	F	572	GLY	3.3
2	H	131	VAL	3.2
3	I	375	ASN	3.2
2	E	103	ILE	3.2
3	I	53	ASP	3.2
3	C	222	LYS	3.2
2	E	78	GLU	3.2
3	F	263	ASP	3.1
3	C	569	TYR	3.1
3	I	408	TYR	3.1
3	L	322	MET	3.1
3	F	314	GLN	3.1
3	I	7	GLN	3.1
3	I	258	CYS	3.1
3	C	58	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
3	L	303	THR	3.1
3	C	295	GLN	3.1
3	I	567	GLN	3.1
3	C	236	HIS	3.0
3	I	2	PRO	3.0
3	I	12	LEU	3.0
3	L	3	GLN	3.0
3	C	562	THR	3.0
3	C	166	PRO	3.0
3	C	294	SER	3.0
3	I	327	LEU	3.0
2	B	50	ASN	3.0
3	I	369	MET	3.0
2	E	137	GLU	3.0
3	L	552	GLY	3.0
3	C	252	THR	3.0
3	I	43	SER	2.9
2	B	34	ASN	2.9
2	H	89	ALA	2.9
1	J	38	ILE	2.9
2	E	139	VAL	2.9
3	F	534	ASP	2.9
2	K	100	THR	2.9
3	I	410	ALA	2.9
3	F	302	SER	2.9
3	I	537	PRO	2.9
2	H	119	GLY	2.9
3	I	38	GLY	2.9
3	C	347	ILE	2.9
3	I	389	SER	2.8
3	F	285	HIS	2.8
3	C	315	ALA	2.8
1	A	78	PRO	2.8
3	I	334	ASP	2.8
3	C	312	ASN	2.8
3	F	232	ASN	2.8
3	L	539	ILE	2.8
3	L	342	VAL	2.8
3	C	54	GLY	2.8
3	I	10	ALA	2.8
3	C	275	THR	2.8
3	L	316	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	39	GLY	2.8
3	C	565	MET	2.8
3	F	2	PRO	2.8
3	L	332	PRO	2.8
2	H	78	GLU	2.8
3	C	339	GLU	2.8
3	I	66	GLY	2.7
1	J	6	ARG	2.7
1	G	2	GLN	2.7
3	C	3	GLN	2.7
3	F	323	VAL	2.7
2	H	41	ILE	2.7
3	C	272	THR	2.7
3	L	168	ASP	2.7
2	H	73	HIS	2.7
3	F	333	ALA	2.7
2	H	124	LEU	2.7
3	L	327	LEU	2.7
3	I	303	THR	2.7
3	L	360	SER	2.7
2	B	52	ASN	2.7
2	B	142	ASN	2.7
2	H	50	ASN	2.7
3	I	36	LEU	2.7
3	L	317	LEU	2.7
1	G	99	ILE	2.7
1	G	44	MET	2.7
2	B	76	PHE	2.7
3	C	313	SER	2.7
3	C	560	ILE	2.6
3	F	537	PRO	2.6
3	I	318	PHE	2.6
3	I	341	ARG	2.6
3	L	341	ARG	2.6
2	H	38	GLY	2.6
2	H	63	THR	2.6
2	H	95	LEU	2.6
3	L	548	VAL	2.6
3	L	72	ILE	2.6
3	C	296	PRO	2.6
3	I	533	ASN	2.6
3	I	570	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
3	L	232	ASN	2.6
3	C	563	ALA	2.6
3	I	338	ALA	2.6
3	I	352	VAL	2.6
3	L	307	LEU	2.6
1	A	99	ILE	2.6
2	K	103	ILE	2.6
3	C	321	ILE	2.6
2	E	80	ASN	2.6
3	C	228	GLY	2.6
2	K	43	ALA	2.6
3	I	388	ALA	2.6
3	L	388	ALA	2.6
3	C	380	MET	2.6
3	F	322	MET	2.6
2	H	117	PRO	2.6
3	F	7	GLN	2.6
3	I	65	ASN	2.6
3	C	316	GLU	2.6
3	C	327	LEU	2.6
2	K	90	ALA	2.6
2	B	103	ILE	2.6
3	C	361	MET	2.6
3	C	571	PHE	2.6
3	C	323	VAL	2.6
3	I	311	VAL	2.6
3	I	315	ALA	2.6
1	D	40	THR	2.6
3	C	258	CYS	2.5
3	I	309	TYR	2.5
3	I	528	HIS	2.5
3	L	308	PRO	2.5
3	F	334	ASP	2.5
