Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:51 AM GMT

PDB ID	:	2UZX
Title	:	STRUCTURE OF THE HUMAN RECEPTOR TYROSINE KINASE MET IN COMPLEX WITH THE LISTERIA MONOCYTOGENES INVASION PROTEIN INLB: CRYSTAL FORM I
Authors	:	Niemann, H.H.; Jager, V.; Butler, P.J.G.; Van Den Heuvel, J.; Schmidt, S.; Ferraris, D.; Gherardi, E.; Heinz, D.W.
Deposited on	:	2007-05-02
Resolution	:	2.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

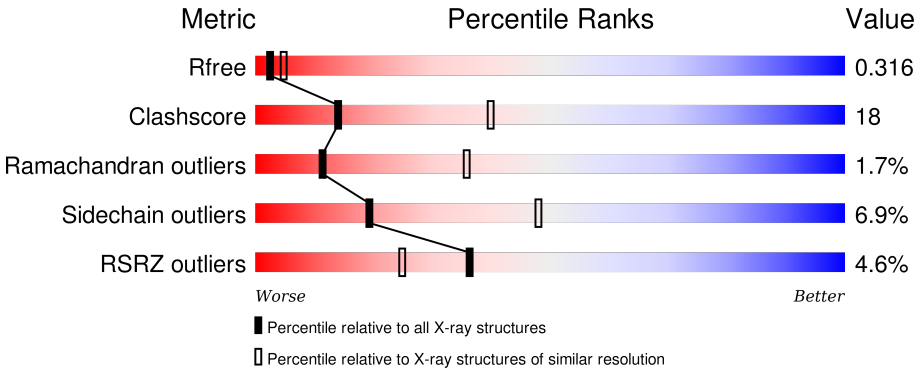
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	289	% 71% 26%
1	C	289	3% 70% 27%
2	B	727	4% 45% 26% 25%
2	D	727	5% 45% 26% 5% 25%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13170 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 INTERNALIN B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2257	1438	379	438	2			
1	C	287	Total	C	N	O	S	0	0	0
			2257	1438	379	438	2			

- Molecule 2 is a protein called HEPATOCYTE GROWTH FACTOR RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	547	Total	C	N	O	S	0	0	1
			4328	2757	732	809	30			
2	D	547	Total	C	N	O	S	0	0	1
			4328	2757	732	809	30			

There are 4 discrepancies between the modelled and reference sequences:

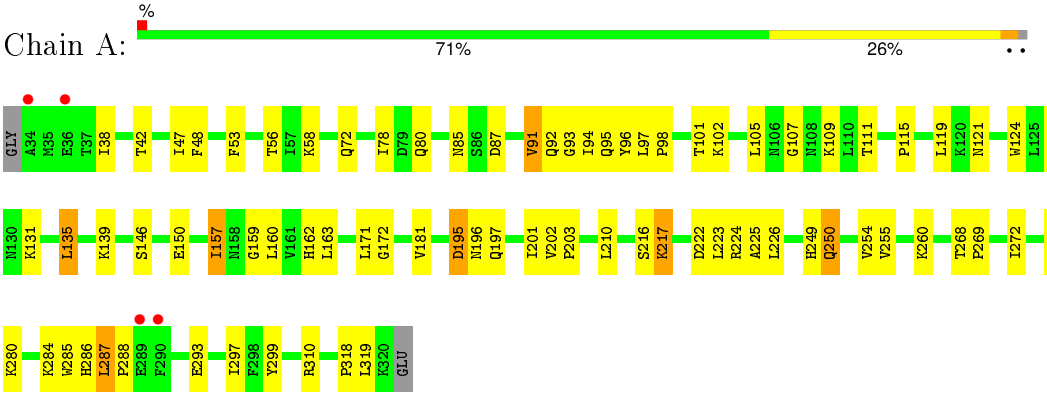
Chain	Residue	Modelled	Actual	Comment	Reference
B	41	CYS	TYR	CONFLICT SEE REMARK 9	UNP P08581
B	344	ALA	GLY	CONFLICT SEE REMARK 9	UNP P08581
D	41	CYS	TYR	CONFLICT SEE REMARK 9	UNP P08581
D	344	ALA	GLY	CONFLICT SEE REMARK 9	UNP P08581

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

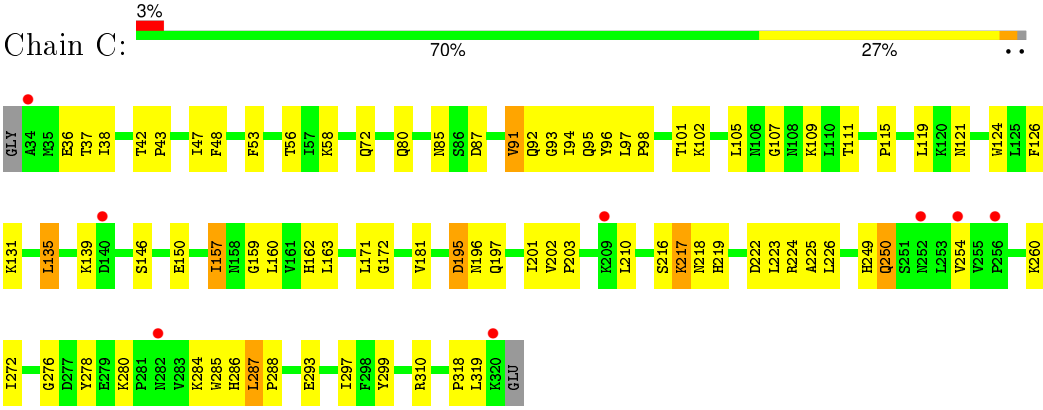
- Molecule 1: INTERNALIN B

Chain A:



