



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:06 AM UTC

PDB ID : 2FNQ / pdb_00002fnq
Title : Insights from the X-ray crystal structure of coral 8R-lipoxygenase: calcium activation via A C2-like domain and a structural basis of product chirality
Authors : Oldham, M.L.; Brash, A.R.; Newcomer, M.E.
Deposited on : 2006-01-11
Resolution : 3.20 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

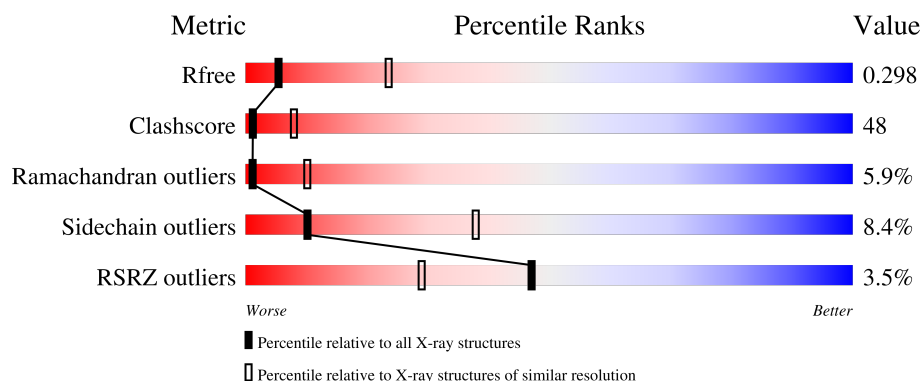
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

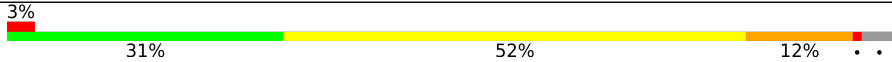
The reported resolution of this entry is 3.20 Å.

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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	699	
1	B	699	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10434 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 Allene oxide synthase-lipoxygenase protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	669	Total	C	N	O	S	0	0	0
			5213	3339	884	977	13			
1	B	669	Total	C	N	O	S	0	0	0
			5213	3339	884	977	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	368	MET	-	cloning artifact	UNP O16025
A	369	HIS	-	cloning artifact	UNP O16025
A	370	HIS	-	cloning artifact	UNP O16025
A	371	HIS	-	cloning artifact	UNP O16025
A	372	HIS	-	cloning artifact	UNP O16025
A	373	HIS	-	cloning artifact	UNP O16025
B	368	MET	-	cloning artifact	UNP O16025
B	369	HIS	-	cloning artifact	UNP O16025
B	370	HIS	-	cloning artifact	UNP O16025
B	371	HIS	-	cloning artifact	UNP O16025
B	372	HIS	-	cloning artifact	UNP O16025
B	373	HIS	-	cloning artifact	UNP O16025

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

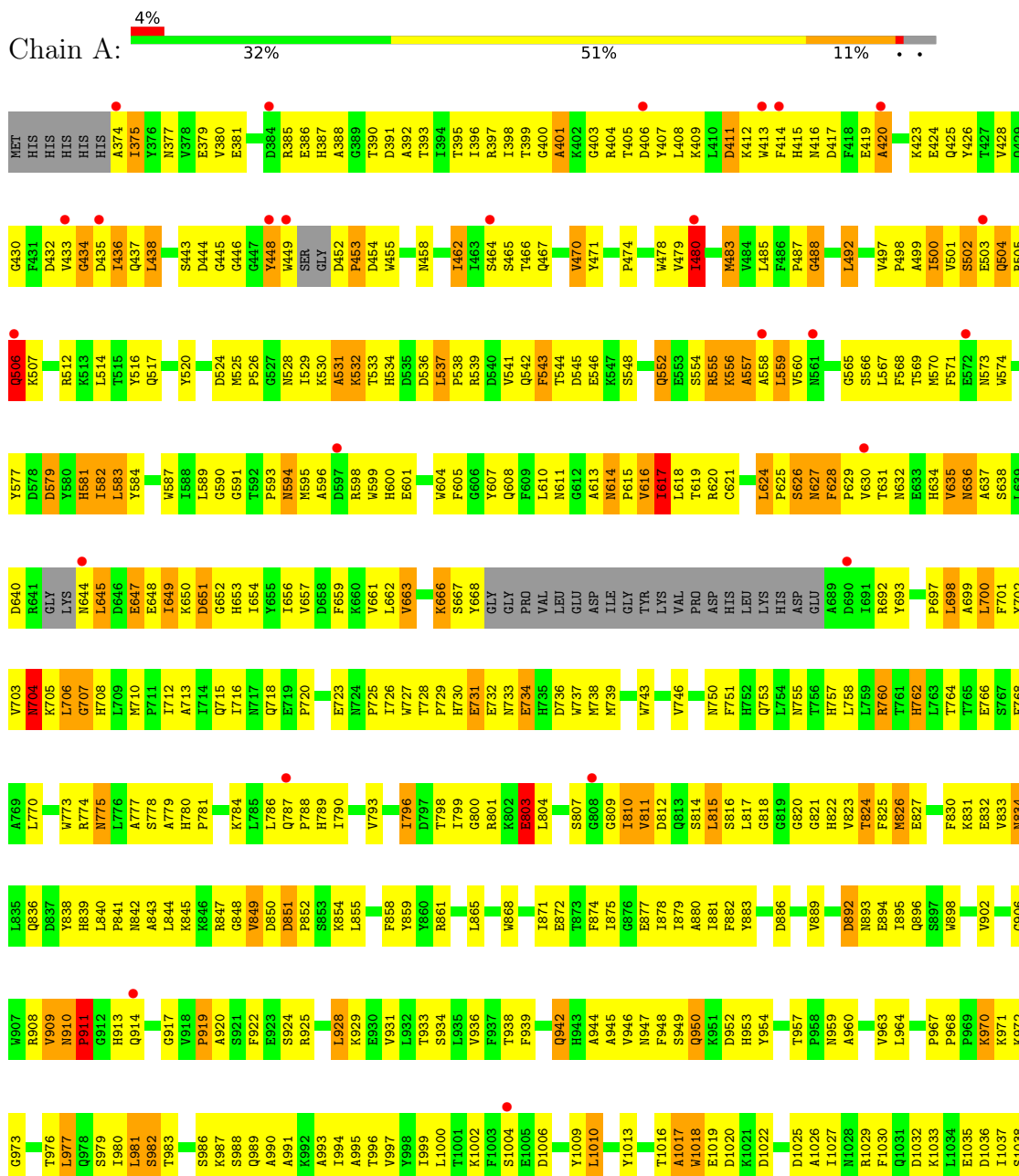
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	Ca 3	0	0
3	B	3	Total 3	Ca 3	0	0

