



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:12 PM UTC

PDB ID : 2ODR / pdb_00002odr
Title : Methanococcus Maripaludis Phosphoseryl-tRNA synthetase
Authors : Steitz, T.A.; Kamtekar, S.
Deposited on : 2006-12-26
Resolution : 3.23 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

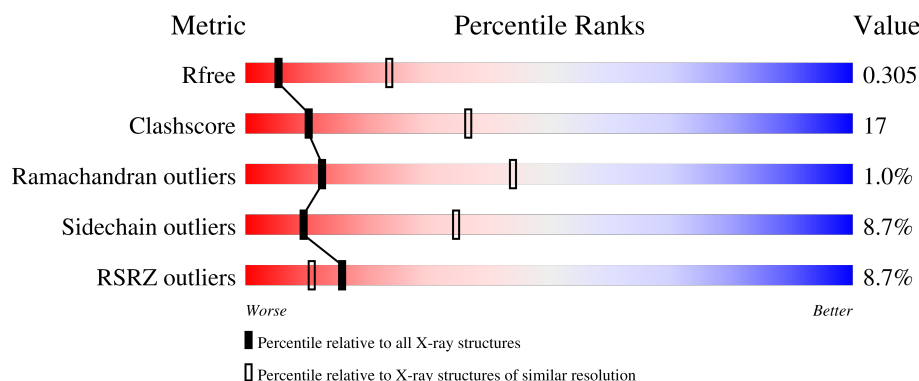
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.23 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	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (3.24-3.20)

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	665	
2	B	648	
3	C	701	
4	D	685	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13538 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 phosphoseryl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			3626	2314	613	682	17			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	cloning artifact	UNP Q6LZE1
A	-17	GLY	-	cloning artifact	UNP Q6LZE1
A	-16	SER	-	cloning artifact	UNP Q6LZE1
A	-15	HIS	-	cloning artifact	UNP Q6LZE1
A	-14	HIS	-	cloning artifact	UNP Q6LZE1
A	-13	HIS	-	cloning artifact	UNP Q6LZE1
A	-12	HIS	-	cloning artifact	UNP Q6LZE1
A	-11	HIS	-	cloning artifact	UNP Q6LZE1
A	-10	HIS	-	cloning artifact	UNP Q6LZE1
A	-9	SER	-	cloning artifact	UNP Q6LZE1
A	-8	SER	-	cloning artifact	UNP Q6LZE1
A	-7	GLY	-	cloning artifact	UNP Q6LZE1
A	-6	LEU	-	cloning artifact	UNP Q6LZE1
A	-5	VAL	-	cloning artifact	UNP Q6LZE1
A	-4	PRO	-	cloning artifact	UNP Q6LZE1
A	-3	ARG	-	cloning artifact	UNP Q6LZE1
A	-2	GLY	-	cloning artifact	UNP Q6LZE1
A	-1	SER	-	cloning artifact	UNP Q6LZE1
A	0	HIS	-	cloning artifact	UNP Q6LZE1

- Molecule 2 is a protein called phosphoseryl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	448	Total	C	N	O	S	0	0	0
			3320	2120	559	625	16			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	MET	-	cloning artifact	UNP Q6LZE1
B	-17	GLY	-	cloning artifact	UNP Q6LZE1
B	-16	SER	-	cloning artifact	UNP Q6LZE1
B	-15	HIS	-	cloning artifact	UNP Q6LZE1
B	-14	HIS	-	cloning artifact	UNP Q6LZE1
B	-13	HIS	-	cloning artifact	UNP Q6LZE1
B	-12	HIS	-	cloning artifact	UNP Q6LZE1
B	-11	HIS	-	cloning artifact	UNP Q6LZE1
B	-10	HIS	-	cloning artifact	UNP Q6LZE1
B	-9	SER	-	cloning artifact	UNP Q6LZE1
B	-8	SER	-	cloning artifact	UNP Q6LZE1
B	-7	GLY	-	cloning artifact	UNP Q6LZE1
B	-6	LEU	-	cloning artifact	UNP Q6LZE1
B	-5	VAL	-	cloning artifact	UNP Q6LZE1
B	-4	PRO	-	cloning artifact	UNP Q6LZE1
B	-3	ARG	-	cloning artifact	UNP Q6LZE1
B	-2	GLY	-	cloning artifact	UNP Q6LZE1
B	-1	SER	-	cloning artifact	UNP Q6LZE1
B	0	HIS	-	cloning artifact	UNP Q6LZE1

- Molecule 3 is a protein called phosphoseryl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	468	Total	C	N	O	S	0	0	0
			3337	2119	577	627	14			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	MET	-	cloning artifact	UNP Q6LZE1
C	-17	GLY	-	cloning artifact	UNP Q6LZE1
C	-16	SER	-	cloning artifact	UNP Q6LZE1
C	-15	HIS	-	cloning artifact	UNP Q6LZE1
C	-14	HIS	-	cloning artifact	UNP Q6LZE1
C	-13	HIS	-	cloning artifact	UNP Q6LZE1
C	-12	HIS	-	cloning artifact	UNP Q6LZE1
C	-11	HIS	-	cloning artifact	UNP Q6LZE1
C	-10	HIS	-	cloning artifact	UNP Q6LZE1
C	-9	SER	-	cloning artifact	UNP Q6LZE1
C	-8	SER	-	cloning artifact	UNP Q6LZE1
C	-7	GLY	-	cloning artifact	UNP Q6LZE1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	LEU	-	cloning artifact	UNP Q6LZE1
C	-5	VAL	-	cloning artifact	UNP Q6LZE1
C	-4	PRO	-	cloning artifact	UNP Q6LZE1
C	-3	ARG	-	cloning artifact	UNP Q6LZE1
C	-2	GLY	-	cloning artifact	UNP Q6LZE1
C	-1	SER	-	cloning artifact	UNP Q6LZE1
C	0	HIS	-	cloning artifact	UNP Q6LZE1

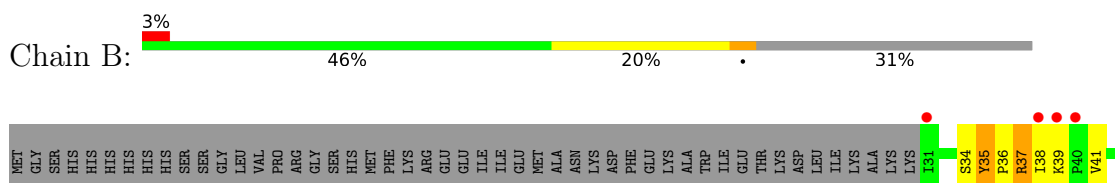
- Molecule 4 is a protein called phosphoseryl-tRNA synthetase.