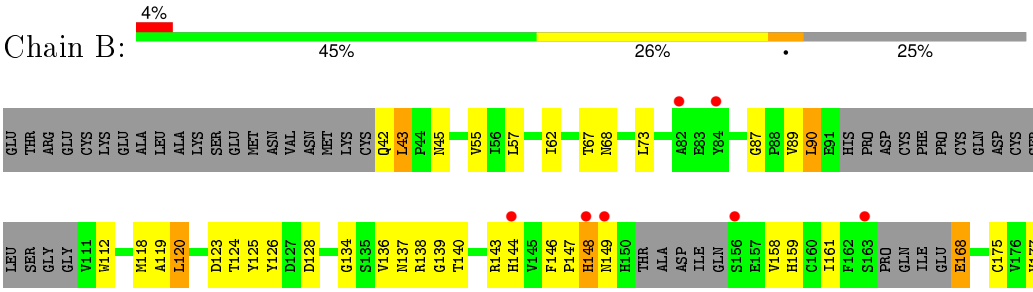
- Molecule 1: INTERNALIN B

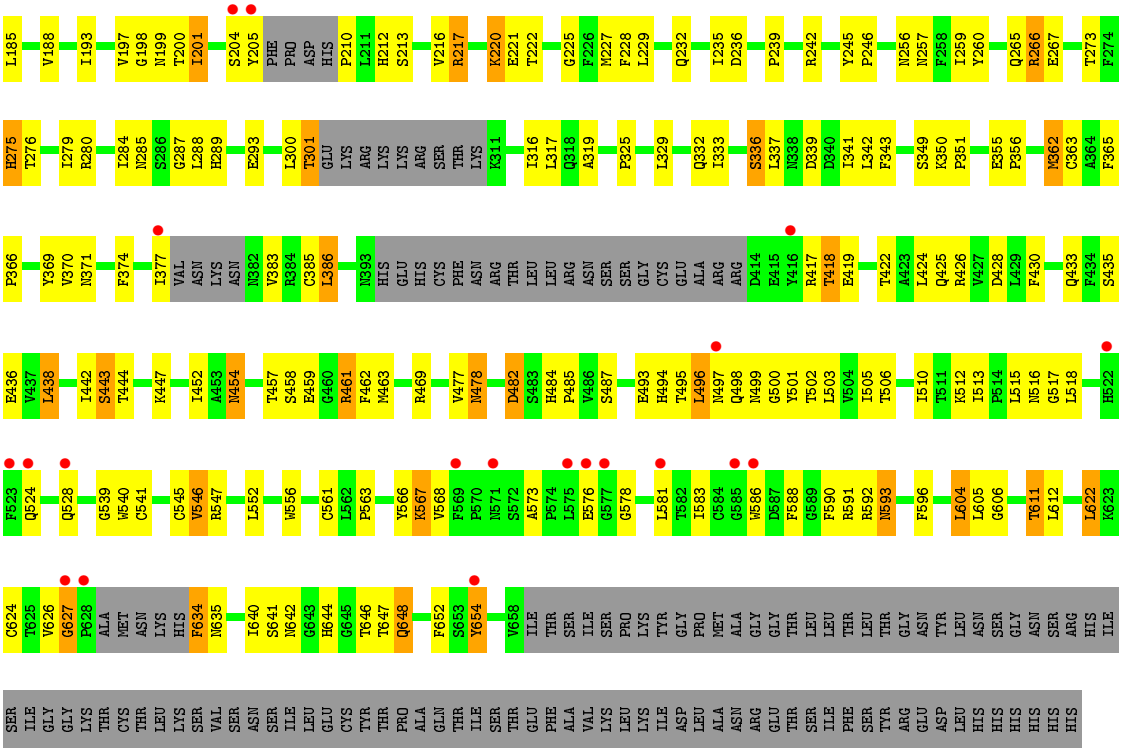
Chain C:



- Molecule 2: HEPATOCYTE GROWTH FACTOR RECEPTOR

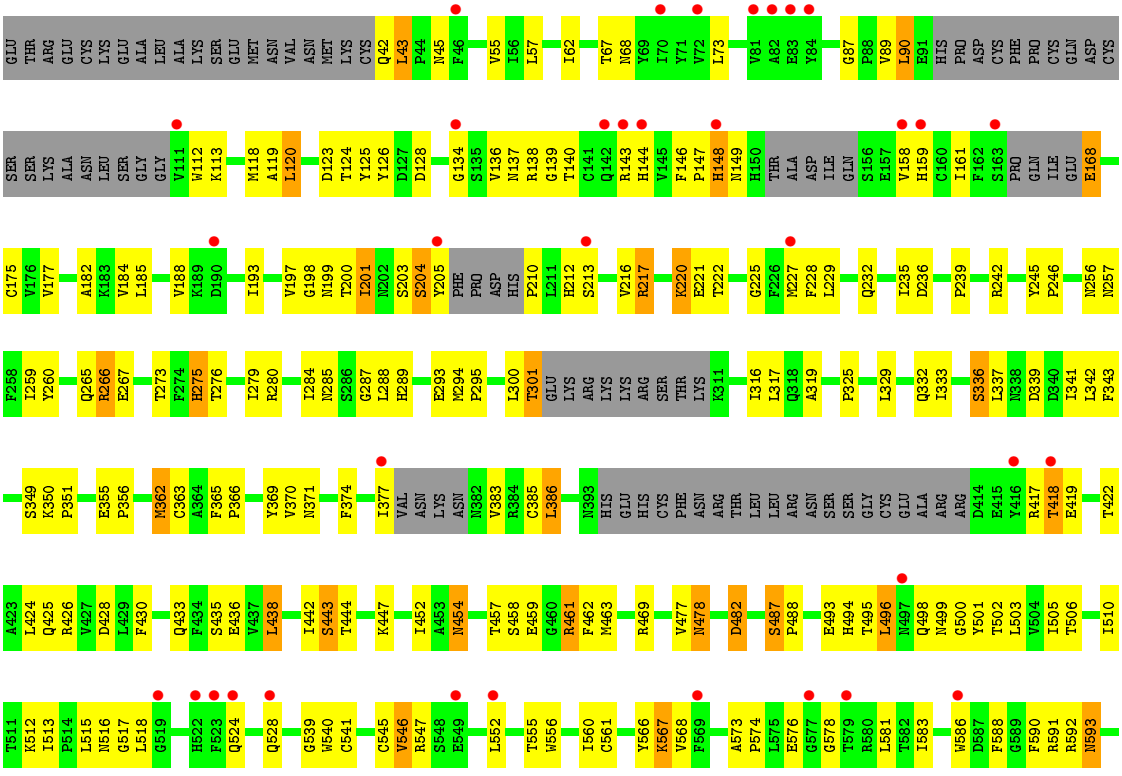
Chain B:

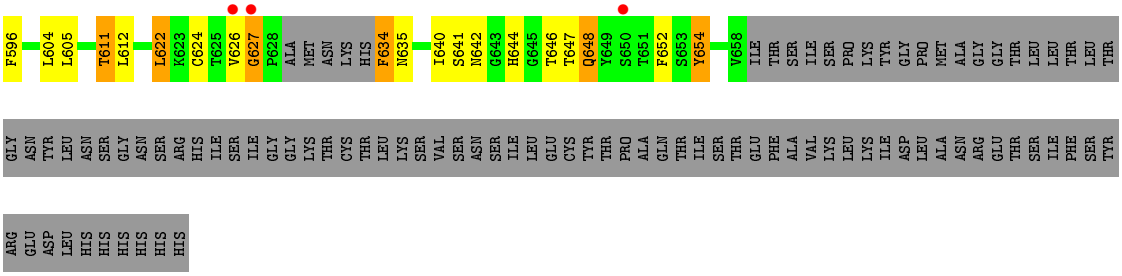




• Molecule 2: HEPATOCYTE GROWTH FACTOR RECEPTOR

Chain D:




F596 L604 L605 T611 L612 L622 K623 G624 T625 V626 G627 F628 ALA MET ASN LYS HIS F634 N635 I640 S641 N642 G643 H644 G645 T646 T647 Q648 Y649 S650 T651 F652 S653 Y654 V658 ILE THR SER ILE SER PRO LYS TYR GLY PRO MET ALA GLY GLY THR LEU LEU THR LEU THR
GLY ASN TYR LEU ASN SER GLY ASN SER ARG HIS ILE SER ILE GLY GLY LYS THR CYS THR LEU LYS SER VAL SER ASN SER ILE LEU GLU CYS TYR THR PRO ALA GLN THR ILE SER THR GLU PHE ALA VAL LYS LEU LYS ILE ASP LEU ALA ASN ARG GLU THR SER ILE PHE SER TYR
ARG GLU ASP LEU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	214.50Å 66.70Å 181.50Å 90.00° 123.30° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 48.39 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.9 (15.00-2.80) 97.2 (48.39-2.80)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.268 , 0.307 0.277 , 0.316	Depositor DCC
R_{free} test set	2482 reflections (4.80%)	DCC
Wilson B-factor (Å^2)	53.2	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 48.9	EDS
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Outliers	0 of 51863 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	13170	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.05 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.8953e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.34	0/2293	0.53	0/3112
1	C	0.34	0/2293	0.53	0/3112
2	B	0.37	0/4427	0.58	0/6001
2	D	0.37	0/4427	0.58	0/6001
All	All	0.36	0/13440	0.56	0/18226

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	3
2	D	0	3
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	168	GLU	Peptide
2	B	210	PRO	Peptide
2	B	627	GLY	Peptide
2	D	168	GLU	Peptide
2	D	210	PRO	Peptide
2	D	627	GLY	Peptide

5.2 Too-close contacts (i)

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	2257	0	2328	69	0
1	C	2257	0	2328	70	0
2	B	4328	0	4212	175	0
2	D	4328	0	4212	171	0
All	All	13170	0	13080	480	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 18.