3 Residue-property plots

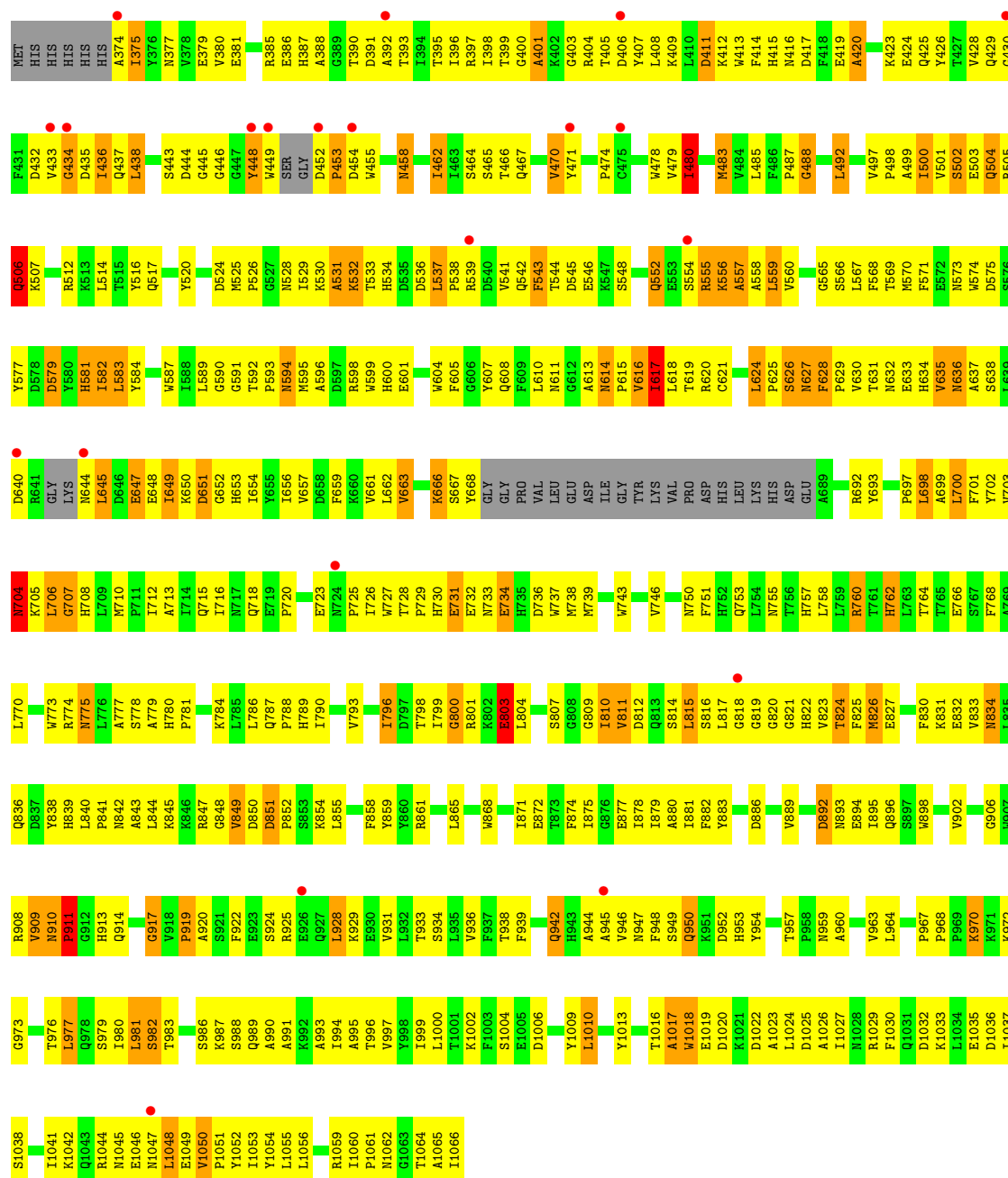
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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





● Molecule 1: Allene oxide synthase-lipoxygenase protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.55Å 78.02Å 176.49Å 90.00° 96.66° 90.00°	Depositor
Resolution (Å)	29.00 – 3.20 29.00 – 3.21	Depositor EDS
% Data completeness (in resolution range)	92.3 (29.00-3.20) 92.8 (29.00-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.81 (at 3.18Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.254 , 0.296 0.255 , 0.298	Depositor DCC
R_{free} test set	1529 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 82.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	10434	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, FE2

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	0.53	0/5358	1.11	47/7315 (0.6%)
1	B	0.53	0/5358	1.11	48/7315 (0.7%)
All	All	0.53	0/10716	1.11	95/14630 (0.6%)

There are no bond length outliers.