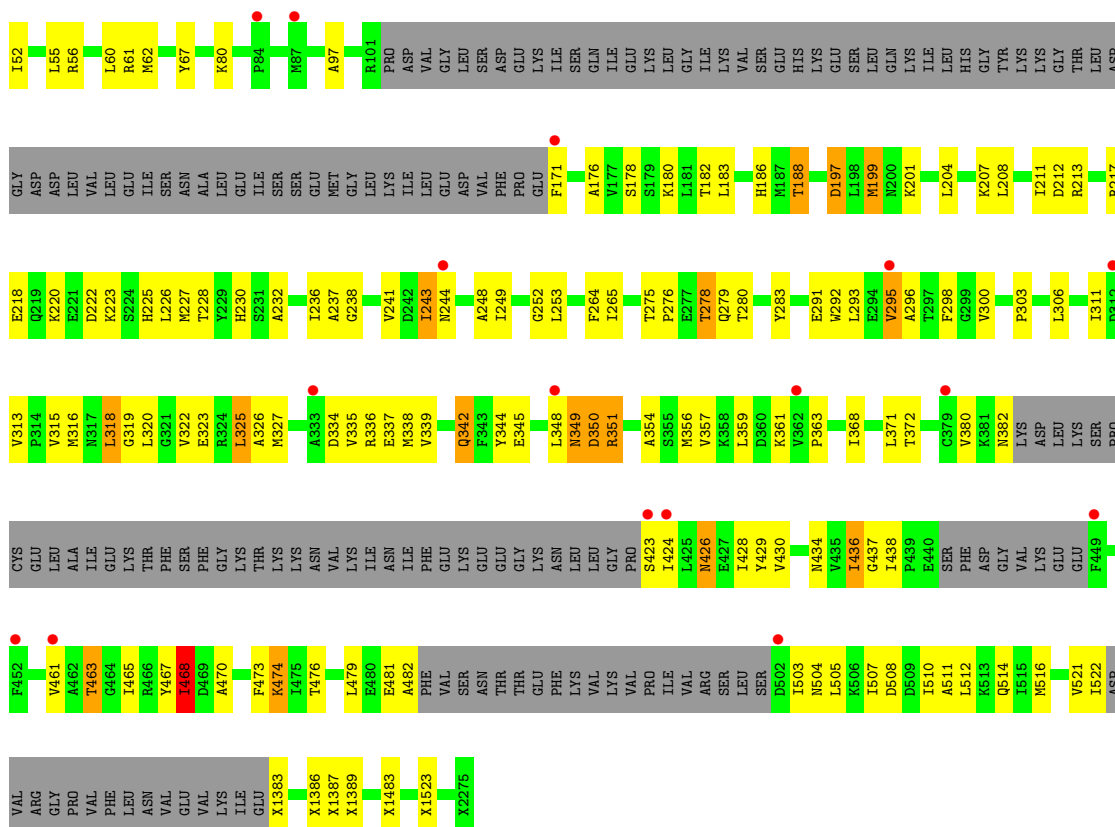
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	451	Total	C	N	O	S	0	0	0
			3255	2071	560	610	14			

There are 19 discrepancies between the modelled and reference sequences:

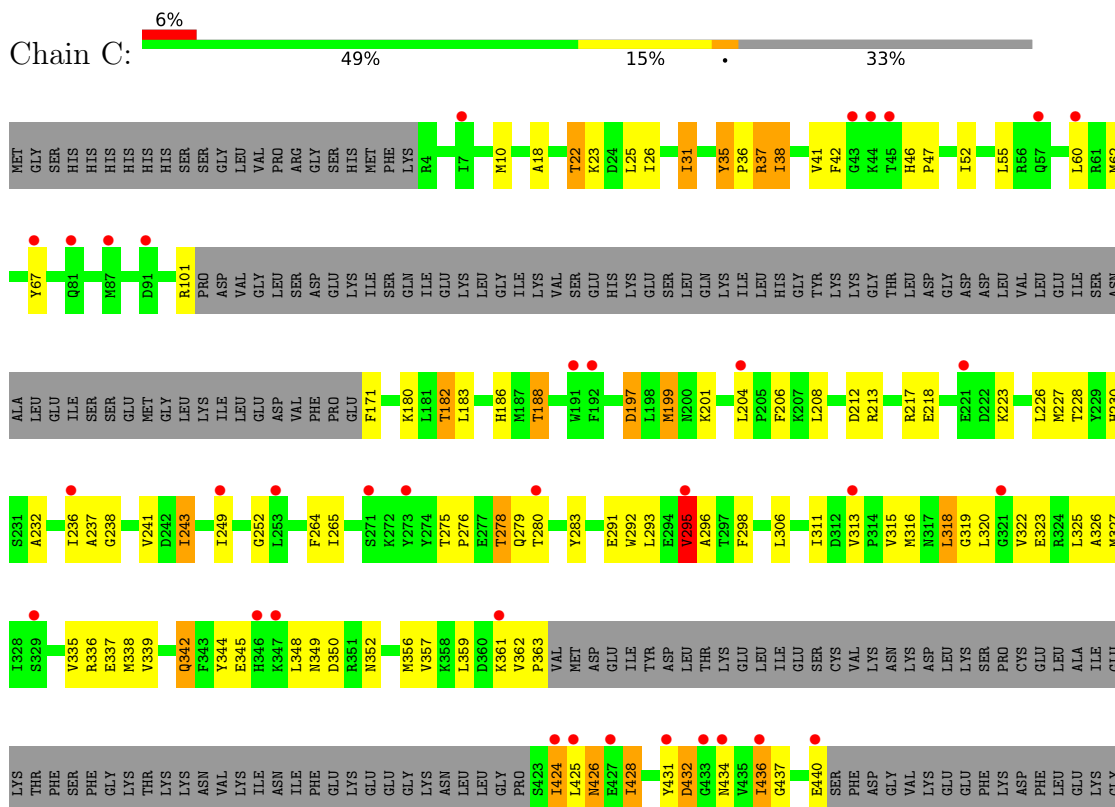
Chain	Residue	Modelled	Actual	Comment	Reference
D	-18	MET	-	cloning artifact	UNP Q6LZE1
D	-17	GLY	-	cloning artifact	UNP Q6LZE1
D	-16	SER	-	cloning artifact	UNP Q6LZE1
D	-15	HIS	-	cloning artifact	UNP Q6LZE1
D	-14	HIS	-	cloning artifact	UNP Q6LZE1
D	-13	HIS	-	cloning artifact	UNP Q6LZE1
D	-12	HIS	-	cloning artifact	UNP Q6LZE1
D	-11	HIS	-	cloning artifact	UNP Q6LZE1
D	-10	HIS	-	cloning artifact	UNP Q6LZE1
D	-9	SER	-	cloning artifact	UNP Q6LZE1
D	-8	SER	-	cloning artifact	UNP Q6LZE1
D	-7	GLY	-	cloning artifact	UNP Q6LZE1
D	-6	LEU	-	cloning artifact	UNP Q6LZE1
D	-5	VAL	-	cloning artifact	UNP Q6LZE1
D	-4	PRO	-	cloning artifact	UNP Q6LZE1
D	-3	ARG	-	cloning artifact	UNP Q6LZE1
D	-2	GLY	-	cloning artifact	UNP Q6LZE1
D	-1	SER	-	cloning artifact	UNP Q6LZE1
D	0	HIS	-	cloning artifact	UNP Q6LZE1

- Molecule 1: phosphoseryl-tRNA synthetase





- Molecule 3: phosphoseryl-tRNA synthetase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	119.17Å 133.94Å 208.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.23 50.00 – 3.23	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.00-3.23) 97.8 (50.00-3.23)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.25Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.292 , 0.306 0.292 , 0.305	Depositor DCC
R_{free} test set	2697 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	123.4	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 164.3	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	0.88	EDS
Total number of atoms	13538	wwPDB-VP
Average B, all atoms (Å ²)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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

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	0.52	0/3142	0.77	2/4229 (0.0%)
2	B	0.53	0/2918	0.77	3/3932 (0.1%)
3	C	0.53	0/2669	0.76	1/3597 (0.0%)
4	D	0.55	0/2671	0.77	1/3597 (0.0%)
All	All	0.53	0/11400	0.77	7/15355 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	436	ILE	N-CA-C	7.25	117.86	110.82
1	A	436	ILE	N-CA-C	7.06	117.63	111.56
2	B	436	ILE	N-CA-C	6.79	117.40	111.56
3	C	436	ILE	N-CA-C	6.39	116.56	110.74
1	A	325	LEU	N-CA-C	-5.21	105.50	111.07
2	B	468	ILE	CB-CA-C	-5.08	105.39	112.04
2	B	325	LEU	N-CA-C	-5.05	105.66	111.07

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	3626	0	3242	126	0
2	B	3320	0	2990	124	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3337	0	2798	100	0
4	D	3255	0	2788	109	1
All	All	13538	0	11818	432	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 17.