All (480) 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:D:329:LEU:HA	2:D:332:GLN:NE2	1.93	0.84
2:D:43:LEU:HD12	2:D:513:ILE:HA	1.61	0.82
2:B:329:LEU:HA	2:B:332:GLN:NE2	1.93	0.82
2:B:43:LEU:HD12	2:B:513:ILE:HA	1.61	0.80
2:B:647:THR:HG22	2:B:648:GLN:H	1.47	0.80
2:D:647:THR:HG22	2:D:648:GLN:H	1.48	0.79
2:B:546:VAL:HG22	2:B:547:ARG:H	1.48	0.78
2:D:546:VAL:HG22	2:D:547:ARG:H	1.47	0.78
1:A:157:ILE:H	1:A:157:ILE:HD13	1.49	0.78
1:C:157:ILE:H	1:C:157:ILE:HD13	1.49	0.76
2:B:329:LEU:HA	2:B:332:GLN:HE21	1.51	0.76
1:A:80:GLN:HB2	1:A:102:LYS:HB2	1.68	0.76
2:B:161:ILE:HG23	2:B:225:GLY:HA2	1.68	0.75
2:B:265:GLN:O	2:B:275:HIS:HB2	1.87	0.75
2:D:561:CYS:H	2:D:644:HIS:HD2	1.32	0.75
1:C:80:GLN:HB2	1:C:102:LYS:HB2	1.68	0.75
2:D:161:ILE:HG23	2:D:225:GLY:HA2	1.68	0.74
2:D:265:GLN:O	2:D:275:HIS:HB2	1.87	0.74
2:B:611:THR:O	2:B:624:CYS:HB2	1.88	0.73
2:D:611:THR:O	2:D:624:CYS:HB2	1.88	0.73
2:B:89:VAL:HB	2:B:136:VAL:HG11	1.71	0.73
1:A:286:HIS:NE2	1:A:288:PRO:HG3	2.03	0.73
1:A:195:ASP:HA	1:A:217:LYS:HB2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:581:LEU:HG	2:B:626:VAL:HG21	1.71	0.72
1:C:195:ASP:HA	1:C:217:LYS:HB2	1.71	0.72
2:D:329:LEU:HA	2:D:332:GLN:HE21	1.50	0.72
1:C:286:HIS:NE2	1:C:288:PRO:HG3	2.04	0.72
2:D:89:VAL:HB	2:D:136:VAL:HG11	1.71	0.72
1:C:135:LEU:HD13	1:C:159:GLY:HA3	1.72	0.71
2:D:581:LEU:HG	2:D:626:VAL:HG21	1.71	0.71
1:A:85:ASN:O	2:D:496:LEU:HD13	1.90	0.71
2:B:300:LEU:HD12	2:B:301:THR:H	1.55	0.71
2:B:566:TYR:O	2:B:567:LYS:HB2	1.90	0.71
1:A:135:LEU:HD13	1:A:159:GLY:HA3	1.72	0.71
2:D:300:LEU:HD12	2:D:301:THR:H	1.55	0.70
2:D:566:TYR:O	2:D:567:LYS:HB2	1.90	0.70
2:B:443:SER:HB2	2:B:454:ASN:OD1	1.90	0.70
2:D:443:SER:HB2	2:D:454:ASN:OD1	1.90	0.70
2:B:583:ILE:HD13	2:B:640:ILE:HD11	1.75	0.68
1:C:87:ASP:OD1	1:C:109:LYS:HE3	1.94	0.68
2:D:583:ILE:HD13	2:D:640:ILE:HD11	1.75	0.67
2:D:216:VAL:CG2	2:D:288:LEU:HD11	2.24	0.67
2:B:216:VAL:CG2	2:B:288:LEU:HD11	2.24	0.67
1:A:87:ASP:OD1	1:A:109:LYS:HE3	1.94	0.66
1:C:286:HIS:CD2	1:C:288:PRO:HG3	2.31	0.66
2:D:498:GLN:HG2	2:D:500:GLY:H	1.61	0.66
1:A:286:HIS:CD2	1:A:288:PRO:HG3	2.31	0.65
2:B:498:GLN:HG2	2:B:500:GLY:H	1.61	0.65
1:C:135:LEU:HD21	1:C:157:ILE:HA	1.79	0.65
2:B:590:PHE:CE1	2:B:644:HIS:CE1	2.85	0.65
2:D:590:PHE:CE1	2:D:644:HIS:CE1	2.85	0.64
1:A:139:LYS:HE2	1:A:162:HIS:CD2	2.32	0.64
2:B:365:PHE:CE2	2:B:426:ARG:HG2	2.33	0.64
2:D:217:ARG:HD2	2:D:217:ARG:H	1.63	0.64
1:A:135:LEU:HD21	1:A:157:ILE:HA	1.79	0.64
1:C:139:LYS:HG2	1:C:162:HIS:CG	2.33	0.64
2:B:43:LEU:H	2:B:43:LEU:HD23	1.63	0.64
1:C:139:LYS:HE2	1:C:162:HIS:CD2	2.32	0.64
2:D:287:GLY:HA2	2:D:289:HIS:NE2	2.14	0.63
2:D:43:LEU:HD23	2:D:43:LEU:H	1.63	0.63
2:D:148:HIS:CD2	2:D:149:ASN:H	2.17	0.63
2:B:280:ARG:NH2	2:B:374:PHE:HB3	2.14	0.63
2:B:217:ARG:HD2	2:B:217:ARG:H	1.63	0.63
1:A:139:LYS:HG2	1:A:162:HIS:CG	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:ASN:HA	1:C:107:GLY:O	1.99	0.62
2:D:365:PHE:CE2	2:D:426:ARG:HG2	2.33	0.62
1:A:85:ASN:HA	1:A:107:GLY:O	1.99	0.62
2:D:626:VAL:HG12	2:D:654:TYR:OH	2.00	0.62
1:C:226:LEU:H	1:C:226:LEU:HD12	1.65	0.62
2:B:148:HIS:CD2	2:B:149:ASN:H	2.17	0.62
2:B:626:VAL:HG12	2:B:654:TYR:OH	1.99	0.62
2:D:280:ARG:NH2	2:D:374:PHE:HB3	2.14	0.62
2:B:287:GLY:HA2	2:B:289:HIS:NE2	2.13	0.62
2:D:220:LYS:HD3	2:D:225:GLY:O	2.00	0.61
2:B:220:LYS:HD3	2:B:225:GLY:O	2.00	0.61
2:D:605:LEU:HD21	2:D:652:PHE:CE2	2.36	0.61
2:D:634:PHE:HD1	2:D:635:ASN:H	1.49	0.60
2:B:583:ILE:HG21	2:B:640:ILE:HD11	1.84	0.60
2:D:235:ILE:HD12	2:D:417:ARG:HG2	1.83	0.60
2:B:605:LEU:HD21	2:B:652:PHE:CE2	2.36	0.60
1:C:139:LYS:HE2	1:C:162:HIS:NE2	2.16	0.60
2:B:634:PHE:HD1	2:B:635:ASN:H	1.49	0.60
1:A:226:LEU:H	1:A:226:LEU:HD12	1.65	0.60
1:A:139:LYS:HE2	1:A:162:HIS:NE2	2.16	0.60
1:A:249:HIS:HD2	1:A:287:LEU:HD23	1.67	0.59
2:B:612:LEU:HA	2:B:624:CYS:CB	2.32	0.59
2:D:583:ILE:HG21	2:D:640:ILE:HD11	1.84	0.59
2:B:517:GLY:O	2:B:518:LEU:HD13	2.03	0.59
2:B:235:ILE:HD12	2:B:417:ARG:HG2	1.83	0.59
1:C:249:HIS:HD2	1:C:287:LEU:HD23	1.67	0.58
2:B:430:PHE:HB3	2:B:433:GLN:HB3	1.85	0.58
2:B:216:VAL:HG21	2:B:288:LEU:HD11	1.85	0.58
2:B:611:THR:C	2:B:624:CYS:HB2	2.24	0.58
2:D:517:GLY:O	2:D:518:LEU:HD13	2.03	0.58
2:D:612:LEU:HA	2:D:624:CYS:CB	2.32	0.58
2:D:430:PHE:HB3	2:D:433:GLN:HB3	1.84	0.58
2:D:578:GLY:HA2	2:D:627:GLY:H	1.67	0.58
2:B:578:GLY:HA2	2:B:627:GLY:H	1.67	0.58
2:D:125:TYR:CE1	2:D:188:VAL:HG11	2.38	0.58
2:B:497:ASN:HD22	2:D:555:THR:HA	1.69	0.58
2:D:611:THR:C	2:D:624:CYS:HB2	2.24	0.58
2:D:216:VAL:HG21	2:D:288:LEU:HD11	1.85	0.58
2:B:125:TYR:CE1	2:B:188:VAL:HG11	2.38	0.57
2:D:287:GLY:HA2	2:D:289:HIS:CE1	2.39	0.57
2:B:287:GLY:HA2	2:B:289:HIS:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:561:CYS:H	2:B:644:HIS:HD2	1.53	0.57
1:A:224:ARG:HH21	1:A:260:LYS:CD	2.18	0.57
2:B:216:VAL:HB	2:B:288:LEU:HD11	1.86	0.57
1:A:201:ILE:HG13	1:A:225:ALA:HB3	1.87	0.56
2:B:539:GLY:HA3	2:B:556:TRP:NE1	2.20	0.56
1:C:224:ARG:HH21	1:C:260:LYS:CD	2.18	0.56
2:D:539:GLY:HA3	2:D:556:TRP:NE1	2.19	0.56
2:D:266:ARG:O	2:D:266:ARG:HG2	2.05	0.56
2:D:216:VAL:HB	2:D:288:LEU:HD11	1.86	0.56
2:B:266:ARG:O	2:B:266:ARG:HG2	2.05	0.56
2:D:200:THR:O	2:D:201:ILE:HG23	2.07	0.55
2:D:229:LEU:HD22	2:D:285:ASN:HB3	1.89	0.55
1:C:201:ILE:HG13	1:C:225:ALA:HB3	1.88	0.55