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	649	ILE	N-CA-C	-9.54	94.70	109.78
1	A	649	ILE	N-CA-C	-9.54	94.71	109.78
1	A	557	ALA	N-CA-C	-8.98	101.58	111.36
1	A	502	SER	N-CA-C	-8.93	96.69	110.17
1	B	557	ALA	N-CA-C	-8.92	101.64	111.36
1	B	502	SER	N-CA-C	-8.90	96.72	110.17
1	B	705	LYS	N-CA-C	-8.67	101.97	112.54
1	A	705	LYS	N-CA-C	-8.64	102.00	112.54
1	B	1050	VAL	CA-C-N	8.40	128.92	119.93
1	B	1050	VAL	C-N-CA	8.40	128.92	119.93
1	A	1050	VAL	CA-C-N	8.37	128.88	119.93
1	A	1050	VAL	C-N-CA	8.37	128.88	119.93
1	A	851	ASP	CA-C-N	8.24	127.54	118.97
1	A	851	ASP	C-N-CA	8.24	127.54	118.97
1	B	851	ASP	CA-C-N	8.22	127.52	118.97
1	B	851	ASP	C-N-CA	8.22	127.52	118.97
1	B	504	GLN	N-CA-C	-7.90	103.77	113.41
1	A	504	GLN	N-CA-C	-7.83	103.86	113.41
1	A	925	ARG	N-CA-C	-7.68	103.52	113.12
1	B	803	GLU	N-CA-C	7.62	120.56	111.33
1	A	851	ASP	N-CA-C	7.60	119.80	109.24
1	A	803	GLU	N-CA-C	7.58	120.51	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	851	ASP	N-CA-C	7.58	119.78	109.24
1	B	506	GLN	N-CA-C	-7.42	102.25	111.75
1	A	506	GLN	N-CA-C	-7.39	102.29	111.75
1	A	760	ARG	N-CA-C	7.36	121.70	112.87
1	A	635	VAL	N-CA-C	7.34	117.32	110.42
1	B	760	ARG	N-CA-C	7.33	121.67	112.87
1	B	635	VAL	N-CA-C	7.33	117.31	110.42
1	A	492	LEU	N-CA-C	-7.13	100.46	110.29
1	A	950	GLN	N-CA-C	7.10	120.05	111.82
1	B	950	GLN	N-CA-C	7.08	120.04	111.82
1	B	492	LEU	N-CA-C	-7.07	100.53	110.29
1	B	640	ASP	N-CA-C	-6.87	100.87	110.35
1	A	640	ASP	N-CA-C	-6.85	100.90	110.35
1	A	914	GLN	N-CA-C	-6.71	100.02	110.42
1	B	914	GLN	N-CA-C	-6.69	100.05	110.42
1	A	651	ASP	N-CA-C	-6.63	103.13	113.02
1	B	651	ASP	N-CA-C	-6.62	103.16	113.02
1	A	391	ASP	N-CA-C	-6.43	102.64	112.99
1	B	391	ASP	N-CA-C	-6.39	102.70	112.99
1	B	925	ARG	N-CA-C	-6.36	103.61	112.45
1	A	380	VAL	N-CA-C	6.01	115.00	106.53
1	B	380	VAL	N-CA-C	5.97	114.95	106.53
1	A	977	LEU	N-CA-C	-5.80	104.96	111.28
1	B	977	LEU	N-CA-C	-5.77	104.99	111.28
1	B	982	SER	N-CA-C	-5.71	105.90	112.92
1	A	500	ILE	N-CA-C	5.68	116.41	110.62
1	B	500	ILE	N-CA-C	5.67	116.41	110.62
1	A	982	SER	N-CA-C	-5.65	105.97	112.92
1	A	811	VAL	N-CA-C	-5.62	105.62	110.74
1	B	849	VAL	N-CA-C	-5.61	107.52	112.90
1	B	811	VAL	N-CA-C	-5.61	105.64	110.74
1	A	920	ALA	N-CA-C	-5.58	105.43	114.09
1	A	849	VAL	N-CA-C	-5.58	107.54	112.90
1	B	920	ALA	N-CA-C	-5.56	105.47	114.09
1	B	605	PHE	N-CA-C	-5.54	105.39	111.82
1	A	605	PHE	N-CA-C	-5.51	105.42	111.82
1	A	981	LEU	N-CA-C	-5.40	106.62	114.12
1	B	981	LEU	N-CA-C	-5.39	106.63	114.12
1	B	707	GLY	N-CA-C	5.37	125.91	113.18
1	A	821	GLY	N-CA-C	-5.36	107.13	113.99
1	A	628	PHE	CA-C-N	5.35	126.53	119.84
1	A	628	PHE	C-N-CA	5.35	126.53	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	821	GLY	N-CA-C	-5.34	107.16	113.99
1	A	707	GLY	N-CA-C	5.33	125.82	113.18
1	A	928	LEU	N-CA-C	-5.31	104.74	111.11
1	B	628	PHE	CA-C-N	5.31	126.47	119.84
1	B	628	PHE	C-N-CA	5.31	126.47	119.84
1	B	928	LEU	N-CA-C	-5.31	104.74	111.11
1	B	647	GLU	N-CA-C	-5.20	105.29	111.69
1	A	718	GLN	N-CA-C	5.19	119.94	111.37
1	A	647	GLU	N-CA-C	-5.18	105.32	111.69
1	B	968	PRO	CA-C-N	5.16	126.28	119.84
1	B	968	PRO	C-N-CA	5.16	126.28	119.84
1	B	718	GLN	N-CA-C	5.14	119.86	111.37
1	B	626	SER	N-CA-C	5.13	119.00	112.34
1	A	968	PRO	CA-C-N	5.12	126.24	119.84
1	A	968	PRO	C-N-CA	5.12	126.24	119.84
1	B	917	GLY	CA-C-N	-5.12	118.33	123.04
1	B	917	GLY	C-N-CA	-5.12	118.33	123.04
1	B	601	GLU	N-CA-C	5.09	117.04	109.25
1	B	910	ASN	CA-C-N	5.09	126.20	119.84
1	B	910	ASN	C-N-CA	5.09	126.20	119.84
1	A	626	SER	N-CA-C	5.08	118.95	112.34
1	A	601	GLU	N-CA-C	5.07	117.01	109.25
1	A	775	ASN	N-CA-C	5.07	120.85	114.31
1	A	624	LEU	N-CA-C	5.04	116.74	109.48
1	B	624	LEU	N-CA-C	5.03	116.73	109.48
1	A	917	GLY	CA-C-N	-5.02	118.42	123.04
1	A	917	GLY	C-N-CA	-5.02	118.42	123.04
1	B	775	ASN	N-CA-C	5.02	120.79	114.31
1	B	800	GLY	N-CA-C	5.02	118.75	112.73
1	A	910	ASN	CA-C-N	5.00	126.09	119.84
1	A	910	ASN	C-N-CA	5.00	126.09	119.84

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	5213	0	4854	483	2
1	B	5213	0	4854	485	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
All	All	10434	0	9708	968	3

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 48.