All (432) 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)
3:C:236:ILE:HD11	3:C:249:ILE:HD11	1.26	1.13
4:D:236:ILE:HD11	4:D:249:ILE:HD11	1.25	1.13
1:A:236:ILE:HD11	1:A:249:ILE:HD11	1.26	1.11
2:B:236:ILE:HD11	2:B:249:ILE:HD11	1.30	1.09
3:C:506:LYS:N	3:C:1505:UNK:C	2.20	1.04
1:A:275:THR:O	1:A:278:THR:HG22	1.58	1.03
3:C:275:THR:O	3:C:278:THR:HG22	1.59	1.02
2:B:275:THR:O	2:B:278:THR:HG22	1.62	1.00
4:D:275:THR:O	4:D:278:THR:HG22	1.61	1.00
1:A:482:ALA:C	1:A:1483:UNK:N	2.25	0.94
4:D:236:ILE:CD1	4:D:249:ILE:HD11	2.00	0.92
2:B:482:ALA:C	2:B:1483:UNK:N	2.27	0.92
1:A:236:ILE:CD1	1:A:249:ILE:HD11	2.01	0.91
3:C:236:ILE:CD1	3:C:249:ILE:HD11	2.01	0.91
1:A:348:LEU:HD11	1:A:510:ILE:HG22	1.54	0.90
4:D:505:LEU:N	4:D:1504:UNK:C	2.34	0.90
4:D:223:LYS:O	4:D:335:VAL:HG22	1.70	0.90
1:A:382:ASN:C	1:A:1383:UNK:N	2.28	0.90
2:B:236:ILE:CD1	2:B:249:ILE:HD11	2.03	0.88
3:C:223:LYS:O	3:C:335:VAL:HG22	1.72	0.87
2:B:223:LYS:O	2:B:335:VAL:HG22	1.72	0.87
1:A:326:ALA:HB3	1:A:338:MET:HE1	1.56	0.87
2:B:382:ASN:C	2:B:1383:UNK:N	2.32	0.86
2:B:348:LEU:HD11	2:B:510:ILE:HG22	1.58	0.86
1:A:223:LYS:O	1:A:335:VAL:HG22	1.76	0.85
3:C:183:LEU:HD11	4:D:183:LEU:HD11	1.56	0.84
3:C:326:ALA:HB3	3:C:338:MET:HE1	1.60	0.83
4:D:326:ALA:HB3	4:D:338:MET:HE1	1.60	0.82
2:B:326:ALA:HB3	2:B:338:MET:HE1	1.61	0.82
4:D:342:GLN:H	4:D:342:GLN:HE21	1.25	0.82
1:A:249:ILE:HD12	1:A:316:MET:HE1	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:342:GLN:H	2:B:342:GLN:HE21	1.27	0.80
1:A:300:VAL:HG11	4:D:26:ILE:HD13	1.65	0.78
1:A:342:GLN:H	1:A:342:GLN:HE21	1.29	0.78
1:A:176:ALA:HB3	2:B:178:SER:OG	1.84	0.77
4:D:521:VAL:C	4:D:1522:UNK:N	2.42	0.77
3:C:342:GLN:H	3:C:342:GLN:HE21	1.31	0.76
2:B:249:ILE:HD12	2:B:316:MET:HE1	1.67	0.74
2:B:368:ILE:O	2:B:476:THR:HG21	1.87	0.74
2:B:368:ILE:O	2:B:476:THR:CG2	2.35	0.74
1:A:31:ILE:HG21	1:A:359:LEU:HD12	1.67	0.73
4:D:199:MET:HE1	4:D:204:LEU:HD11	1.69	0.73
1:A:31:ILE:CG2	1:A:359:LEU:HD12	2.18	0.73
1:A:178:SER:OG	2:B:176:ALA:HB3	1.89	0.73
3:C:337:GLU:HG2	3:C:344:TYR:CD2	2.25	0.71
3:C:199:MET:HE1	3:C:204:LEU:HD11	1.73	0.71
2:B:512:LEU:HD21	2:B:516:MET:HE3	1.73	0.71
1:A:368:ILE:O	1:A:476:THR:CG2	2.38	0.71
4:D:199:MET:CE	4:D:199:MET:HA	2.21	0.70
1:A:327:MET:SD	1:A:335:VAL:HG13	2.32	0.70
3:C:249:ILE:HD12	3:C:316:MET:HE1	1.73	0.69
1:A:512:LEU:HD21	1:A:516:MET:HE3	1.75	0.69
4:D:249:ILE:HD12	4:D:316:MET:HE1	1.74	0.69
1:A:327:MET:SD	1:A:335:VAL:CG1	2.81	0.69
2:B:368:ILE:HG22	2:B:476:THR:HG22	1.73	0.69
3:C:199:MET:HA	3:C:199:MET:CE	2.23	0.69
1:A:368:ILE:O	1:A:476:THR:HG21	1.92	0.68
3:C:298:PHE:HB3	3:C:318:LEU:HD23	1.75	0.68
1:A:298:PHE:HB3	1:A:318:LEU:HD23	1.75	0.68
1:A:295:VAL:O	1:A:320:LEU:HD12	1.94	0.68
2:B:199:MET:CE	2:B:199:MET:HA	2.24	0.68
1:A:348:LEU:HD11	1:A:510:ILE:CG2	2.23	0.67
1:A:2256:UNK:CB	1:A:2262:UNK:HA	2.24	0.67
1:A:368:ILE:HG22	1:A:476:THR:HG22	1.76	0.66
2:B:295:VAL:O	2:B:320:LEU:HD12	1.95	0.66
2:B:298:PHE:HB3	2:B:318:LEU:HD23	1.75	0.66
4:D:428:ILE:HD13	4:D:505:LEU:CD1	2.25	0.66
1:A:382:ASN:C	1:A:1383:UNK:H	2.03	0.66
1:A:482:ALA:C	1:A:1483:UNK:H	2.04	0.66
1:A:199:MET:HE1	1:A:204:LEU:HD11	1.78	0.66
2:B:204:LEU:HD22	2:B:313:VAL:HG11	1.78	0.66
2:B:291:GLU:OE1	2:B:293:LEU:HD21	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:295:VAL:O	3:C:320:LEU:HD12	1.95	0.65
1:A:326:ALA:CB	1:A:338:MET:HE1	2.26	0.65
1:A:199:MET:HA	1:A:199:MET:CE	2.26	0.65
1:A:363:PRO:HG3	1:A:476:THR:HG22	1.79	0.64
4:D:298:PHE:HB3	4:D:318:LEU:HD23	1.77	0.64
1:A:507:ILE:HG22	1:A:508:ASP:O	1.98	0.64
2:B:348:LEU:HD11	2:B:510:ILE:CG2	2.27	0.64
2:B:199:MET:HE1	2:B:204:LEU:HD11	1.79	0.64
1:A:31:ILE:HG21	1:A:359:LEU:CD1	2.27	0.64
4:D:204:LEU:HD22	4:D:313:VAL:HG11	1.78	0.64
4:D:521:VAL:HG12	4:D:1522:UNK:H	1.64	0.63
1:A:62:MET:HE3	1:A:252:GLY:HA3	1.79	0.63
2:B:243:ILE:HD11	2:B:278:THR:HA	1.80	0.63
1:A:291:GLU:OE1	1:A:293:LEU:HD21	1.98	0.63
3:C:204:LEU:HD22	3:C:313:VAL:HG11	1.80	0.63
3:C:291:GLU:OE1	3:C:293:LEU:HD21	1.99	0.63
1:A:199:MET:HE1	1:A:204:LEU:HD21	1.81	0.63
3:C:62:MET:HE3	3:C:252:GLY:HA3	1.81	0.63
2:B:507:ILE:HG22	2:B:508:ASP:O	1.98	0.63
2:B:482:ALA:C	2:B:1483:UNK:H	2.06	0.62
3:C:363:PRO:C	3:C:1364:UNK:N	2.57	0.62
2:B:237:ALA:HB2	2:B:315:VAL:HG22	1.82	0.62
4:D:291:GLU:OE1	4:D:293:LEU:HD21	1.98	0.62
1:A:204:LEU:HD22	1:A:313:VAL:HG11	1.80	0.62
2:B:199:MET:HE1	2:B:204:LEU:HD21	1.81	0.62
3:C:326:ALA:CB	3:C:338:MET:HE1	2.29	0.62
4:D:327:MET:SD	4:D:335:VAL:HG13	2.40	0.62
2:B:382:ASN:C	2:B:1383:UNK:H	2.05	0.62
2:B:300:VAL:HG11	3:C:26:ILE:HD13	1.82	0.62
2:B:467:TYR:CG	2:B:503:ILE:HD11	2.34	0.62
3:C:243:ILE:HD11	3:C:278:THR:HA	1.81	0.61
2:B:62:MET:HE3	2:B:252:GLY:HA3	1.82	0.61
1:A:243:ILE:HD11	1:A:278:THR:HA	1.82	0.60
4:D:356:MET:HE2	4:D:508:ASP:HB2	1.83	0.60
4:D:326:ALA:CB	4:D:338:MET:HE1	2.30	0.60
1:A:300:VAL:CG1	4:D:26:ILE:HD13	2.30	0.60
1:A:467:TYR:CG	1:A:503:ILE:HD11	2.37	0.60
4:D:199:MET:HA	4:D:199:MET:HE2	1.83	0.59
1:A:349:ASN:OD1	1:A:350:ASP:N	2.35	0.59
1:A:232:ALA:HB3	1:A:320:LEU:HB3	1.83	0.59
1:A:238:GLY:O	1:A:241:VAL:HG23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:236:ILE:HD11	4:D:249:ILE:CD1	2.18	0.59
4:D:264:PHE:HB3	4:D:280:THR:HG21	1.85	0.59
4:D:243:ILE:HD11	4:D:278:THR:HA	1.85	0.59
4:D:295:VAL:O	4:D:320:LEU:HD12	2.01	0.59
4:D:428:ILE:CD1	4:D:505:LEU:HD12	2.32	0.59
4:D:359:LEU:HD23	4:D:505:LEU:HD22	1.85	0.59
2:B:349:ASN:OD1	2:B:350:ASP:N	2.35	0.59
1:A:265:ILE:HD12	1:A:283:TYR:CD1	2.38	0.59
2:B:424:ILE:HB	2:B:468:ILE:HG23	1.85	0.59
3:C:199:MET:HA	3:C:199:MET:HE2	1.85	0.59
3:C:35:TYR:O	3:C:37:ARG:N	2.36	0.58
1:A:264:PHE:HB3	1:A:280:THR:HG21	1.85	0.58
4:D:67:TYR:CE1	4:D:208:LEU:HD22	2.38	0.58
2:B:306:LEU:HD22	2:B:311:ILE:HG21	1.85	0.58
2:B:264:PHE:HB3	2:B:280:THR:HG21	1.85	0.58
3:C:264:PHE:HB3	3:C:280:THR:HG21	1.84	0.58
2:B:363:PRO:HG3	2:B:476:THR:HG22	1.86	0.58
4:D:306:LEU:HD22	4:D:311:ILE:HG21	1.86	0.58
4:D:237:ALA:HB2	4:D:315:VAL:HG22	1.86	0.58
2:B:326:ALA:CB	2:B:338:MET:HE1	2.33	0.58
1:A:249:ILE:HD12	1:A:316:MET:CE	2.33	0.57
3:C:35:TYR:O	3:C:36:PRO:C	2.46	0.57
4:D:199:MET:CE	4:D:204:LEU:HD11	2.32	0.57
3:C:67:TYR:CE1	3:C:208:LEU:HD22	2.39	0.57
3:C:506:LYS:N	3:C:1505:UNK:O	2.37	0.57
2:B:249:ILE:HD12	2:B:316:MET:CE	2.35	0.57
1:A:67:TYR:CE1	1:A:208:LEU:HD22	2.40	0.57
1:A:424:ILE:HB	1:A:468:ILE:HG23	1.87	0.57
1:A:318:LEU:HD22	1:A:319:GLY:H	1.70	0.57
4:D:363:PRO:C	4:D:1364:UNK:N	2.63	0.56