2:B:287:GLY:CA	2:B:289:HIS:NE2	2.69	0.55
1:A:285:TRP:HB3	1:A:287:LEU:HD13	1.89	0.55
1:A:101:THR:HG22	1:A:121:ASN:O	2.07	0.55
1:C:101:THR:HG22	1:C:121:ASN:O	2.07	0.55
2:D:287:GLY:CA	2:D:289:HIS:NE2	2.70	0.54
2:D:583:ILE:HG21	2:D:640:ILE:CD1	2.37	0.54
2:B:592:ARG:HD3	2:B:593:ASN:H	1.73	0.54
2:D:284:ILE:O	2:D:285:ASN:HB2	2.08	0.54
1:C:285:TRP:HB3	1:C:287:LEU:HD13	1.89	0.54
2:B:144:HIS:ND1	2:B:158:VAL:HG22	2.22	0.54
2:B:200:THR:O	2:B:201:ILE:HG23	2.07	0.54
1:A:48:PHE:HA	1:A:92:GLN:O	2.08	0.54
2:B:260:TYR:HA	2:B:279:ILE:O	2.08	0.54
2:B:647:THR:HG22	2:B:648:GLN:N	2.20	0.54
2:B:499:ASN:O	2:B:515:LEU:HB2	2.08	0.54
2:D:118:MET:CB	2:D:177:VAL:HG11	2.38	0.54
2:B:284:ILE:O	2:B:285:ASN:HB2	2.08	0.54
2:B:125:TYR:HE1	1:C:43:PRO:HD3	1.73	0.54
2:B:583:ILE:HG21	2:B:640:ILE:CD1	2.37	0.54
2:D:592:ARG:HD3	2:D:593:ASN:H	1.73	0.54
2:B:457:THR:HG22	2:B:458:SER:N	2.22	0.54
2:D:198:GLY:HA2	2:D:213:SER:O	2.08	0.54
2:D:457:THR:HG22	2:D:458:SER:N	2.22	0.53
2:D:260:TYR:HA	2:D:279:ILE:O	2.08	0.53
2:B:229:LEU:HD22	2:B:285:ASN:HB3	1.89	0.53
1:C:48:PHE:HA	1:C:92:GLN:O	2.08	0.53
2:D:463:MET:HB3	2:D:478:ASN:HA	1.89	0.53
1:C:318:PRO:O	1:C:319:LEU:HD23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:144:HIS:ND1	2:D:158:VAL:HG22	2.22	0.53
2:B:198:GLY:HA2	2:B:213:SER:O	2.08	0.53
2:D:499:ASN:O	2:D:515:LEU:HB2	2.07	0.53
2:B:362:MET:O	2:B:428:ASP:HA	2.08	0.53
2:B:591:ARG:HB2	2:B:596:PHE:CZ	2.43	0.53
2:B:118:MET:CB	2:B:177:VAL:HG11	2.38	0.53
2:D:316:ILE:O	2:D:316:ILE:HG22	2.09	0.53
1:C:286:HIS:O	1:C:288:PRO:HD3	2.09	0.53
2:D:591:ARG:HB2	2:D:596:PHE:CZ	2.43	0.53
2:D:216:VAL:CB	2:D:288:LEU:HD11	2.39	0.53
2:D:362:MET:O	2:D:428:ASP:HA	2.08	0.53
2:D:424:LEU:HD23	2:D:425:GLN:N	2.24	0.53
2:B:424:LEU:HD23	2:B:425:GLN:N	2.25	0.52
2:B:463:MET:HB3	2:B:478:ASN:HA	1.90	0.52
1:A:318:PRO:O	1:A:319:LEU:HD23	2.09	0.52
2:D:647:THR:HG22	2:D:648:GLN:N	2.20	0.52
2:B:216:VAL:CB	2:B:288:LEU:HD11	2.39	0.52
1:C:285:TRP:HB3	1:C:287:LEU:CD1	2.39	0.52
1:A:285:TRP:HB3	1:A:287:LEU:CD1	2.39	0.52
2:B:539:GLY:HA3	2:B:556:TRP:CE2	2.44	0.52
2:B:482:ASP:OD1	2:B:506:THR:HB	2.09	0.52
2:D:539:GLY:HA3	2:D:556:TRP:CE2	2.44	0.52
2:D:482:ASP:OD1	2:D:506:THR:HB	2.09	0.52
2:B:612:LEU:HA	2:B:624:CYS:HB3	1.91	0.52
2:B:452:ILE:HD12	2:B:452:ILE:N	2.25	0.52
1:A:297:ILE:HD12	1:A:297:ILE:N	2.25	0.52
1:C:128:ASP:OD2	1:C:150:GLU:N	2.32	0.52
2:B:43:LEU:HD11	2:B:513:ILE:HG12	1.92	0.52
1:C:299:TYR:OH	1:C:310:ARG:HD2	2.10	0.52
2:D:612:LEU:HA	2:D:624:CYS:HB3	1.91	0.52
2:B:498:GLN:HE21	2:B:500:GLY:HA2	1.74	0.52
2:D:452:ILE:N	2:D:452:ILE:HD12	2.25	0.52
2:D:612:LEU:HD23	2:D:624:CYS:HB3	1.93	0.51
2:B:300:LEU:HD12	2:B:301:THR:N	2.25	0.51
2:D:216:VAL:HG23	2:D:288:LEU:HD21	1.92	0.51
2:D:317:LEU:HD11	2:D:319:ALA:O	2.11	0.51
1:A:128:ASP:OD2	1:A:150:GLU:N	2.32	0.51
2:D:540:TRP:CZ3	2:D:545:CYS:HB2	2.45	0.51
1:C:297:ILE:HD12	1:C:297:ILE:N	2.25	0.51
2:B:612:LEU:HD23	2:B:624:CYS:HB3	1.92	0.51
1:A:286:HIS:O	1:A:288:PRO:HD3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:ILE:HG12	1:C:181:VAL:HG11	1.93	0.51
2:B:342:LEU:HB3	2:B:365:PHE:HB2	1.93	0.51
2:D:287:GLY:HA3	2:D:289:HIS:CD2	2.45	0.51
2:B:287:GLY:HA3	2:B:289:HIS:CD2	2.45	0.51
1:A:97:LEU:O	1:A:119:LEU:HD22	2.11	0.51
2:B:317:LEU:HD11	2:B:319:ALA:O	2.11	0.51
2:D:276:THR:HG21	2:D:317:LEU:HB2	1.93	0.51
1:A:299:TYR:OH	1:A:310:ARG:HD2	2.10	0.51
2:B:239:PRO:HG3	2:B:242:ARG:NH2	2.26	0.51
2:D:288:LEU:N	2:D:288:LEU:HD12	2.27	0.50
2:B:288:LEU:HD12	2:B:288:LEU:N	2.26	0.50
1:A:139:LYS:HG2	1:A:162:HIS:CD2	2.46	0.50
2:D:316:ILE:HD13	2:D:349:SER:HB3	1.92	0.50
1:C:97:LEU:O	1:C:119:LEU:HD22	2.11	0.50
2:B:316:ILE:HG22	2:B:316:ILE:O	2.09	0.50
2:B:454:ASN:HB2	2:B:462:PHE:CZ	2.46	0.50
2:B:216:VAL:HG23	2:B:288:LEU:HD21	1.92	0.50
2:B:563:PRO:HG3	2:B:642:ASN:ND2	2.26	0.50
2:B:143:ARG:HB2	2:B:159:HIS:HB2	1.93	0.50
2:B:316:ILE:HD13	2:B:349:SER:HB3	1.92	0.50
2:D:454:ASN:HB2	2:D:462:PHE:CZ	2.46	0.50
1:A:157:ILE:HG12	1:A:181:VAL:HG11	1.93	0.50
2:D:573:ALA:HB3	2:D:652:PHE:CZ	2.46	0.50
2:B:540:TRP:CZ3	2:B:545:CYS:HB2	2.45	0.50
1:C:124:TRP:CD1	1:C:146:SER:HB3	2.46	0.50
2:D:495:THR:O	2:D:498:GLN:HB3	2.12	0.50
2:D:342:LEU:HB3	2:D:365:PHE:HB2	1.93	0.50
2:D:239:PRO:HG3	2:D:242:ARG:NH2	2.27	0.50
2:B:276:THR:HG21	2:B:317:LEU:HB2	1.93	0.50
1:C:272:ILE:HG21	1:C:276:GLY:HA3	1.93	0.50
1:A:254:VAL:HG22	1:A:284:LYS:HG2	1.94	0.50
2:B:454:ASN:HB2	2:B:462:PHE:CE1	2.47	0.50
2:D:498:GLN:HE21	2:D:500:GLY:HA2	1.75	0.50
1:A:272:ILE:HG21	1:A:276:GLY:HA3	1.94	0.50
1:C:268:THR:HG22	1:C:278:TYR:HE2	1.77	0.50
2:D:447:LYS:HE3	2:D:516:ASN:OD1	2.12	0.50
2:B:573:ALA:HB3	2:B:652:PHE:CZ	2.46	0.49
2:B:495:THR:O	2:B:498:GLN:HB3	2.12	0.49
2:D:43:LEU:HD11	2:D:513:ILE:HG12	1.92	0.49
1:A:224:ARG:NH2	1:A:260:LYS:HD2	2.28	0.49
1:C:139:LYS:HG2	1:C:162:HIS:CD2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:185:LEU:HD12	2:D:259:ILE:HG23	1.94	0.49
2:B:447:LYS:HE3	2:B:516:ASN:OD1	2.12	0.49
1:C:254:VAL:HG22	1:C:284:LYS:HG2	1.94	0.49
2:B:185:LEU:HD12	2:B:259:ILE:HG23	1.94	0.49
2:D:143:ARG:HB2	2:D:159:HIS:HB2	1.93	0.49
2:D:184:VAL:HG22	2:D:197:VAL:HG22	1.95	0.49
2:D:279:ILE:HG13	2:D:293:GLU:HG2	1.95	0.49
1:C:111:THR:HG22	1:C:131:LYS:HB2	1.94	0.49
1:C:38:ILE:HG12	1:C:72:GLN:OE1	2.13	0.49
2:D:217:ARG:HB3	2:D:228:PHE:CE2	2.48	0.49