All (968) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:ALA:HB3	1:B:434:GLY:HA3	1.26	1.16
1:A:401:ALA:HB3	1:A:434:GLY:HA3	1.26	1.12
1:A:436:ILE:HD12	1:A:462:ILE:HD11	1.36	1.05
1:A:662:LEU:O	1:A:663:VAL:HG23	1.58	1.04
1:B:436:ILE:HD12	1:B:462:ILE:HD11	1.36	1.03
1:B:662:LEU:O	1:B:663:VAL:HG23	1.58	1.02
1:B:631:THR:H	1:B:634:HIS:HD2	1.05	1.01
1:B:834:ASN:ND2	1:B:836:GLN:H	1.60	0.99
1:A:631:THR:H	1:A:634:HIS:HD2	1.05	0.98
1:A:834:ASN:ND2	1:A:836:GLN:H	1.60	0.97
1:A:834:ASN:HD22	1:A:836:GLN:H	0.98	0.97
1:B:616:VAL:C	1:B:847:ARG:HH12	1.74	0.96
1:A:616:VAL:C	1:A:847:ARG:HH12	1.74	0.95
1:B:631:THR:H	1:B:634:HIS:CD2	1.85	0.94
1:A:631:THR:H	1:A:634:HIS:CD2	1.85	0.94
1:A:644:ASN:HD22	1:A:647:GLU:H	1.15	0.93
1:B:644:ASN:HD22	1:B:647:GLU:H	1.15	0.92
1:B:573:ASN:ND2	1:B:982:SER:HA	1.85	0.91
1:A:446:GLY:HA3	1:A:453:PRO:HB3	1.53	0.91
1:B:446:GLY:HA3	1:B:453:PRO:HB3	1.53	0.91
1:B:834:ASN:HD22	1:B:836:GLN:H	0.98	0.90
1:A:573:ASN:ND2	1:A:982:SER:HA	1.85	0.89
1:A:753:GLN:HE22	1:A:950:GLN:HE22	1.22	0.87
1:A:700:LEU:HD12	1:A:712:ILE:HD11	1.57	0.86
1:A:644:ASN:ND2	1:A:647:GLU:H	1.72	0.86
1:B:502:SER:C	1:B:504:GLN:H	1.84	0.86
1:B:970:LYS:H	1:B:970:LYS:HD2	1.41	0.85
1:A:595:MET:HG2	1:A:608:GLN:NE2	1.91	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:MET:HG2	1:B:608:GLN:NE2	1.91	0.85
1:A:804:LEU:HA	1:A:810:ILE:HD11	1.59	0.85
1:A:502:SER:C	1:A:504:GLN:H	1.84	0.85
1:B:573:ASN:HD22	1:B:982:SER:HA	1.39	0.85
1:B:700:LEU:HD12	1:B:712:ILE:HD11	1.57	0.85
1:A:573:ASN:HD22	1:A:982:SER:HA	1.39	0.84
1:B:644:ASN:ND2	1:B:647:GLU:H	1.72	0.84
1:A:970:LYS:H	1:A:970:LYS:HD2	1.41	0.84
1:A:608:GLN:HE22	1:A:959:ASN:HD21	1.23	0.84
1:B:753:GLN:HE22	1:B:950:GLN:HE22	1.22	0.84
1:B:608:GLN:HE22	1:B:959:ASN:HD21	1.23	0.83
1:B:804:LEU:HA	1:B:810:ILE:HD11	1.59	0.83
1:B:488:GLY:HA2	1:B:1019:GLU:HG3	1.61	0.83
1:A:1045:ASN:HA	1:A:1048:LEU:HD22	1.58	0.83
1:A:488:GLY:HA2	1:A:1019:GLU:HG3	1.61	0.83
1:B:666:LYS:H	1:B:666:LYS:HD3	1.45	0.82
1:B:1045:ASN:HA	1:B:1048:LEU:HD22	1.58	0.82
1:A:644:ASN:ND2	1:A:647:GLU:HG3	1.95	0.82
1:A:839:HIS:CD2	1:A:841:PRO:HD2	2.15	0.82
1:B:480:ILE:HD12	1:B:480:ILE:H	1.44	0.82
1:B:644:ASN:ND2	1:B:647:GLU:HG3	1.95	0.81
1:A:480:ILE:H	1:A:480:ILE:HD12	1.44	0.81
1:B:839:HIS:CD2	1:B:841:PRO:HD2	2.15	0.81
1:B:780:HIS:CD2	1:B:781:PRO:HD2	2.16	0.81
1:A:938:THR:HA	1:A:942:GLN:HB2	1.62	0.81
1:A:666:LYS:H	1:A:666:LYS:HD3	1.45	0.81
1:A:834:ASN:HD22	1:A:836:GLN:N	1.78	0.81
1:A:632:ASN:ND2	1:A:645:LEU:H	1.79	0.80
1:B:408:LEU:HB3	1:B:428:VAL:HG21	1.63	0.80
1:B:631:THR:N	1:B:634:HIS:HD2	1.79	0.80
1:A:537:LEU:HD13	1:A:541:VAL:HG23	1.64	0.80
1:A:659:PHE:HB3	1:A:662:LEU:HD23	1.63	0.80
1:A:780:HIS:CD2	1:A:781:PRO:HD2	2.16	0.80
1:B:537:LEU:HD13	1:B:541:VAL:HG23	1.64	0.80
1:A:631:THR:N	1:A:634:HIS:HD2	1.79	0.80
1:B:938:THR:HA	1:B:942:GLN:HB2	1.62	0.80
1:B:632:ASN:ND2	1:B:645:LEU:H	1.80	0.79
1:A:408:LEU:HB3	1:A:428:VAL:HG21	1.63	0.79
1:B:834:ASN:HD22	1:B:836:GLN:N	1.78	0.78
1:B:659:PHE:HB3	1:B:662:LEU:HD23	1.63	0.78
1:B:910:ASN:HB3	1:B:911:PRO:HD2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:632:ASN:HD21	1:B:645:LEU:H	1.30	0.77
1:A:632:ASN:HD21	1:A:645:LEU:H	1.30	0.77
1:A:532:LYS:H	1:A:532:LYS:HE3	1.50	0.77
1:B:840:LEU:HB3	1:B:841:PRO:HD3	1.67	0.77
1:B:577:TYR:OH	1:B:980:ILE:HD11	1.86	0.76
1:A:840:LEU:HB3	1:A:841:PRO:HD3	1.67	0.76
1:A:910:ASN:HB3	1:A:911:PRO:HD2	1.67	0.75
1:A:577:TYR:OH	1:A:980:ILE:HD11	1.86	0.75