3	F	342	VAL	2.5
2	E	89	ALA	2.5
3	I	157	ALA	2.5
1	D	99	ILE	2.5
2	E	116	ILE	2.5
2	K	101	THR	2.5
2	H	42	LEU	2.5
2	H	83	LEU	2.5
3	I	103	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
3	L	535	GLN	2.5
3	C	229	ALA	2.5
3	C	319	ASP	2.5
3	C	564	ALA	2.5
3	F	253	ASP	2.5
3	I	69	ASP	2.5
3	C	376	TRP	2.5
2	K	42	LEU	2.5
3	C	56	GLY	2.5
3	F	6	ARG	2.5
2	H	79	VAL	2.5
3	C	231	ALA	2.5
3	L	315	ALA	2.5
3	I	374	GLU	2.5
2	H	96	ASN	2.5
3	C	561	ASP	2.5
3	L	328	ASN	2.5
3	I	55	MET	2.5
2	B	91	TYR	2.5
3	L	333	ALA	2.5
3	I	119	VAL	2.5
3	C	567	GLN	2.5
3	I	322	MET	2.4
2	H	118	PHE	2.4
3	F	20	LYS	2.4
3	I	319	ASP	2.4
1	A	93	VAL	2.4
3	I	539	ILE	2.4
2	H	40	CYS	2.4
1	G	79	ASN	2.4
2	E	65	ASP	2.4
3	I	39	TYR	2.4
2	B	82	ALA	2.4
3	C	356	MET	2.4
2	E	37	LEU	2.4
2	K	34	ASN	2.4
1	A	49	ASP	2.4
1	A	97	ASP	2.4
3	C	53	ASP	2.4
3	C	84	VAL	2.4
3	C	60	HIS	2.4
3	C	282	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	88	ALA	2.4
3	C	4	ILE	2.4
3	C	555	ALA	2.4
3	C	369	MET	2.4
2	B	144	GLU	2.4
2	K	134	TRP	2.4
3	F	287	PRO	2.4
3	I	562	THR	2.4
3	L	242	ASP	2.4
2	H	125	TYR	2.3
3	F	567	GLN	2.3
3	I	381	GLN	2.3
1	J	54	GLU	2.3
2	H	46	PRO	2.3
3	C	153	SER	2.3
2	K	35	THR	2.3
3	L	76	THR	2.3
3	L	532	ARG	2.3
2	H	128	ASN	2.3
2	K	129	ASN	2.3
3	F	384	ASN	2.3
3	I	569	TYR	2.3
2	B	147	ASP	2.3
1	G	21	PHE	2.3
2	E	42	LEU	2.3
3	C	276	PHE	2.3
2	B	78	GLU	2.3
2	E	79	VAL	2.3
3	C	311	VAL	2.3
3	C	344	PRO	2.3
3	I	344	PRO	2.3
3	L	2	PRO	2.3
2	B	39	GLY	2.3
3	C	227	TRP	2.3
3	F	11	GLY	2.3
3	I	399	GLY	2.3
3	L	290	ILE	2.3
3	L	309	TYR	2.3
3	C	317	LEU	2.3
3	L	304	ASN	2.3
3	L	533	ASN	2.3
3	L	567	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	548	VAL	2.3
3	F	311	VAL	2.3
3	I	292	VAL	2.3
3	C	343	ARG	2.3
3	F	329	PRO	2.3
3	C	286	ALA	2.3
3	F	10	ALA	2.3
1	G	1	MET	2.3
3	C	382	THR	2.3
3	F	313	SER	2.3
3	I	306	THR	2.3
2	K	40	CYS	2.3
3	F	168	ASP	2.3
3	I	535	GLN	2.3
3	I	343	ARG	2.3
3	C	24	GLY	2.3
3	L	369	MET	2.3
2	K	145	ARG	2.3
3	L	367	GLN	2.3
3	F	544	GLU	2.2
3	L	338	ALA	2.2
3	L	361	MET	2.2
3	C	268	PHE	2.2
3	I	354	HIS	2.2
3	C	375	ASN	2.2
3	C	379	VAL	2.2
3	I	116	VAL	2.2
3	C	288	ASP	2.2
3	C	558	GLU	2.2
3	F	56	GLY	2.2
3	F	280	GLY	2.2
3	F	338	ALA	2.2
2	K	91	TYR	2.2
1	A	30	LEU	2.2
3	C	355	ASP	2.2
1	J	33	PRO	2.2
3	I	393	LEU	2.2
3	L	291	ARG	2.2
3	C	264	THR	2.2