1:A:38:ILE:HG12	1:A:72:GLN:OE1	2.13	0.49
2:D:560:ILE:HA	2:D:644:HIS:CD2	2.48	0.49
1:A:202:VAL:N	1:A:203:PRO:CD	2.76	0.49
1:A:124:TRP:CD1	1:A:146:SER:HB3	2.46	0.49
2:D:454:ASN:HB2	2:D:462:PHE:CE1	2.47	0.49
2:D:438:LEU:HB3	2:D:458:SER:HB3	1.95	0.49
2:D:188:VAL:HG22	2:D:193:ILE:HG12	1.95	0.49
2:B:457:THR:HG22	2:B:459:GLU:N	2.27	0.49
2:B:188:VAL:HG22	2:B:193:ILE:HG12	1.95	0.48
2:D:199:ASN:HB2	2:D:212:HIS:O	2.13	0.48
2:D:43:LEU:HD12	2:D:512:LYS:O	2.13	0.48
2:B:217:ARG:HB3	2:B:228:PHE:CE2	2.48	0.48
2:B:438:LEU:HB3	2:B:458:SER:HB3	1.94	0.48
2:B:43:LEU:HD12	2:B:512:LYS:O	2.13	0.48
2:D:457:THR:HG22	2:D:459:GLU:N	2.27	0.48
1:A:268:THR:HG22	1:A:278:TYR:HE2	1.77	0.48
1:C:224:ARG:NH2	1:C:260:LYS:HD2	2.28	0.48
2:B:418:THR:OG1	2:B:419:GLU:N	2.46	0.48
1:C:202:VAL:N	1:C:203:PRO:CD	2.76	0.48
1:A:111:THR:HG22	1:A:131:LYS:HB2	1.95	0.48
2:B:279:ILE:HG13	2:B:293:GLU:HG2	1.95	0.48
2:B:184:VAL:HG22	2:B:197:VAL:HG22	1.95	0.48
1:C:124:TRP:HB3	1:C:126:PHE:HE1	1.79	0.48
2:B:199:ASN:HB2	2:B:212:HIS:O	2.13	0.48
2:B:325:PRO:HG3	2:B:341:ILE:HG13	1.96	0.48
2:D:138:ARG:HH22	2:D:205:TYR:C	2.17	0.47
2:B:546:VAL:HG22	2:B:547:ARG:N	2.25	0.47
1:A:201:ILE:HG13	1:A:225:ALA:CB	2.44	0.47
1:C:58:LYS:HD2	1:C:58:LYS:C	2.35	0.47
2:B:220:LYS:HD2	2:B:227:MET:HG2	1.96	0.47
2:D:220:LYS:HD2	2:D:227:MET:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:493:GLU:HB2	2:B:501:TYR:CZ	2.49	0.47
1:A:157:ILE:HB	1:A:160:LEU:HD12	1.97	0.47
2:D:300:LEU:HD12	2:D:301:THR:N	2.25	0.47
2:D:493:GLU:HB2	2:D:501:TYR:CZ	2.49	0.47
2:D:546:VAL:HG22	2:D:547:ARG:N	2.25	0.47
1:A:157:ILE:CD1	1:A:157:ILE:H	2.25	0.47
1:C:157:ILE:HB	1:C:160:LEU:HD12	1.97	0.47
2:B:232:GLN:HB3	2:B:417:ARG:HH22	1.80	0.47
1:C:111:THR:HG22	1:C:131:LYS:CB	2.44	0.47
2:D:325:PRO:HG3	2:D:341:ILE:HG13	1.96	0.47
2:B:581:LEU:HG	2:B:626:VAL:CG2	2.44	0.47
2:D:350:LYS:HB3	2:D:351:PRO:HD2	1.96	0.47
2:B:498:GLN:HG2	2:B:499:ASN:N	2.30	0.47
1:A:124:TRP:HB3	1:A:126:PHE:HE1	1.79	0.47
1:A:111:THR:HG22	1:A:131:LYS:CB	2.44	0.47
2:B:385:CYS:O	2:B:386:LEU:C	2.53	0.47
2:D:113:LYS:HE3	2:D:113:LYS:HB3	1.53	0.47
2:B:137:ASN:HB2	2:B:140:THR:HG22	1.97	0.47
1:C:150:GLU:HG2	1:C:172:GLY:N	2.30	0.47
2:B:217:ARG:HG3	2:B:217:ARG:HH11	1.80	0.46
2:D:498:GLN:HG2	2:D:499:ASN:N	2.30	0.46
2:B:148:HIS:CD2	2:B:149:ASN:N	2.83	0.46
1:C:171:LEU:HA	1:C:171:LEU:HD23	1.78	0.46
2:B:161:ILE:N	2:B:161:ILE:HD12	2.30	0.46
2:D:213:SER:OG	2:D:236:ASP:HA	2.15	0.46
2:B:540:TRP:HZ3	2:B:545:CYS:HB2	1.81	0.46
2:D:62:ILE:HB	2:D:73:LEU:HB2	1.97	0.46
1:A:58:LYS:C	1:A:58:LYS:HD2	2.35	0.46
1:C:38:ILE:HD11	1:C:72:GLN:N	2.31	0.46
2:D:461:ARG:HB3	2:D:461:ARG:HE	1.59	0.46
2:B:138:ARG:HH22	2:B:205:TYR:C	2.17	0.46
2:B:568:VAL:CG1	2:B:581:LEU:HD22	2.45	0.46
2:D:147:PRO:O	2:D:148:HIS:CB	2.63	0.46
2:D:239:PRO:HA	2:D:242:ARG:NE	2.30	0.46
2:D:245:TYR:HA	2:D:246:PRO:HD3	1.61	0.46
2:D:43:LEU:CD1	2:D:513:ILE:HA	2.40	0.46
1:C:201:ILE:HG13	1:C:225:ALA:CB	2.45	0.46
2:B:147:PRO:O	2:B:148:HIS:CB	2.63	0.46
2:D:232:GLN:HB3	2:D:417:ARG:HH22	1.80	0.46
2:D:137:ASN:HB2	2:D:140:THR:HG22	1.97	0.46
2:B:220:LYS:HB2	2:B:222:THR:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:568:VAL:CG1	2:D:581:LEU:HD22	2.45	0.46
2:B:239:PRO:HA	2:B:242:ARG:NE	2.30	0.46
1:A:38:ILE:HD11	1:A:72:GLN:N	2.31	0.46
2:D:641:SER:HB2	2:D:646:THR:HG22	1.98	0.46
2:D:581:LEU:HG	2:D:626:VAL:CG2	2.44	0.46
2:D:463:MET:HB2	2:D:477:VAL:O	2.16	0.46
2:B:213:SER:OG	2:B:236:ASP:HA	2.15	0.46
1:A:150:GLU:HG2	1:A:172:GLY:N	2.30	0.46
2:D:217:ARG:O	2:D:217:ARG:HG2	2.16	0.45
2:B:350:LYS:HB3	2:B:351:PRO:HD2	1.96	0.45
2:D:161:ILE:N	2:D:161:ILE:HD12	2.31	0.45
1:A:249:HIS:CD2	1:A:287:LEU:HD23	2.50	0.45
2:B:642:ASN:OD1	2:B:644:HIS:HB2	2.16	0.45
2:B:417:ARG:HD2	2:B:417:ARG:N	2.32	0.45
2:B:641:SER:HB2	2:B:646:THR:HG22	1.98	0.45
2:B:377:ILE:HD12	2:B:377:ILE:O	2.17	0.45
2:B:62:ILE:HB	2:B:73:LEU:HB2	1.97	0.45
2:D:385:CYS:O	2:D:386:LEU:C	2.53	0.45
2:B:457:THR:HG22	2:B:459:GLU:H	1.82	0.45
2:B:329:LEU:CD1	2:B:333:ILE:HD13	2.47	0.45
2:D:590:PHE:CE1	2:D:644:HIS:ND1	2.85	0.45
2:B:590:PHE:CE1	2:B:644:HIS:ND1	2.85	0.45
2:D:457:THR:CG2	2:D:458:SER:N	2.80	0.45
2:D:540:TRP:HZ3	2:D:545:CYS:HB2	1.81	0.45
2:B:256:ASN:O	2:B:257:ASN:HB2	2.17	0.45
2:D:503:LEU:HB3	2:D:510:ILE:HD11	1.99	0.45
2:D:418:THR:OG1	2:D:419:GLU:N	2.47	0.45
2:B:370:VAL:HG12	2:B:371:ASN:N	2.32	0.45
1:A:96:TYR:O	1:A:98:PRO:HD3	2.17	0.45
2:D:561:CYS:H	2:D:644:HIS:CD2	2.22	0.45
2:B:43:LEU:CD1	2:B:513:ILE:HA	2.40	0.45
2:D:220:LYS:HB2	2:D:222:THR:HG22	1.98	0.45
2:B:605:LEU:HD22	2:B:626:VAL:HG13	1.99	0.45
2:D:417:ARG:N	2:D:417:ARG:HD2	2.31	0.45
1:C:272:ILE:CG2	1:C:276:GLY:HA3	2.47	0.45
2:D:256:ASN:O	2:D:257:ASN:HB2	2.17	0.45
2:D:329:LEU:CD1	2:D:333:ILE:HD13	2.47	0.45
2:B:457:THR:CG2	2:B:458:SER:N	2.80	0.45
2:B:463:MET:HB2	2:B:477:VAL:O	2.17	0.45
1:A:272:ILE:CG2	1:A:276:GLY:HA3	2.47	0.44
2:D:642:ASN:OD1	2:D:644:HIS:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:148:HIS:CD2	2:D:149:ASN:N	2.83	0.44
1:A:128:ASP:O	1:A:129:GLU:HB2	2.18	0.44
2:B:182:ALA:HA	2:B:198:GLY:O	2.17	0.44
2:B:161:ILE:CG2	2:B:225:GLY:HA2	2.44	0.44
2:B:496:LEU:HD13	1:C:85:ASN:O	2.17	0.44
2:B:503:LEU:HB3	2:B:510:ILE:HD11	1.99	0.44
2:D:217:ARG:HH11	2:D:217:ARG:HG3	1.81	0.44
2:B:217:ARG:O	2:B:217:ARG:HG2	2.16	0.44