1:B:532:LYS:HE3	1:B:532:LYS:H	1.50	0.75
1:A:504:GLN:O	1:A:507:LYS:HB3	1.86	0.75
1:B:400:GLY:HA2	1:B:437:GLN:HG3	1.67	0.75
1:B:504:GLN:O	1:B:507:LYS:HB3	1.86	0.75
1:A:812:ASP:O	1:A:818:GLY:HA3	1.87	0.75
1:B:812:ASP:O	1:B:818:GLY:HA3	1.87	0.74
1:A:400:GLY:HA2	1:A:437:GLN:HG3	1.67	0.74
1:B:728:THR:OG1	1:B:729:PRO:HD2	1.88	0.74
1:B:1048:LEU:HD21	1:B:1051:PRO:HA	1.70	0.74
1:A:1045:ASN:C	1:A:1047:ASN:H	1.95	0.74
1:B:1045:ASN:C	1:B:1047:ASN:H	1.95	0.74
1:A:446:GLY:CA	1:A:453:PRO:HB3	2.18	0.73
1:A:1048:LEU:HD21	1:A:1051:PRO:HA	1.70	0.73
1:B:503:GLU:HA	1:B:506:GLN:HG2	1.69	0.73
1:A:503:GLU:HA	1:A:506:GLN:HG2	1.69	0.73
1:B:608:GLN:NE2	1:B:959:ASN:HD21	1.86	0.73
1:A:728:THR:OG1	1:A:729:PRO:HD2	1.88	0.73
1:A:503:GLU:O	1:A:507:LYS:HB2	1.89	0.73
1:A:624:LEU:HD11	1:A:630:VAL:HB	1.71	0.73
1:A:843:ALA:O	1:A:847:ARG:HG3	1.89	0.72
1:A:608:GLN:NE2	1:A:959:ASN:HD21	1.86	0.72
1:B:503:GLU:O	1:B:507:LYS:HB2	1.89	0.72
1:B:728:THR:HG23	1:B:730:HIS:H	1.55	0.72
1:B:820:GLY:O	1:B:823:VAL:HG22	1.88	0.72
1:B:624:LEU:HD11	1:B:630:VAL:HB	1.71	0.72
1:A:417:ASP:HB3	1:A:426:TYR:OH	1.89	0.72
1:A:820:GLY:O	1:A:823:VAL:HG22	1.88	0.72
1:B:417:ASP:HB3	1:B:426:TYR:OH	1.89	0.72
1:B:446:GLY:CA	1:B:453:PRO:HB3	2.18	0.72
1:B:843:ALA:O	1:B:847:ARG:HG3	1.89	0.72
1:A:845:LYS:HA	1:A:850:ASP:HB2	1.72	0.72
1:B:875:ILE:HD12	1:B:933:THR:HA	1.72	0.71
1:A:480:ILE:H	1:A:480:ILE:CD1	1.99	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:753:GLN:HE22	1:B:950:GLN:NE2	1.87	0.71
1:B:645:LEU:C	1:B:645:LEU:HD12	2.15	0.71
1:B:845:LYS:HA	1:B:850:ASP:HB2	1.72	0.71
1:A:875:ILE:HD12	1:A:933:THR:HA	1.72	0.70
1:B:452:ASP:C	1:B:454:ASP:H	2.00	0.70
1:A:552:GLN:O	1:A:555:ARG:HB3	1.92	0.70
1:A:753:GLN:HE22	1:A:950:GLN:NE2	1.87	0.70
1:A:1038:SER:O	1:A:1042:LYS:HG3	1.91	0.70
1:A:753:GLN:O	1:A:758:LEU:HD13	1.92	0.70
1:A:438:LEU:C	1:A:438:LEU:HD12	2.17	0.69
1:A:728:THR:HG23	1:A:730:HIS:H	1.55	0.69
1:A:942:GLN:O	1:A:946:VAL:HG12	1.92	0.69
1:B:942:GLN:O	1:B:946:VAL:HG12	1.92	0.69
1:B:1038:SER:O	1:B:1042:LYS:HG3	1.91	0.69
1:A:452:ASP:C	1:A:454:ASP:H	1.99	0.69
1:A:811:VAL:HG13	1:A:815:LEU:HD21	1.73	0.69
1:B:552:GLN:O	1:B:555:ARG:HB3	1.92	0.69
1:A:645:LEU:C	1:A:645:LEU:HD12	2.15	0.69
1:B:528:ASN:HB2	1:B:766:GLU:OE2	1.92	0.69
1:A:528:ASN:HB2	1:A:766:GLU:OE2	1.92	0.69
1:A:555:ARG:C	1:A:557:ALA:H	2.01	0.69
1:B:438:LEU:C	1:B:438:LEU:HD12	2.17	0.69
1:B:753:GLN:O	1:B:758:LEU:HD13	1.92	0.69
1:B:811:VAL:HG13	1:B:815:LEU:HD21	1.73	0.69
1:A:728:THR:O	1:A:731:GLU:HG2	1.92	0.69
1:B:412:LYS:HB2	1:B:415:HIS:CD2	2.29	0.68
1:B:728:THR:O	1:B:731:GLU:HG2	1.92	0.68
1:B:644:ASN:HD22	1:B:647:GLU:N	1.91	0.68
1:B:598:ARG:HH12	1:B:1049:GLU:HG2	1.59	0.68
1:B:820:GLY:HA2	1:B:822:HIS:CE1	2.29	0.68
1:A:996:THR:O	1:A:1000:LEU:HD23	1.94	0.68
1:A:502:SER:C	1:A:504:GLN:N	2.52	0.67
1:A:820:GLY:HA2	1:A:822:HIS:CE1	2.29	0.67
1:B:996:THR:O	1:B:1000:LEU:HD23	1.94	0.67
1:A:645:LEU:HD12	1:A:645:LEU:O	1.95	0.67
1:B:555:ARG:C	1:B:557:ALA:H	2.01	0.67
1:A:598:ARG:HH12	1:A:1049:GLU:HG2	1.59	0.67
1:B:532:LYS:HG2	1:B:536:ASP:OD2	1.94	0.67
1:B:616:VAL:CA	1:B:847:ARG:HH12	2.08	0.67
1:B:492:LEU:HD11	1:B:882:PHE:O	1.95	0.67
1:B:607:TYR:CE2	1:B:611:ASN:HB2	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:970:LYS:H	1:B:970:LYS:CD	2.04	0.67
1:A:412:LYS:HB2	1:A:415:HIS:CD2	2.29	0.67
1:A:492:LEU:HD11	1:A:882:PHE:O	1.95	0.67
1:A:607:TYR:CE2	1:A:611:ASN:HB2	2.30	0.67
1:B:1045:ASN:HA	1:B:1048:LEU:CD2	2.25	0.67