3	C	274	HIS	2.2
2	H	52	ASN	2.2
2	K	124	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	F	327	LEU	2.2
2	E	82	ALA	2.2
3	I	57	ALA	2.2
3	F	337	PHE	2.2
3	I	37	ARG	2.2
3	F	536	THR	2.2
3	I	128	HIS	2.2
3	L	306	THR	2.2
3	L	382	THR	2.2
3	C	309	TYR	2.2
3	C	408	TYR	2.2
3	C	530	LEU	2.2
3	C	65	ASN	2.2
3	L	395	GLU	2.2
3	C	145	PRO	2.2
1	G	63	VAL	2.1
1	J	93	VAL	2.1
3	C	342	VAL	2.1
3	I	78	VAL	2.1
3	I	560	ILE	2.1
3	L	381	GLN	2.1
3	C	249	SER	2.1
3	C	461	ALA	2.1
3	L	54	GLY	2.1
1	D	93	VAL	2.1
2	H	75	HIS	2.1
3	I	71	VAL	2.1
3	C	138	THR	2.1
3	L	198	ILE	2.1
3	L	569	TYR	2.1
2	B	89	ALA	2.1
3	I	555	ALA	2.1
2	H	136	GLY	2.1
3	C	389	SER	2.1
2	E	41	ILE	2.1
2	E	135	THR	2.1
3	C	273	ILE	2.1
3	F	176	THR	2.1
3	F	341	ARG	2.1
3	C	381	GLN	2.1
2	K	144	GLU	2.1
3	C	570	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
3	I	364	SER	2.1
3	L	29	PHE	2.1
3	F	372	VAL	2.1
3	C	128	HIS	2.1
3	C	299	LEU	2.1
3	F	290	ILE	2.1
3	F	319	ASP	2.1
3	I	47	GLY	2.1
3	L	11	GLY	2.1
2	H	105	PHE	2.1
2	K	78	GLU	2.1
3	I	571	PHE	2.1
2	K	98	SER	2.1
3	C	364	SER	2.1
1	A	79	ASN	2.1
2	B	96	ASN	2.1
1	A	6	ARG	2.1
3	C	23	LEU	2.1
3	C	142	LEU	2.1
3	C	152	LEU	2.1
3	F	369	MET	2.1
3	F	286	ALA	2.1
3	I	333	ALA	2.1
2	H	114	PRO	2.1
3	C	350	GLU	2.1
3	L	313	SER	2.0
1	G	6	ARG	2.0
3	C	291	ARG	2.0
3	C	538	ASN	2.0
3	C	568	ARG	2.0
3	I	23	LEU	2.0
1	G	43	ALA	2.0
1	G	60	ALA	2.0
3	C	293	ALA	2.0
3	F	53	ASP	2.0
2	K	92	GLY	2.0
3	F	191	GLY	2.0
3	I	106	GLY	2.0
2	B	36	PRO	2.0
2	H	146	PRO	2.0
2	E	93	LYS	2.0
3	L	339	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
3	L	550	VAL	2.0
1	G	3	LEU	2.0
2	H	56	THR	2.0
3	F	303	THR	2.0
3	F	383	ALA	2.0
1	J	55	ASP	2.0
3	C	310	GLY	2.0
2	B	122	GLN	2.0
3	L	527	LYS	2.0
2	E	70	VAL	2.0
2	E	84	GLU	2.0
2	H	84	GLU	2.0
3	I	409	VAL	2.0
3	I	558	GLU	2.0
3	F	291	ARG	2.0
2	B	130	LEU	2.0
2	K	41	ILE	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
4	NI	F	601	1/1	0.88	0.10	53,53,53,53	0
4	NI	F	602	1/1	0.93	0.15	45,45,45,45	0
4	NI	L	601	1/1	0.94	0.09	52,52,52,52	0
4	NI	I	601	1/1	0.96	0.09	41,41,41,41	0
4	NI	C	601	1/1	0.96	0.09	81,81,81,81	0
4	NI	C	602	1/1	0.97	0.06	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NI	L	602	1/1	0.97	0.07	43,43,43,43	0
4	NI	I	602	1/1	0.99	0.13	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.