1:C:201:ILE:CD1	1:C:226:LEU:HD11	2.47	0.44
2:D:605:LEU:HD22	2:D:626:VAL:HG13	1.99	0.44
1:A:201:ILE:CD1	1:A:226:LEU:HD11	2.47	0.44
1:C:96:TYR:O	1:C:98:PRO:HD3	2.17	0.44
2:B:284:ILE:HD13	2:B:289:HIS:HD2	1.83	0.44
2:D:137:ASN:HB2	2:D:140:THR:CG2	2.48	0.44
2:D:67:THR:O	2:D:68:ASN:HB2	2.18	0.44
2:D:457:THR:HG22	2:D:459:GLU:H	1.81	0.44
2:D:366:PRO:O	2:D:369:TYR:HB3	2.17	0.44
2:D:329:LEU:HD13	2:D:333:ILE:HD13	2.00	0.44
1:C:157:ILE:H	1:C:157:ILE:CD1	2.25	0.43
2:D:377:ILE:HD12	2:D:377:ILE:O	2.17	0.43
2:B:90:LEU:HD23	2:B:90:LEU:H	1.83	0.43
1:C:105:LEU:HB2	1:C:127:LEU:HD23	2.00	0.43
2:D:284:ILE:HD13	2:D:289:HIS:HD2	1.83	0.43
1:C:249:HIS:CD2	1:C:287:LEU:HD23	2.50	0.43
2:B:67:THR:O	2:B:68:ASN:HB2	2.18	0.43
2:B:461:ARG:HE	2:B:461:ARG:HB3	1.60	0.43
2:B:566:TYR:HB2	2:B:586:TRP:CZ3	2.53	0.43
2:D:566:TYR:HB2	2:D:586:TRP:CZ3	2.53	0.43
1:A:269:PRO:HD2	1:A:278:TYR:CD2	2.54	0.43
1:C:42:THR:HB	1:C:47:ILE:HD11	2.00	0.43
2:B:55:VAL:CG2	2:B:505:ILE:HD11	2.49	0.43
2:D:370:VAL:HG12	2:D:371:ASN:N	2.32	0.43
2:B:329:LEU:HD13	2:B:333:ILE:HD13	2.00	0.43
2:D:146:PHE:HA	2:D:147:PRO:HD3	1.79	0.43
2:B:366:PRO:O	2:B:369:TYR:HB3	2.17	0.43
1:C:250:GLN:HE21	1:C:250:GLN:HB2	1.67	0.43
2:B:284:ILE:H	2:B:287:GLY:H	1.66	0.43
2:D:182:ALA:HA	2:D:198:GLY:O	2.17	0.43
1:A:196:ASN:HB3	1:A:197:GLN:H	1.58	0.43
1:C:269:PRO:HD2	1:C:278:TYR:CD2	2.54	0.43
2:B:245:TYR:HA	2:B:246:PRO:HD3	1.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:500:GLY:HA3	2:D:515:LEU:HD12	2.01	0.43
2:B:43:LEU:CD2	2:B:43:LEU:H	2.31	0.43
1:A:105:LEU:HB2	1:A:127:LEU:HD23	2.00	0.43
1:C:128:ASP:O	1:C:129:GLU:HB2	2.17	0.43
2:D:138:ARG:NH1	2:D:205:TYR:O	2.52	0.43
1:A:95:GLN:CD	1:A:95:GLN:H	2.22	0.43
2:D:55:VAL:CG2	2:D:505:ILE:HD11	2.48	0.43
2:B:588:PHE:CD2	2:B:622:LEU:HD13	2.54	0.43
2:B:566:TYR:O	2:B:566:TYR:CG	2.72	0.42
2:D:138:ARG:HG3	2:D:175:CYS:HB3	2.01	0.42
2:D:343:PHE:CE1	2:D:444:THR:HG21	2.54	0.42
1:C:223:LEU:HB3	1:C:226:LEU:HD13	2.00	0.42
2:B:125:TYR:CE1	1:C:43:PRO:HD3	2.54	0.42
2:B:137:ASN:HB2	2:B:140:THR:CG2	2.48	0.42
1:C:157:ILE:HB	1:C:160:LEU:CD1	2.49	0.42
1:C:95:GLN:CD	1:C:95:GLN:H	2.22	0.42
2:D:494:HIS:HB2	2:D:515:LEU:CD1	2.49	0.42
1:A:223:LEU:HB3	1:A:226:LEU:HD13	2.00	0.42
1:A:42:THR:HB	1:A:47:ILE:HD11	2.00	0.42
2:B:567:LYS:HD2	2:B:567:LYS:HA	1.88	0.42
2:B:500:GLY:HA3	2:B:515:LEU:HD12	2.01	0.42
2:B:138:ARG:NH1	2:B:205:TYR:O	2.52	0.42
1:A:210:LEU:HA	1:A:210:LEU:HD23	1.84	0.42
2:D:90:LEU:H	2:D:90:LEU:HD23	1.84	0.42
2:D:566:TYR:CG	2:D:566:TYR:O	2.72	0.42
2:D:119:ALA:O	2:D:120:LEU:HD13	2.20	0.42
2:B:343:PHE:CE1	2:B:444:THR:HG21	2.54	0.42
1:A:94:ILE:HG22	1:A:115:PRO:HB3	2.01	0.42
2:D:294:MET:HA	2:D:295:PRO:HD3	1.74	0.42
1:A:157:ILE:N	1:A:157:ILE:HD13	2.26	0.42
2:D:284:ILE:HB	2:D:289:HIS:CD2	2.55	0.42
1:C:196:ASN:HB3	1:C:197:GLN:H	1.57	0.42
2:B:484:HIS:HA	2:B:485:PRO:HD3	1.94	0.42
1:A:53:PHE:O	1:A:56:THR:HB	2.19	0.42
1:C:53:PHE:O	1:C:56:THR:HB	2.19	0.42
1:A:157:ILE:HB	1:A:160:LEU:CD1	2.49	0.42
1:C:94:ILE:HG22	1:C:115:PRO:HB3	2.02	0.42
2:B:355:GLU:HA	2:B:356:PRO:HD3	1.85	0.42
2:D:355:GLU:HA	2:D:356:PRO:HD3	1.85	0.42
2:B:119:ALA:O	2:B:120:LEU:HD13	2.20	0.42
2:D:43:LEU:H	2:D:43:LEU:CD2	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:494:HIS:HB2	2:B:515:LEU:CD1	2.49	0.41
1:A:48:PHE:CE1	1:A:93:GLY:O	2.73	0.41
2:B:267:GLU:HA	2:B:275:HIS:ND1	2.35	0.41
2:D:284:ILE:H	2:D:287:GLY:H	1.67	0.41
2:B:138:ARG:HG3	2:B:175:CYS:HB3	2.01	0.41
2:B:350:LYS:HB3	2:B:351:PRO:CD	2.50	0.41
1:C:216:SER:C	1:C:217:LYS:HG2	2.41	0.41
2:B:325:PRO:HD3	2:B:339:ASP:O	2.20	0.41
2:D:524:GLN:HB2	2:D:528:GLN:HE22	1.86	0.41
1:C:218:ASN:HB3	1:C:219:HIS:H	1.71	0.41
2:B:627:GLY:HA2	2:B:654:TYR:OH	2.21	0.41
2:D:588:PHE:CD2	2:D:622:LEU:HD13	2.54	0.41
1:A:268:THR:HA	1:A:269:PRO:HD3	1.86	0.41
2:D:203:SER:O	2:D:204:SER:HB3	2.20	0.41
2:D:134:GLY:O	2:D:139:GLY:HA2	2.20	0.41
1:A:171:LEU:HA	1:A:171:LEU:HD23	1.78	0.41
2:D:284:ILE:H	2:D:287:GLY:HA3	1.86	0.41
1:C:268:THR:HA	1:C:269:PRO:HD3	1.86	0.41
2:D:647:THR:CG2	2:D:648:GLN:H	2.26	0.41
1:A:216:SER:C	1:A:217:LYS:HG2	2.41	0.41
2:B:336:SER:O	2:B:339:ASP:HB2	2.21	0.41
2:D:336:SER:O	2:D:339:ASP:HB2	2.21	0.41
2:B:124:THR:HG22	2:B:128:ASP:HA	2.03	0.41
2:B:612:LEU:HA	2:B:624:CYS:HB2	2.03	0.41
2:B:284:ILE:HB	2:B:289:HIS:CD2	2.55	0.41
2:D:487:SER:HA	2:D:488:PRO:HD3	1.85	0.41
2:B:647:THR:CG2	2:B:648:GLN:H	2.26	0.41
2:D:573:ALA:HA	2:D:574:PRO:HD3	1.82	0.41
1:C:48:PHE:CE1	1:C:93:GLY:O	2.73	0.41
2:B:134:GLY:O	2:B:139:GLY:HA2	2.21	0.41
2:D:612:LEU:HA	2:D:624:CYS:HB2	2.03	0.41
2:B:146:PHE:HA	2:B:147:PRO:HD3	1.79	0.41
2:B:229:LEU:CD2	2:B:285:ASN:HB3	2.51	0.41
1:A:224:ARG:NH2	1:A:260:LYS:CD	2.84	0.41
2:D:267:GLU:HA	2:D:275:HIS:ND1	2.35	0.40
2:D:124:THR:HG22	2:D:128:ASP:HA	2.03	0.40
1:A:255:VAL:HB	1:A:285:TRP:HZ3	1.86	0.40
2:D:325:PRO:HD3	2:D:339:ASP:O	2.21	0.40
1:A:250:GLN:HB2	1:A:250:GLN:HE21	1.68	0.40
2:B:605:LEU:HD12	2:B:605:LEU:HA	1.93	0.40
2:B:515:LEU:HD23	2:B:515:LEU:HA	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:524:GLN:HB2	2:B:528:GLN:HE22	1.86	0.40
1:C:226:LEU:HD12	1:C:226:LEU:N	2.34	0.40
1:C:36:GLU:O	1:C:37:THR:HB	2.22	0.40
1:C:210:LEU:HD23	1:C:210:LEU:HA	1.84	0.40
1:A:78:ILE:HD12	1:A:97:LEU:HD21	2.04	0.40
2:B:604:LEU:HD12	2:B:606:GLY:O	2.22	0.40