1:A:533:THR:HG22	1:A:534:HIS:H	1.60	0.67
1:A:532:LYS:HG2	1:A:536:ASP:OD2	1.94	0.66
1:B:645:LEU:HD12	1:B:645:LEU:O	1.95	0.66
1:A:1045:ASN:HA	1:A:1048:LEU:CD2	2.25	0.66
1:A:608:GLN:HE22	1:A:959:ASN:ND2	1.94	0.66
1:A:635:VAL:O	1:A:637:ALA:N	2.29	0.66
1:B:635:VAL:O	1:B:637:ALA:N	2.29	0.66
1:B:594:ASN:HB2	1:B:595:MET:CE	2.25	0.66
1:A:594:ASN:HB2	1:A:595:MET:CE	2.25	0.66
1:A:977:LEU:O	1:A:981:LEU:HB2	1.96	0.66
1:B:608:GLN:HE22	1:B:959:ASN:ND2	1.94	0.66
1:A:616:VAL:CA	1:A:847:ARG:HH12	2.08	0.66
1:B:844:LEU:HD12	1:B:865:LEU:HD21	1.78	0.65
1:A:532:LYS:HE3	1:A:532:LYS:N	2.12	0.65
1:A:644:ASN:O	1:A:648:GLU:HB2	1.97	0.65
1:B:533:THR:HG22	1:B:534:HIS:H	1.60	0.65
1:B:804:LEU:HA	1:B:810:ILE:CD1	2.27	0.65
1:A:374:ALA:HA	1:A:430:GLY:O	1.95	0.65
1:A:804:LEU:HA	1:A:810:ILE:CD1	2.27	0.65
1:B:762:HIS:CE1	1:B:1066:ILE:C	2.74	0.65
1:B:970:LYS:HD2	1:B:970:LYS:N	2.12	0.65
1:B:624:LEU:CD1	1:B:630:VAL:HB	2.27	0.65
1:A:624:LEU:CD1	1:A:630:VAL:HB	2.27	0.65
1:A:844:LEU:HD12	1:A:865:LEU:HD21	1.78	0.65
1:B:644:ASN:O	1:B:648:GLU:HB2	1.97	0.65
1:B:374:ALA:HA	1:B:430:GLY:O	1.96	0.65
1:A:533:THR:HG22	1:A:534:HIS:N	2.13	0.64
1:A:613:ALA:C	1:A:615:PRO:HD3	2.23	0.64
1:B:977:LEU:O	1:B:981:LEU:HB2	1.96	0.64
1:A:757:HIS:CE1	1:A:947:ASN:HD22	2.14	0.64
1:B:555:ARG:HG3	1:B:556:LYS:N	2.12	0.64
1:A:635:VAL:HG11	1:A:712:ILE:HD12	1.80	0.64
1:A:762:HIS:CE1	1:A:1066:ILE:C	2.74	0.64
1:B:757:HIS:CE1	1:B:947:ASN:HD22	2.14	0.64
1:B:796:ILE:HG13	1:B:1065:ALA:O	1.97	0.64
1:B:555:ARG:O	1:B:557:ALA:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:796:ILE:HG13	1:A:1065:ALA:O	1.97	0.64
1:B:416:ASN:OD1	1:B:419:GLU:HG2	1.98	0.64
1:A:400:GLY:HA3	1:A:433:VAL:CG1	2.27	0.64
1:B:408:LEU:CB	1:B:428:VAL:HG21	2.28	0.64
1:B:444:ASP:O	1:B:446:GLY:N	2.31	0.64
1:B:532:LYS:HE3	1:B:532:LYS:N	2.12	0.64
1:B:613:ALA:C	1:B:615:PRO:HD3	2.23	0.64
1:A:555:ARG:HG3	1:A:556:LYS:N	2.12	0.64
1:B:524:ASP:O	1:B:525:MET:HE2	1.98	0.64
1:B:816:SER:OG	1:B:963:VAL:HA	1.97	0.64
1:A:524:ASP:O	1:A:525:MET:HE2	1.98	0.63
1:A:416:ASN:OD1	1:A:419:GLU:HG2	1.98	0.63
1:A:574:TRP:NE1	1:A:987:LYS:HA	2.14	0.63
1:A:816:SER:OG	1:A:963:VAL:HA	1.97	0.63
1:B:892:ASP:O	1:B:896:GLN:HG2	1.99	0.63
1:A:408:LEU:CB	1:A:428:VAL:HG21	2.28	0.63
1:A:617:ILE:O	1:A:619:THR:HG23	1.99	0.63
1:B:617:ILE:O	1:B:619:THR:HG23	1.99	0.63
1:A:444:ASP:O	1:A:446:GLY:N	2.31	0.63
1:B:400:GLY:HA3	1:B:433:VAL:CG1	2.28	0.63
1:A:555:ARG:O	1:A:557:ALA:N	2.31	0.63
1:A:644:ASN:HD22	1:A:647:GLU:N	1.91	0.63
1:A:970:LYS:HD2	1:A:970:LYS:N	2.12	0.62
1:B:533:THR:HG22	1:B:534:HIS:N	2.13	0.62
1:B:635:VAL:HG11	1:B:712:ILE:HD12	1.79	0.62
1:A:666:LYS:HD3	1:A:666:LYS:N	2.14	0.62
1:A:798:THR:HA	1:A:801:ARG:HH12	1.65	0.62
1:B:574:TRP:NE1	1:B:987:LYS:HA	2.13	0.62
1:A:403:GLY:O	1:A:433:VAL:HG22	1.99	0.62
1:A:892:ASP:O	1:A:896:GLN:HG2	1.99	0.62
1:B:403:GLY:O	1:B:433:VAL:HG22	1.99	0.62
1:A:377:ASN:O	1:A:462:ILE:HA	2.00	0.62
1:A:498:PRO:HG2	1:A:501:VAL:CG2	2.30	0.62
1:A:1059:ARG:O	1:A:1061:PRO:HD3	1.99	0.62
1:B:502:SER:C	1:B:504:GLN:N	2.52	0.62
1:B:1059:ARG:O	1:B:1061:PRO:HD3	1.99	0.62
1:A:942:GLN:HA	1:A:942:GLN:OE1	1.99	0.62
1:B:942:GLN:HA	1:B:942:GLN:OE1	1.99	0.62
1:A:390:THR:HG22	1:A:453:PRO:C	2.25	0.61
1:A:875:ILE:O	1:A:879:ILE:HG13	2.00	0.61
1:B:377:ASN:HB3	1:B:425:GLN:HE22	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:815:LEU:N	1:B:815:LEU:HD22	2.16	0.61
1:A:424:GLU:HB3	1:A:426:TYR:CE1	2.35	0.61
1:B:436:ILE:HB	1:B:471:TYR:CE2	2.35	0.61