1:A:306:LEU:HD22	1:A:311:ILE:HG21	1.87	0.56
1:A:1387:UNK:C	1:A:1389:UNK:H2	2.18	0.56
2:B:67:TYR:CE1	2:B:208:LEU:HD22	2.40	0.56
3:C:428:ILE:HA	3:C:437:GLY:HA2	1.87	0.56
4:D:1364:UNK:O	4:D:1365:UNK:C	2.53	0.56
2:B:351:ARG:HA	2:B:461:VAL:HG21	1.87	0.56
1:A:351:ARG:HA	1:A:461:VAL:HG21	1.88	0.56
1:A:429:TYR:CD1	1:A:438:ILE:HD12	2.40	0.56
2:B:428:ILE:HA	2:B:437:GLY:HA2	1.88	0.56
3:C:232:ALA:HB3	3:C:320:LEU:HB3	1.86	0.56
1:A:176:ALA:HB3	2:B:178:SER:CB	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:199:MET:CE	3:C:204:LEU:HD11	2.36	0.56
4:D:62:MET:HE3	4:D:252:GLY:HA3	1.87	0.56
2:B:278:THR:HG23	2:B:279:GLN:N	2.21	0.56
4:D:265:ILE:HD12	4:D:283:TYR:CD1	2.41	0.56
4:D:327:MET:SD	4:D:335:VAL:CG1	2.94	0.56
1:A:26:ILE:HD11	4:D:275:THR:OG1	2.05	0.55
1:A:213:ARG:HE	1:A:228:THR:CG2	2.18	0.55
2:B:265:ILE:HD12	2:B:283:TYR:CD1	2.41	0.55
2:B:344:TYR:O	2:B:345:GLU:C	2.49	0.55
2:B:429:TYR:CD1	2:B:438:ILE:HD12	2.41	0.55
2:B:327:MET:SD	2:B:335:VAL:HG13	2.46	0.55
2:B:1387:UNK:C	2:B:1389:UNK:H2	2.18	0.55
4:D:337:GLU:HG2	4:D:344:TYR:CD2	2.42	0.55
1:A:327:MET:SD	1:A:335:VAL:HG12	2.45	0.55
4:D:335:VAL:O	4:D:339:VAL:HG23	2.07	0.55
1:A:428:ILE:HG23	1:A:463:THR:OG1	2.07	0.55
3:C:265:ILE:HD12	3:C:283:TYR:CD1	2.41	0.55
4:D:428:ILE:HA	4:D:437:GLY:HA2	1.89	0.55
2:B:199:MET:HA	2:B:199:MET:HE2	1.87	0.55
2:B:232:ALA:HB3	2:B:320:LEU:HB3	1.87	0.55
3:C:327:MET:SD	3:C:335:VAL:HG13	2.46	0.55
1:A:183:LEU:HD11	2:B:183:LEU:HD11	1.89	0.55
2:B:465:ILE:HG21	2:B:505:LEU:HD21	1.88	0.55
2:B:213:ARG:HE	2:B:228:THR:CG2	2.20	0.55
1:A:237:ALA:HB2	1:A:315:VAL:HG22	1.88	0.55
3:C:237:ALA:HB2	3:C:315:VAL:HG22	1.89	0.55
4:D:218:GLU:O	4:D:227:MET:HE2	2.06	0.54
3:C:296:ALA:HB2	3:C:320:LEU:HD13	1.88	0.54
1:A:199:MET:CE	1:A:204:LEU:HD11	2.37	0.54
4:D:362:VAL:HG13	4:D:363:PRO:HD2	1.90	0.54
2:B:1386:UNK:O	2:B:1387:UNK:C	2.56	0.54
4:D:232:ALA:HB3	4:D:320:LEU:HB3	1.88	0.54
2:B:62:MET:HE1	2:B:249:ILE:HA	1.90	0.54
2:B:199:MET:CE	2:B:204:LEU:HD11	2.37	0.54
3:C:356:MET:HE2	3:C:508:ASP:HB2	1.88	0.54
2:B:248:ALA:HB2	3:C:38:ILE:HG21	1.90	0.54
1:A:295:VAL:O	1:A:320:LEU:CD1	2.56	0.54
3:C:278:THR:HG23	3:C:279:GLN:N	2.22	0.54
3:C:318:LEU:HD22	3:C:319:GLY:H	1.72	0.54
4:D:357:VAL:HG11	4:D:428:ILE:HD11	1.90	0.54
2:B:35:TYR:O	2:B:38:ILE:N	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:GLU:O	1:A:227:MET:HE2	2.08	0.54
2:B:361:LYS:HE3	2:B:474:LYS:HZ2	1.74	0.53
1:A:178:SER:CB	2:B:176:ALA:HB3	2.39	0.53
4:D:226:LEU:HD21	4:D:336:ARG:HG2	1.90	0.53
4:D:521:VAL:C	4:D:1522:UNK:H2	2.16	0.53
1:A:428:ILE:HA	1:A:437:GLY:HA2	1.90	0.53
2:B:318:LEU:HD22	2:B:319:GLY:H	1.74	0.53
2:B:337:GLU:HG2	2:B:344:TYR:CD2	2.44	0.53
3:C:249:ILE:HD12	3:C:316:MET:CE	2.38	0.53
4:D:359:LEU:HD23	4:D:505:LEU:CD2	2.38	0.53
1:A:465:ILE:HG21	1:A:505:LEU:HD21	1.90	0.53
2:B:295:VAL:O	2:B:320:LEU:CD1	2.56	0.53
1:A:265:ILE:HD12	1:A:283:TYR:CE1	2.43	0.53
2:B:265:ILE:HD12	2:B:283:TYR:CE1	2.44	0.53
2:B:226:LEU:HD21	2:B:336:ARG:HG2	1.90	0.53
2:B:470:ALA:HB1	2:B:503:ILE:O	2.09	0.53
3:C:213:ARG:HE	3:C:228:THR:CG2	2.22	0.53
4:D:249:ILE:HD12	4:D:316:MET:CE	2.38	0.53
4:D:306:LEU:HD22	4:D:311:ILE:CG2	2.39	0.53
4:D:278:THR:HG23	4:D:279:GLN:N	2.23	0.52
3:C:230:HIS:N	3:C:323:GLU:OE2	2.40	0.52
3:C:337:GLU:HG2	3:C:344:TYR:CG	2.43	0.52
3:C:236:ILE:HD11	3:C:249:ILE:CD1	2.18	0.52
3:C:327:MET:SD	3:C:335:VAL:CG1	2.98	0.52
3:C:1364:UNK:O	3:C:1365:UNK:C	2.57	0.52
3:C:362:VAL:HG13	3:C:363:PRO:HD2	1.91	0.52
1:A:361:LYS:HE3	1:A:474:LYS:HZ2	1.75	0.52
2:B:327:MET:SD	2:B:335:VAL:CG1	2.98	0.52
3:C:218:GLU:O	3:C:227:MET:HE2	2.09	0.52
4:D:213:ARG:HE	4:D:228:THR:CG2	2.23	0.52
4:D:428:ILE:CD1	4:D:505:LEU:CD1	2.88	0.52
1:A:521:VAL:HG12	1:A:522:ILE:N	2.25	0.52
1:A:199:MET:HA	1:A:199:MET:HE2	1.91	0.52
1:A:26:ILE:CD1	4:D:275:THR:OG1	2.58	0.51
1:A:55:LEU:HD13	1:A:232:ALA:HB2	1.92	0.51
3:C:212:ASP:OD1	3:C:213:ARG:N	2.38	0.51
3:C:265:ILE:HD12	3:C:283:TYR:CE1	2.45	0.51
3:C:306:LEU:HD22	3:C:311:ILE:HG21	1.91	0.51
2:B:35:TYR:O	2:B:36:PRO:C	2.54	0.51
3:C:62:MET:HE1	3:C:249:ILE:HA	1.91	0.51
1:A:318:LEU:HD22	1:A:319:GLY:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:237:ALA:CB	2:B:315:VAL:HG22	2.40	0.51
3:C:425:LEU:O	3:C:426:ASN:C	2.53	0.51
2:B:372:THR:HG21	2:B:473:PHE:CD1	2.46	0.51
2:B:428:ILE:HG23	2:B:463:THR:OG1	2.11	0.51
1:A:372:THR:HG21	1:A:473:PHE:CD1	2.45	0.51
2:B:306:LEU:HD22	2:B:311:ILE:CG2	2.40	0.51
2:B:521:VAL:HG12	2:B:522:ILE:N	2.26	0.51
3:C:226:LEU:HD21	3:C:336:ARG:HG2	1.91	0.51
3:C:357:VAL:HG11	3:C:428:ILE:HD11	1.93	0.51
1:A:62:MET:HE1	1:A:249:ILE:HA	1.92	0.50
2:B:212:ASP:OD1	2:B:213:ARG:N	2.36	0.50
3:C:516:MET:HA	3:C:516:MET:HE2	1.93	0.50
4:D:31:ILE:HG21	4:D:359:LEU:HD11	1.91	0.50
4:D:357:VAL:HG22	4:D:507:ILE:HG13	1.92	0.50
4:D:199:MET:HE1	4:D:204:LEU:HD21	1.94	0.50
1:A:236:ILE:HD11	1:A:249:ILE:CD1	2.20	0.50
1:A:356:MET:HE2	1:A:508:ASP:HB2	1.93	0.50
2:B:334:ASP:C	2:B:334:ASP:OD1	2.54	0.50
2:B:335:VAL:O	2:B:339:VAL:HG23	2.12	0.50
1:A:230:HIS:N	1:A:323:GLU:OE2	2.40	0.50
1:A:361:LYS:HG2	1:A:504:ASN:OD1	2.12	0.50
4:D:265:ILE:HD12	4:D:283:TYR:CE1	2.46	0.50
3:C:199:MET:HE1	3:C:204:LEU:HD21	1.93	0.49
1:A:22:THR:HG23	4:D:303:PRO:HG2	1.94	0.49
1:A:1386:UNK:O	1:A:1387:UNK:C	2.59	0.49
4:D:37:ARG:HA	4:D:355:SER:HA	1.95	0.49
1:A:278:THR:HG23	1:A:279:GLN:N	2.26	0.49
4:D:62:MET:HE1	4:D:249:ILE:HA	1.95	0.49
1:A:380:VAL:HG22	1:A:468:ILE:HD13	1.94	0.49
2:B:348:LEU:HB2	2:B:514:GLN:OE1	2.12	0.49
3:C:318:LEU:HD22	3:C:319:GLY:N	2.28	0.49
1:A:61:ARG:CZ	3:C:60:LEU:HD13	2.41	0.49
1:A:334:ASP:OD1	1:A:334:ASP:C	2.56	0.49
1:A:199:MET:HA	1:A:199:MET:HE3	1.94	0.49
2:B:296:ALA:HB2	2:B:320:LEU:HD13	1.94	0.49
4:D:31:ILE:HG21	4:D:359:LEU:CD1	2.42	0.49
4:D:362:VAL:CG1	4:D:363:PRO:HD2	2.43	0.49
4:D:197:ASP:O	4:D:201:LYS:HD2	2.13	0.49
1:A:212:ASP:OD1	1:A:213:ARG:N	2.39	0.49
2:B:55:LEU:HD13	2:B:232:ALA:HB2	1.95	0.49
3:C:295:VAL:O	3:C:320:LEU:CD1	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ALA:HB2	1:A:320:LEU:HD13	1.94	0.48
2:B:35:TYR:O	2:B:37:ARG:N	2.46	0.48
1:A:197:ASP:O	1:A:201:LYS:HD2	2.13	0.48
2:B:199:MET:HA	2:B:199:MET:HE3	1.95	0.48
1:A:2272:UNK:O	1:A:2276:UNK:C	2.61	0.48
4:D:238:GLY:O	4:D:241:VAL:HG23	2.13	0.48
1:A:306:LEU:HD22	1:A:311:ILE:CG2	2.43	0.48
3:C:55:LEU:HD13	3:C:232:ALA:HB2	1.94	0.48
4:D:199:MET:HA	4:D:199:MET:HE3	1.95	0.48
3:C:348:LEU:H	3:C:514:GLN:HE22	1.62	0.48
3:C:436:ILE:HD11	3:C:1456:UNK:CB	2.43	0.48