There are no symmetry-related clashes.

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	285/289 (99%)	253 (89%)	30 (10%)	2 (1%)	26	62
1	C	285/289 (99%)	252 (88%)	31 (11%)	2 (1%)	26	62
2	B	529/727 (73%)	450 (85%)	67 (13%)	12 (2%)	8	26
2	D	529/727 (73%)	451 (85%)	66 (12%)	12 (2%)	8	26
All	All	1628/2032 (80%)	1406 (86%)	194 (12%)	28 (2%)	11	36

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	148	HIS
2	D	148	HIS
2	B	87	GLY
2	B	386	LEU
2	B	552	LEU
2	D	87	GLY
2	D	386	LEU
2	D	552	LEU
2	B	204	SER

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Mol	Chain	Res	Type
2	B	478	ASN
2	B	546	VAL
2	B	567	LYS
2	D	204	SER
2	D	478	ASN
2	D	546	VAL
2	D	567	LYS
2	B	266	ARG
2	B	482	ASP
2	B	593	ASN
2	D	266	ARG
2	D	482	ASP
2	D	593	ASN
1	A	280	LYS
1	C	280	LYS
2	B	126	TYR
2	D	126	TYR
1	A	91	VAL
1	C	91	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	264/265 (100%)	254 (96%)	10 (4%)	40	74
1	C	264/265 (100%)	254 (96%)	10 (4%)	40	74
2	B	493/654 (75%)	451 (92%)	42 (8%)	13	36
2	D	493/654 (75%)	451 (92%)	42 (8%)	13	36
All	All	1514/1838 (82%)	1410 (93%)	104 (7%)	19	48