1:A:377:ASN:HB3	1:A:425:GLN:HE22	1.65	0.61
1:A:436:ILE:HB	1:A:471:TYR:CE2	2.35	0.61
1:A:500:ILE:O	1:A:504:GLN:HB2	2.01	0.61
1:B:424:GLU:HB3	1:B:426:TYR:CE1	2.35	0.61
1:B:498:PRO:HG2	1:B:501:VAL:CG2	2.30	0.61
1:B:500:ILE:O	1:B:504:GLN:HB2	2.01	0.61
1:B:390:THR:HG22	1:B:453:PRO:C	2.25	0.61
1:B:555:ARG:HG3	1:B:556:LYS:H	1.66	0.61
1:A:616:VAL:C	1:A:847:ARG:NH1	2.54	0.61
1:B:875:ILE:O	1:B:879:ILE:HG13	2.00	0.61
1:B:377:ASN:O	1:B:462:ILE:HA	2.00	0.61
1:A:1045:ASN:C	1:A:1047:ASN:N	2.57	0.61
1:A:1056:LEU:O	1:A:1060:ILE:HG13	2.01	0.60
1:B:798:THR:HA	1:B:801:ARG:HH12	1.65	0.60
1:A:544:THR:HG22	1:A:546:GLU:H	1.67	0.60
1:A:970:LYS:H	1:A:970:LYS:CD	2.04	0.60
1:A:815:LEU:HD22	1:A:815:LEU:N	2.16	0.60
1:B:616:VAL:HG12	1:B:617:ILE:H	1.67	0.60
1:B:839:HIS:CD2	1:B:842:ASN:H	2.20	0.60
1:B:1056:LEU:O	1:B:1060:ILE:HG13	2.01	0.60
1:B:913:HIS:H	1:B:913:HIS:CD2	2.19	0.60
1:A:555:ARG:HG3	1:A:556:LYS:H	1.66	0.60
1:A:839:HIS:CD2	1:A:842:ASN:H	2.20	0.60
1:B:706:LEU:HD12	1:B:708:HIS:CE1	2.37	0.60
1:A:788:PRO:O	1:A:1062:ASN:HB3	2.01	0.60
1:B:798:THR:HA	1:B:801:ARG:NH1	2.17	0.60
1:B:788:PRO:O	1:B:1062:ASN:HB3	2.01	0.60
1:B:666:LYS:HD3	1:B:666:LYS:N	2.14	0.59
1:B:480:ILE:HD12	1:B:480:ILE:N	2.16	0.59
1:A:798:THR:HA	1:A:801:ARG:NH1	2.17	0.59
1:B:381:GLU:HB2	1:B:423:LYS:HG3	1.84	0.59
1:A:531:ALA:HA	1:A:532:LYS:HE3	1.83	0.59
1:B:390:THR:CG2	1:B:455:TRP:HB2	2.32	0.59
1:B:544:THR:HG22	1:B:546:GLU:H	1.67	0.59
1:A:448:TYR:HD1	1:A:448:TYR:C	2.11	0.59
1:B:381:GLU:HA	1:B:423:LYS:HA	1.84	0.59
1:B:393:THR:N	1:B:444:ASP:OD1	2.35	0.59
1:B:448:TYR:C	1:B:448:TYR:HD1	2.11	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:663:VAL:O	1:B:663:VAL:HG12	2.02	0.59
1:B:831:LYS:HG2	1:B:913:HIS:CD2	2.37	0.59
1:A:831:LYS:HG2	1:A:913:HIS:CD2	2.37	0.59
1:A:666:LYS:HA	1:A:816:SER:O	2.02	0.59
1:A:913:HIS:CD2	1:A:913:HIS:H	2.19	0.59
1:B:531:ALA:HA	1:B:532:LYS:HE3	1.84	0.59
1:A:470:VAL:O	1:A:470:VAL:HG22	2.03	0.59
1:A:706:LEU:HD12	1:A:708:HIS:CE1	2.37	0.59
1:B:644:ASN:ND2	1:B:647:GLU:N	2.50	0.59
1:B:666:LYS:HA	1:B:816:SER:O	2.02	0.59
1:A:616:VAL:HG12	1:A:617:ILE:H	1.67	0.59
1:B:470:VAL:HG22	1:B:470:VAL:O	2.03	0.59
1:B:556:LYS:O	1:B:559:LEU:HD23	2.03	0.59
1:B:616:VAL:HG12	1:B:617:ILE:N	2.18	0.59
1:B:627:ASN:C	1:B:629:PRO:HD3	2.28	0.59
1:B:994:ILE:HD12	1:B:994:ILE:H	1.68	0.59
1:A:390:THR:CG2	1:A:455:TRP:HB2	2.32	0.58
1:A:555:ARG:C	1:A:557:ALA:N	2.61	0.58
1:A:556:LYS:O	1:A:559:LEU:HD23	2.03	0.58
1:B:395:THR:HG22	1:B:409:LYS:HA	1.85	0.58
1:A:395:THR:HG22	1:A:409:LYS:HA	1.85	0.58
1:A:381:GLU:HA	1:A:423:LYS:HA	1.84	0.58
1:A:480:ILE:HD12	1:A:480:ILE:N	2.16	0.58
1:A:582:ILE:O	1:A:584:TYR:N	2.37	0.58
1:A:663:VAL:HG12	1:A:663:VAL:O	2.02	0.58
1:A:627:ASN:C	1:A:629:PRO:HD3	2.28	0.58
1:B:502:SER:O	1:B:504:GLN:N	2.37	0.58
1:A:823:VAL:CG2	1:A:824:THR:N	2.66	0.58
1:A:849:VAL:CG1	1:A:858:PHE:CE2	2.87	0.58
1:B:823:VAL:HG23	1:B:824:THR:N	2.18	0.58
1:A:616:VAL:HG12	1:A:617:ILE:N	2.18	0.58
1:B:582:ILE:O	1:B:584:TYR:N	2.37	0.58
1:B:823:VAL:CG2	1:B:824:THR:N	2.66	0.58
1:A:994:ILE:HD12	1:A:994:ILE:H	1.68	0.57
1:A:393:THR:N	1:A:444:ASP:OD1	2.35	0.57
1:A:910:ASN:HB3	1:A:911:PRO:CD	2.34	0.57
1:A:381:GLU:HB2	1:A:423:LYS:HG3	1.84	0.57
1:B:595:MET:HE2	1:B:595:MET:H	1.69	0.57
1:B:1045:ASN:C	1:B:1047:ASN:N	2.57	0.57
1:B:448:TYR:C	1:B:448:TYR:CD1	2.81	0.57
1:A:448:TYR:C	1:A:448:TYR:CD1	2.81	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:ILE:O	1:A:883:TYR:HB2	2.05	0.57