2:B:230:HIS:N	2:B:323:GLU:OE2	2.45	0.48
3:C:199:MET:HA	3:C:199:MET:HE3	1.95	0.48
3:C:18:ALA:O	3:C:22:THR:HB	2.14	0.48
3:C:424:ILE:HG23	3:C:1528:UNK:CB	2.44	0.48
4:D:31:ILE:O	4:D:37:ARG:NH1	2.47	0.48
4:D:318:LEU:HD22	4:D:319:GLY:H	1.77	0.48
2:B:318:LEU:HD22	2:B:319:GLY:N	2.27	0.47
3:C:357:VAL:HG22	3:C:507:ILE:HG13	1.96	0.47
1:A:226:LEU:HD21	1:A:336:ARG:HG2	1.95	0.47
1:A:248:ALA:HB2	4:D:38:ILE:HG21	1.96	0.47
1:A:426:ASN:N	1:A:426:ASN:HD22	2.13	0.47
2:B:218:GLU:O	2:B:227:MET:HE2	2.14	0.47
2:B:238:GLY:O	2:B:241:VAL:HG23	2.15	0.47
3:C:197:ASP:O	3:C:201:LYS:HD2	2.14	0.47
3:C:512:LEU:O	3:C:513:LYS:C	2.57	0.47
4:D:296:ALA:HB2	4:D:320:LEU:HD13	1.96	0.47
4:D:436:ILE:HD11	4:D:1456:UNK:CB	2.45	0.47
1:A:326:ALA:CB	1:A:338:MET:CE	2.93	0.47
2:B:361:LYS:HG2	2:B:504:ASN:OD1	2.14	0.47
1:A:359:LEU:HD21	1:A:470:ALA:HA	1.97	0.47
1:A:368:ILE:HG22	1:A:476:THR:CG2	2.43	0.47
2:B:467:TYR:CD2	2:B:503:ILE:HD11	2.50	0.47
4:D:230:HIS:N	4:D:323:GLU:OE2	2.44	0.47
3:C:238:GLY:O	3:C:241:VAL:HG23	2.14	0.47
3:C:425:LEU:HD13	3:C:440:GLU:OE2	2.15	0.47
4:D:237:ALA:CB	4:D:315:VAL:HG22	2.45	0.47
1:A:503:ILE:HG23	1:A:505:LEU:HG	1.97	0.47
2:B:356:MET:HE2	2:B:508:ASP:HB2	1.95	0.47
3:C:306:LEU:HD22	3:C:311:ILE:CG2	2.45	0.47
3:C:362:VAL:CG1	3:C:363:PRO:HD2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:348:LEU:H	4:D:514:GLN:HE22	1.63	0.46
4:D:356:MET:HE2	4:D:508:ASP:CB	2.46	0.46
4:D:55:LEU:HD13	4:D:232:ALA:HB2	1.97	0.46
2:B:503:ILE:HG23	2:B:505:LEU:HG	1.97	0.46
1:A:18:ALA:O	1:A:22:THR:HB	2.14	0.46
1:A:354:ALA:HA	1:A:430:VAL:HG21	1.98	0.46
2:B:213:ARG:HE	2:B:228:THR:HG21	1.80	0.46
2:B:303:PRO:HG2	3:C:22:THR:HG23	1.97	0.46
2:B:380:VAL:HG22	2:B:468:ILE:HD13	1.97	0.46
4:D:516:MET:HE2	4:D:516:MET:HA	1.98	0.46
2:B:197:ASP:O	2:B:201:LYS:HD2	2.15	0.45
2:B:244:ASN:HB3	3:C:38:ILE:HD12	1.98	0.45
1:A:213:ARG:HE	1:A:228:THR:HG21	1.80	0.45
1:A:275:THR:OG1	4:D:26:ILE:HD12	2.16	0.45
2:B:186:HIS:HB3	2:B:188:THR:HG23	1.98	0.45
4:D:505:LEU:HD21	4:D:1470:UNK:CB	2.47	0.45
2:B:507:ILE:CG2	2:B:511:ALA:HB3	2.47	0.45
3:C:431:TYR:O	3:C:432:ASP:C	2.59	0.45
1:A:507:ILE:CG2	1:A:511:ALA:HB3	2.47	0.45
1:A:52:ILE:HG13	1:A:322:VAL:HG11	1.98	0.45
3:C:335:VAL:O	3:C:339:VAL:HG23	2.17	0.45
4:D:18:ALA:O	4:D:22:THR:HB	2.17	0.45
4:D:318:LEU:HD22	4:D:319:GLY:N	2.32	0.45
2:B:60:LEU:HD13	4:D:61:ARG:CZ	2.47	0.45
2:B:222:ASP:OD1	2:B:225:HIS:N	2.50	0.45
2:B:354:ALA:HA	2:B:430:VAL:HG21	1.98	0.45
3:C:52:ILE:HG13	3:C:322:VAL:HG11	1.97	0.45
4:D:295:VAL:O	4:D:320:LEU:CD1	2.65	0.44
3:C:237:ALA:CB	3:C:315:VAL:HG22	2.46	0.44
1:A:348:LEU:HB2	1:A:514:GLN:OE1	2.17	0.44
1:A:237:ALA:CB	1:A:315:VAL:HG22	2.47	0.44
2:B:300:VAL:CG1	3:C:26:ILE:HD13	2.47	0.44
3:C:2241:UNK:O	3:C:2242:UNK:C	2.65	0.44
4:D:56:ARG:HB3	4:D:211:ILE:HD13	2.00	0.44
2:B:336:ARG:HB3	2:B:344:TYR:OH	2.18	0.44
3:C:349:ASN:HB3	3:C:352:ASN:ND2	2.33	0.44
4:D:428:ILE:HD12	4:D:505:LEU:HD12	1.99	0.44
2:B:426:ASN:N	2:B:426:ASN:HD22	2.16	0.44
3:C:436:ILE:CD1	3:C:1456:UNK:CB	2.96	0.44
3:C:1463:UNK:O	3:C:1464:UNK:CB	2.66	0.44
4:D:212:ASP:OD1	4:D:213:ARG:N	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ARG:HE	1:A:228:THR:HG22	1.82	0.44
2:B:61:ARG:CZ	4:D:60:LEU:HD13	2.48	0.44
2:B:326:ALA:CB	2:B:338:MET:CE	2.96	0.44
4:D:223:LYS:C	4:D:335:VAL:HG22	2.42	0.44
2:B:428:ILE:C	2:B:463:THR:HG1	2.26	0.43
3:C:101:ARG:O	3:C:2210:UNK:C	2.66	0.43
2:B:292:TRP:O	2:B:293:LEU:HD23	2.17	0.43
3:C:31:ILE:HG21	3:C:359:LEU:HD11	2.00	0.43
3:C:1365:UNK:O	3:C:1366:UNK:C	2.66	0.43
4:D:436:ILE:CD1	4:D:1456:UNK:CB	2.96	0.43
1:A:335:VAL:O	1:A:339:VAL:HG23	2.19	0.43
3:C:22:THR:O	3:C:23:LYS:C	2.62	0.43
3:C:213:ARG:HE	3:C:228:THR:HG22	1.83	0.43
1:A:467:TYR:CD2	1:A:503:ILE:HD11	2.53	0.43
1:A:186:HIS:HB3	1:A:188:THR:HG23	2.00	0.43
2:B:368:ILE:HG22	2:B:476:THR:CG2	2.44	0.43
1:A:206:PHE:CE1	1:A:237:ALA:HB3	2.54	0.43
4:D:206:PHE:CE1	4:D:237:ALA:HB3	2.54	0.43
2:B:359:LEU:HD21	2:B:470:ALA:HA	2.01	0.43
4:D:431:TYR:O	4:D:432:ASP:C	2.62	0.42
4:D:334:ASP:OD1	4:D:334:ASP:C	2.62	0.42
4:D:348:LEU:CD1	4:D:510:ILE:HG22	2.49	0.42
1:A:22:THR:CG2	4:D:303:PRO:HD2	2.50	0.42
2:B:207:LYS:O	2:B:208:LEU:HD23	2.18	0.42
3:C:101:ARG:HH12	3:C:2248:UNK:CB	2.33	0.42
4:D:434:ASN:HD22	4:D:521:VAL:H	1.67	0.42
1:A:470:ALA:HB1	1:A:503:ILE:O	2.19	0.42
2:B:357:VAL:HG22	2:B:507:ILE:HG12	2.02	0.42
4:D:349:ASN:HB3	4:D:352:ASN:ND2	2.34	0.42
4:D:512:LEU:O	4:D:513:LYS:C	2.61	0.42
2:B:52:ILE:HG13	2:B:322:VAL:HG11	2.00	0.42
1:A:2254:UNK:O	1:A:2258:UNK:CB	2.67	0.42
3:C:206:PHE:CE1	3:C:237:ALA:HB3	2.55	0.42
3:C:326:ALA:CB	3:C:338:MET:CE	2.98	0.42
3:C:186:HIS:HB3	3:C:188:THR:HG23	2.02	0.42
3:C:292:TRP:O	3:C:293:LEU:HD23	2.20	0.42
1:A:222:ASP:OD1	1:A:225:HIS:N	2.53	0.41
1:A:242:ASP:OD2	1:A:244:ASN:ND2	2.53	0.41
1:A:503:ILE:HG21	1:A:505:LEU:HD12	2.02	0.41
4:D:1365:UNK:O	4:D:1366:UNK:C	2.68	0.41
1:A:62:MET:CE	1:A:252:GLY:HA3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:LEU:O	1:A:1483:UNK:N	2.54	0.41
2:B:253:LEU:HD23	2:B:320:LEU:HD22	2.03	0.41
2:B:361:LYS:HD2	2:B:474:LYS:HZ1	1.86	0.41
2:B:479:LEU:O	2:B:1483:UNK:N	2.53	0.41
1:A:26:ILE:HD13	4:D:300:VAL:HG11	2.02	0.41
2:B:34:SER:O	2:B:35:TYR:C	2.63	0.41
2:B:62:MET:HG2	3:C:42:PHE:HB3	2.03	0.41
2:B:423:SER:HB2	2:B:426:ASN:HD21	1.86	0.41
1:A:303:PRO:HD2	4:D:22:THR:CG2	2.51	0.41
2:B:303:PRO:HD2	3:C:22:THR:CG2	2.51	0.41
3:C:10:MET:HG2	3:C:18:ALA:HB2	2.03	0.41
3:C:356:MET:HE2	3:C:508:ASP:CB	2.50	0.41
4:D:213:ARG:HE	4:D:228:THR:HG22	1.83	0.41
4:D:222:ASP:OD1	4:D:225:HIS:N	2.54	0.41
4:D:326:ALA:CB	4:D:338:MET:CE	2.98	0.41
4:D:1463:UNK:O	4:D:1464:UNK:CB	2.68	0.41
3:C:46:HIS:CG	3:C:47:PRO:HD2	2.56	0.41
3:C:348:LEU:CD1	3:C:510:ILE:HG22	2.51	0.41
4:D:363:PRO:C	4:D:1364:UNK:HA	2.46	0.41
1:A:97:ALA:HB2	2:B:97:ALA:HB2	2.03	0.41
1:A:223:LYS:C	1:A:335:VAL:HG22	2.44	0.41
1:A:372:THR:HG21	1:A:473:PHE:CG	2.56	0.40
2:B:503:ILE:HG21	2:B:505:LEU:HD12	2.02	0.40
2:B:213:ARG:NE	2:B:228:THR:HG21	2.35	0.40
2:B:436:ILE:HA	2:B:1523:UNK:H	1.86	0.40
1:A:213:ARG:NE	1:A:228:THR:HG21	2.36	0.40
2:B:56:ARG:HB3	2:B:211:ILE:HD13	2.03	0.40
4:D:45:THR:HG23	4:D:50:ASP:OD2	2.22	0.40
4:D:186:HIS:HB3	4:D:188:THR:HG23	2.02	0.40
1:A:22:THR:O	1:A:23:LYS:C	2.65	0.40
3:C:182:THR:CG2	3:C:183:LEU:N	2.85	0.40
4:D:215:PHE:CE2	4:D:228:THR:HG23	2.57	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)
2:B:220:LYS:NZ	4:D:518:LYS:CD[3_655]	1.94	0.26