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	VAL
1	A	135	LEU

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Mol	Chain	Res	Type
1	A	157	ILE
1	A	163	LEU
1	A	195	ASP
1	A	217	LYS
1	A	222	ASP
1	A	250	GLN
1	A	287	LEU
1	A	293	GLU
2	B	42	GLN
2	B	43	LEU
2	B	45	ASN
2	B	57	LEU
2	B	90	LEU
2	B	112	TRP
2	B	120	LEU
2	B	123	ASP
2	B	168	GLU
2	B	201	ILE
2	B	217	ARG
2	B	220	LYS
2	B	221	GLU
2	B	273	THR
2	B	275	HIS
2	B	301	THR
2	B	336	SER
2	B	337	LEU
2	B	362	MET
2	B	363	CYS
2	B	383	VAL
2	B	418	THR
2	B	422	THR
2	B	435	SER
2	B	436	GLU
2	B	438	LEU
2	B	442	ILE
2	B	443	SER
2	B	454	ASN
2	B	461	ARG
2	B	469	ARG
2	B	487	SER
2	B	496	LEU
2	B	502	THR

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Mol	Chain	Res	Type
2	B	541	CYS
2	B	576	GLU
2	B	604	LEU
2	B	611	THR
2	B	622	LEU
2	B	634	PHE
2	B	648	GLN
2	B	654	TYR
1	C	91	VAL
1	C	135	LEU
1	C	157	ILE
1	C	163	LEU
1	C	195	ASP
1	C	217	LYS
1	C	222	ASP
1	C	250	GLN
1	C	287	LEU
1	C	293	GLU
2	D	42	GLN
2	D	43	LEU
2	D	45	ASN
2	D	57	LEU
2	D	90	LEU
2	D	112	TRP
2	D	120	LEU
2	D	123	ASP
2	D	168	GLU
2	D	201	ILE
2	D	217	ARG
2	D	220	LYS
2	D	221	GLU
2	D	273	THR
2	D	275	HIS
2	D	301	THR
2	D	336	SER
2	D	337	LEU
2	D	362	MET
2	D	363	CYS
2	D	383	VAL
2	D	418	THR
2	D	422	THR
2	D	435	SER

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Mol	Chain	Res	Type
2	D	436	GLU
2	D	438	LEU
2	D	442	ILE
2	D	443	SER
2	D	454	ASN
2	D	461	ARG
2	D	469	ARG
2	D	487	SER
2	D	496	LEU
2	D	502	THR
2	D	541	CYS
2	D	576	GLU
2	D	604	LEU
2	D	611	THR
2	D	622	LEU
2	D	634	PHE
2	D	648	GLN
2	D	654	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	GLN
2	B	45	ASN
2	B	148	HIS
2	B	265	GLN
2	B	285	ASN
2	B	289	HIS
2	B	332	GLN
2	B	494	HIS
2	B	498	GLN
1	C	250	GLN
2	D	45	ASN
2	D	148	HIS
2	D	265	GLN
2	D	285	ASN
2	D	289	HIS
2	D	332	GLN
2	D	494	HIS
2	D	498	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	287/289 (99%)	-0.00	4 (1%)	78	69	29, 55, 82, 116	0
1	C	287/289 (99%)	0.12	8 (2%)	56	44	36, 60, 91, 111	0
2	B	547/727 (75%)	0.11	27 (4%)	33	22	17, 55, 95, 119	0
2	D	547/727 (75%)	0.48	38 (6%)	20	11	43, 74, 117, 155	0
All	All	1668/2032 (82%)	0.21	77 (4%)	36	25	17, 62, 103, 155	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	82	ALA	6.9
2	D	84	TYR	5.7
2	D	416	TYR	5.2
1	C	34	ALA	5.1
2	B	576	GLU	5.1
2	D	377	ILE	4.9
1	C	254	VAL	4.7
2	D	70	ILE	4.6
2	D	134	GLY	4.5
2	D	586	TRP	4.5
2	B	524	GLN	4.4
2	D	111	VAL	4.3
2	D	163	SER	4.3
1	A	34	ALA	4.2
2	B	522	HIS	4.1
2	D	83	GLU	4.1
2	B	586	TRP	4.1
2	D	148	HIS	4.0
2	D	522	HIS	3.9
2	D	552	LEU	3.9
2	B	577	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
2	D	627	GLY	3.8
2	D	523	PHE	3.7
1	C	320	LYS	3.6
2	D	46	PHE	3.4
2	D	519	GLY	3.4
2	B	416	TYR	3.3
2	B	148	HIS	3.3
2	D	418	THR	3.3
1	C	140	ASP	3.3
2	B	84	TYR	3.3
2	B	523	PHE	3.2
1	C	282	ASN	3.2
2	D	577	GLY	3.1
2	D	205	TYR	3.0
2	B	156	SER	3.0
2	B	377	ILE	3.0
1	A	36	GLU	3.0
2	D	497	ASN	2.9
2	D	144	HIS	2.9
2	D	142	GLN	2.8
1	C	209	LYS	2.8
2	D	524	GLN	2.8
2	D	72	VAL	2.8
1	C	252	ASN	2.7
2	D	569	PHE	2.6
2	B	82	ALA	2.6
2	B	569	PHE	2.5
2	B	205	TYR	2.5
2	B	144	HIS	2.5
2	D	143	ARG	2.5
2	D	227	MET	2.5
2	D	159	HIS	2.5
2	D	549	GLU	2.5
2	B	204	SER	2.4
2	D	528	GLN	2.4
2	B	163	SER	2.4
2	B	627	GLY	2.4
2	B	575	LEU	2.3
1	A	289	GLU	2.3
2	D	213	SER	2.3
2	B	571	ASN	2.3
2	B	581	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	579	THR	2.3
2	D	650	SER	2.3
2	B	628	PRO	2.3
2	B	497	ASN	2.2
2	B	654	TYR	2.2
2	D	81	VAL	2.2
2	B	528	GLN	2.1
1	A	290	PHE	2.1
2	D	158	VAL	2.1
2	B	585	GLY	2.1
2	D	190	ASP	2.1
2	B	149	ASN	2.1
2	D	626	VAL	2.1
1	C	256	PRO	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 carbohydrates 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.