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	372/665 (56%)	345 (93%)	24 (6%)	3 (1%)	16	48
2	B	346/648 (53%)	320 (92%)	22 (6%)	4 (1%)	10	40
3	C	315/701 (45%)	283 (90%)	27 (9%)	5 (2%)	7	35
4	D	315/685 (46%)	287 (91%)	26 (8%)	2 (1%)	21	55
All	All	1348/2699 (50%)	1235 (92%)	99 (7%)	14 (1%)	12	44

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	349	ASN
2	B	35	TYR
2	B	349	ASN
3	C	35	TYR
3	C	426	ASN
3	C	432	ASP
1	A	276	PRO
2	B	276	PRO
3	C	276	PRO
4	D	276	PRO
1	A	295	VAL
2	B	295	VAL
3	C	295	VAL
4	D	295	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	339/497 (68%)	311 (92%)	28 (8%)	10	37
2	B	316/497 (64%)	291 (92%)	25 (8%)	11	39
3	C	286/497 (58%)	259 (91%)	27 (9%)	8	31
4	D	286/498 (57%)	259 (91%)	27 (9%)	8	31
All	All	1227/1989 (62%)	1120 (91%)	107 (9%)	9	35

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	25	LEU
1	A	37	ARG
1	A	41	VAL
1	A	80	LYS
1	A	171	PHE
1	A	180	LYS
1	A	182	THR
1	A	188	THR
1	A	197	ASP
1	A	199	MET
1	A	217	ARG
1	A	243	ILE
1	A	253	LEU
1	A	278	THR
1	A	295	VAL
1	A	318	LEU
1	A	325	LEU
1	A	342	GLN
1	A	350	ASP
1	A	351	ARG
1	A	371	LEU
1	A	426	ASN
1	A	434	ASN
1	A	463	THR
1	A	468	ILE
1	A	474	LYS
1	A	481	GLU
2	B	37	ARG
2	B	39	LYS
2	B	41	VAL
2	B	80	LYS
2	B	171	PHE

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Mol	Chain	Res	Type
2	B	180	LYS
2	B	182	THR
2	B	188	THR
2	B	197	ASP
2	B	199	MET
2	B	217	ARG
2	B	243	ILE
2	B	278	THR
2	B	318	LEU
2	B	325	LEU
2	B	342	GLN
2	B	350	ASP
2	B	351	ARG
2	B	371	LEU
2	B	426	ASN
2	B	434	ASN
2	B	463	THR
2	B	468	ILE
2	B	474	LYS
2	B	481	GLU
3	C	22	THR
3	C	25	LEU
3	C	31	ILE
3	C	37	ARG
3	C	38	ILE
3	C	41	VAL
3	C	171	PHE
3	C	180	LYS
3	C	182	THR
3	C	188	THR
3	C	197	ASP
3	C	199	MET
3	C	217	ARG
3	C	243	ILE
3	C	278	THR
3	C	295	VAL
3	C	318	LEU
3	C	325	LEU
3	C	342	GLN
3	C	345	GLU
3	C	350	ASP
3	C	361	LYS

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Mol	Chain	Res	Type
3	C	424	ILE
3	C	428	ILE
3	C	434	ASN
3	C	507	ILE
3	C	512	LEU
4	D	22	THR
4	D	25	LEU
4	D	33	GLU
4	D	37	ARG
4	D	38	ILE
4	D	41	VAL
4	D	171	PHE
4	D	180	LYS
4	D	182	THR
4	D	188	THR
4	D	197	ASP
4	D	199	MET
4	D	217	ARG
4	D	243	ILE
4	D	278	THR
4	D	295	VAL
4	D	318	LEU
4	D	325	LEU
4	D	342	GLN
4	D	345	GLU
4	D	350	ASP
4	D	361	LYS
4	D	428	ILE
4	D	434	ASN
4	D	507	ILE
4	D	512	LEU
4	D	521	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	186	HIS
1	A	342	GLN
1	A	382	ASN
1	A	426	ASN
2	B	57	GLN

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Mol	Chain	Res	Type
2	B	186	HIS
2	B	342	GLN
2	B	382	ASN
2	B	426	ASN
3	C	186	HIS
3	C	342	GLN
3	C	514	GLN
4	D	186	HIS
4	D	342	GLN
4	D	514	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	D	12
3	C	11

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Mol	Chain	Number of breaks
2	B	9
1	A	9

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1997:UNK	C	2215:UNK	N	104.15
1	A	1997:UNK	C	2214:UNK	N	90.88
1	D	1537:UNK	C	2216:UNK	N	85.04
1	C	1537:UNK	C	2210:UNK	N	80.26
1	D	1411:UNK	C	1449:UNK	N	31.12
1	C	1411:UNK	C	1449:UNK	N	31.10
1	A	1412:UNK	C	1483:UNK	N	26.38
1	B	1412:UNK	C	1483:UNK	N	26.38
1	B	1523:UNK	C	1533:UNK	N	20.81
1	D	2224:UNK	C	2233:UNK	N	19.66
1	A	1537:UNK	C	1991:UNK	N	18.38
1	B	1495:UNK	C	1523:UNK	N	16.23
1	C	2225:UNK	C	2229:UNK	N	16.19
1	C	1505:UNK	C	1527:UNK	N	15.40
1	D	1504:UNK	C	1522:UNK	N	14.45
1	B	1537:UNK	C	1991:UNK	N	14.36
1	B	2222:UNK	C	2233:UNK	N	14.10
1	B	2243:UNK	C	2250:UNK	N	13.12
1	D	2243:UNK	C	2250:UNK	N	13.11
1	A	2225:UNK	C	2230:UNK	N	12.78
1	D	1382:UNK	C	1389:UNK	N	10.02
1	D	2256:UNK	C	2266:UNK	N	10.02
1	C	1382:UNK	C	1389:UNK	N	9.96
1	A	2243:UNK	C	2248:UNK	N	9.76
1	C	1495:UNK	C	1503:UNK	N	9.66
1	D	1495:UNK	C	1503:UNK	N	9.65
1	D	1523:UNK	C	1527:UNK	N	9.14
1	C	2243:UNK	C	2247:UNK	N	7.78
1	C	2259:UNK	C	2265:UNK	N	7.25
1	C	1486:UNK	C	1489:UNK	N	6.40
1	D	1486:UNK	C	1489:UNK	N	6.40
1	B	2256:UNK	C	2265:UNK	N	6.11
1	A	1495:UNK	C	1527:UNK	N	6.07
1	C	1395:UNK	C	1405:UNK	N	5.85
1	D	1395:UNK	C	1405:UNK	N	5.85
1	A	2262:UNK	C	2267:UNK	N	5.09
1	A	1530:UNK	C	1533:UNK	N	3.04

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1387:UNK	C	1389:UNK	N	3.01
1	B	1387:UNK	C	1389:UNK	N	3.01
1	D	1530:UNK	C	1533:UNK	N	2.91
1	C	1530:UNK	C	1533:UNK	N	2.89

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	382/665 (57%)	0.72	28 (7%) 21 13	132, 140, 141, 144	0
2	B	356/648 (54%)	0.64	20 (5%) 30 19	130, 140, 141, 147	0
3	C	323/701 (46%)	1.06	41 (12%) 8 6	126, 140, 141, 157	0
4	D	323/685 (47%)	0.89	31 (9%) 13 9	126, 140, 141, 146	0
All	All	1384/2699 (51%)	0.82	120 (8%) 16 11	126, 140, 141, 157	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	431	TYR	6.4
1	A	436	ILE	5.6
4	D	244	ASN	5.2
3	C	91	ASP	4.7
1	A	7	ILE	4.4
3	C	44	LYS	4.3
2	B	502	ASP	3.9
3	C	7	ILE	3.8
1	A	521	VAL	3.7
3	C	507	ILE	3.7
3	C	436	ILE	3.7
1	A	18	ALA	3.7
3	C	60	LEU	3.6
2	B	379	CYS	3.6
4	D	362	VAL	3.4
1	A	15	PHE	3.4
2	B	312	ASP	3.4
3	C	434	ASN	3.3
3	C	273	TYR	3.3
4	D	7	ILE	3.2
3	C	515	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	84	PRO	3.2
4	D	43	GLY	3.1
3	C	67	TYR	3.1
3	C	45	THR	3.1
3	C	271	SER	3.0
1	A	28	ALA	3.0
2	B	40	PRO	3.0
1	A	63	GLY	3.0
4	D	171	PHE	3.0
4	D	431	TYR	2.9
3	C	425	LEU	2.9
4	D	515	ILE	2.9
2	B	362	VAL	2.9
4	D	60	LEU	2.8
1	A	503	ILE	2.8
4	D	516	MET	2.8
4	D	1481	GLU	2.8
1	A	31	ILE	2.8
3	C	424	ILE	2.7
4	D	42	PHE	2.7
4	D	31	ILE	2.7
2	B	244	ASN	2.7
4	D	341	PRO	2.7
1	A	16	GLU	2.7
1	A	260	THR	2.7
2	B	39	LYS	2.6
3	C	43	GLY	2.6
3	C	433	GLY	2.6
3	C	204	LEU	2.6
1	A	355	SER	2.6
2	B	423	SER	2.6
4	D	345	GLU	2.6
1	A	181	LEU	2.6
1	A	19	TRP	2.6
2	B	38	ILE	2.6
4	D	297	THR	2.6
2	B	449	PHE	2.5
3	C	57	GLN	2.5
2	B	295	VAL	2.5
1	A	68	ILE	2.5
4	D	38	ILE	2.5
3	C	280	THR	2.5

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Mol	Chain	Res	Type	RSRZ
4	D	436	ILE	2.4
1	A	42	PHE	2.4
3	C	346	HIS	2.4
4	D	63	GLY	2.4
4	D	346	HIS	2.4
1	A	336	ARG	2.4
4	D	439	PRO	2.4
1	A	67	TYR	2.4
3	C	295	VAL	2.4
3	C	87	MET	2.4
1	A	61	ARG	2.3
3	C	249	ILE	2.3
4	D	91	ASP	2.3
3	C	427	GLU	2.3
4	D	440	GLU	2.3
2	B	87	MET	2.3
3	C	81	GLN	2.3
3	C	510	ILE	2.3
2	B	333	ALA	2.3
4	D	55	LEU	2.3
3	C	236	ILE	2.2
4	D	29	LYS	2.2
4	D	65	GLU	2.2
3	C	253	LEU	2.2
3	C	329	SER	2.2
1	A	226	LEU	2.2
3	C	516	MET	2.2
4	D	512	LEU	2.2
3	C	313	VAL	2.2
4	D	322	VAL	2.2
2	B	424	ILE	2.2
1	A	37	ARG	2.2
1	A	171	PHE	2.2
1	A	41	VAL	2.1
4	D	435	VAL	2.1
3	C	361	LYS	2.1
1	A	237	ALA	2.1
3	C	440	GLU	2.1
3	C	321	GLY	2.1
2	B	171	PHE	2.1
4	D	180	LYS	2.1
4	D	363	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	347	LYS	2.1
1	A	38	ILE	2.1
1	A	340	TYR	2.1
3	C	519	ASN	2.1
3	C	191	TRP	2.1
3	C	508	ASP	2.1
4	D	4	ARG	2.0
3	C	192	PHE	2.0
3	C	221	GLU	2.0
2	B	461	VAL	2.0
1	A	368	ILE	2.0
2	B	31	ILE	2.0
2	B	452	PHE	2.0
1	A	39	LYS	2.0
2	B	348	LEU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.