1:B:398:ILE:HG21	1:B:436:ILE:HD13	1.87	0.57
1:B:616:VAL:C	1:B:847:ARG:NH1	2.54	0.57
1:B:849:VAL:CG1	1:B:858:PHE:CE2	2.87	0.57
1:B:879:ILE:O	1:B:883:TYR:HB2	2.05	0.57
1:B:1045:ASN:O	1:B:1047:ASN:N	2.37	0.57
1:A:400:GLY:CA	1:A:433:VAL:HG13	2.34	0.57
1:B:555:ARG:C	1:B:557:ALA:N	2.61	0.57
1:A:950:GLN:HB3	1:A:997:VAL:HG13	1.87	0.57
1:B:780:HIS:HD2	1:B:781:PRO:HD2	1.65	0.57
1:A:750:ASN:ND2	1:A:815:LEU:HB3	2.19	0.57
1:A:1045:ASN:O	1:A:1047:ASN:N	2.37	0.57
1:A:405:THR:HG23	1:A:433:VAL:HG23	1.87	0.57
1:B:400:GLY:CA	1:B:433:VAL:HG13	2.34	0.57
1:A:396:ILE:O	1:A:407:TYR:HA	2.05	0.56
1:A:398:ILE:HG21	1:A:436:ILE:HD13	1.87	0.56
1:B:452:ASP:O	1:B:454:ASP:N	2.38	0.56
1:B:950:GLN:HB3	1:B:997:VAL:HG13	1.87	0.56
1:A:823:VAL:HG23	1:A:824:THR:N	2.18	0.56
1:B:811:VAL:HG13	1:B:815:LEU:CD2	2.36	0.56
1:A:811:VAL:HG13	1:A:815:LEU:CD2	2.36	0.56
1:A:875:ILE:CD1	1:A:933:THR:HA	2.35	0.56
1:B:479:VAL:HG13	1:B:483:MET:HB2	1.86	0.56
1:B:750:ASN:ND2	1:B:815:LEU:HB3	2.19	0.56
1:A:479:VAL:HG13	1:A:483:MET:HB2	1.86	0.56
1:A:595:MET:HE2	1:A:595:MET:H	1.69	0.56
1:B:530:LYS:O	1:B:531:ALA:HB2	2.05	0.56
1:B:594:ASN:HB2	1:B:595:MET:HE2	1.87	0.56
1:B:944:ALA:HA	1:B:948:PHE:HD1	1.69	0.56
1:B:396:ILE:O	1:B:407:TYR:HA	2.05	0.56
1:B:405:THR:HG23	1:B:433:VAL:HG23	1.87	0.56
1:A:598:ARG:HH12	1:A:1049:GLU:CG	2.19	0.56
1:A:464:SER:C	1:A:466:THR:H	2.14	0.56
1:A:530:LYS:O	1:A:531:ALA:HB2	2.05	0.56
1:A:944:ALA:HA	1:A:948:PHE:HD1	1.69	0.56
1:B:910:ASN:HB3	1:B:911:PRO:CD	2.34	0.56
1:B:598:ARG:HH12	1:B:1049:GLU:CG	2.19	0.56
1:A:697:PRO:HB3	1:A:716:ILE:O	2.06	0.56
1:A:727:TRP:HA	1:A:731:GLU:OE2	2.06	0.56
1:B:537:LEU:HD13	1:B:541:VAL:CG2	2.36	0.56
1:A:452:ASP:O	1:A:454:ASP:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:PHE:N	1:B:571:PHE:CD1	2.74	0.55
1:A:502:SER:O	1:A:504:GLN:N	2.37	0.55
1:A:571:PHE:N	1:A:571:PHE:CD1	2.74	0.55
1:A:594:ASN:HB2	1:A:595:MET:HE2	1.87	0.55
1:B:594:ASN:ND2	1:B:952:ASP:HB3	2.21	0.55
1:B:875:ILE:CD1	1:B:933:THR:HA	2.35	0.55
1:B:949:SER:HA	1:B:1054:TYR:CE2	2.42	0.55
1:A:621:CYS:HB3	1:A:654:ILE:HG22	1.88	0.55
1:B:727:TRP:HA	1:B:731:GLU:OE2	2.06	0.55
1:A:949:SER:HA	1:A:1054:TYR:CE2	2.42	0.55
1:A:594:ASN:ND2	1:A:952:ASP:HB3	2.22	0.55
1:B:424:GLU:HB3	1:B:426:TYR:HE1	1.71	0.55
1:B:464:SER:C	1:B:466:THR:H	2.14	0.55
1:B:697:PRO:HB3	1:B:716:ILE:O	2.06	0.55
1:B:621:CYS:HB3	1:B:654:ILE:HG22	1.88	0.54
1:A:624:LEU:HD23	1:A:625:PRO:HD2	1.90	0.54
1:A:892:ASP:HB3	1:A:895:ILE:HG22	1.90	0.54
1:B:464:SER:HB3	1:B:467:GLN:HG2	1.89	0.54
1:B:537:LEU:HD12	1:B:542:GLN:HG3	1.89	0.54
1:B:1027:ILE:O	1:B:1030:PHE:HB3	2.08	0.54
1:A:644:ASN:ND2	1:A:647:GLU:N	2.50	0.54
1:B:390:THR:HG23	1:B:455:TRP:HB2	1.90	0.54
1:B:892:ASP:HB3	1:B:895:ILE:HG22	1.90	0.54
1:B:810:ILE:HD12	1:B:811:VAL:H	1.72	0.54
1:B:1029:ARG:HG3	1:B:1029:ARG:HH11	1.72	0.54
1:A:502:SER:O	1:A:503:GLU:HB3	2.08	0.54
1:B:392:ALA:HB2	1:B:446:GLY:HA2	1.90	0.54
1:A:625:PRO:HG2	1:A:628:PHE:HB3	1.89	0.54
1:A:790:ILE:HG22	1:A:939:PHE:CE1	2.43	0.54
1:B:411:ASP:HA	1:B:426:TYR:HE2	1.73	0.54
1:A:537:LEU:HD13	1:A:541:VAL:CG2	2.36	0.54
1:B:790:ILE:HG22	1:B:939:PHE:CE1	2.43	0.54
1:A:390:THR:HG23	1:A:455:TRP:HB2	1.89	0.53
1:A:595:MET:HG2	1:A:608:GLN:CD	2.34	0.53
1:A:810:ILE:HD12	1:A:811:VAL:H	1.72	0.53
1:A:537:LEU:HD12	1:A:542:GLN:HG3	1.89	0.53
1:B:398:ILE:CG2	1:B:436:ILE:HD13	2.39	0.53
1:B:995:ALA:O	1:B:999:ILE:HG13	2.08	0.53
1:A:398:ILE:CG2	1:A:436:ILE:HD13	2.39	0.53
1:A:411:ASP:HA	1:A:426:TYR:HE2	1.73	0.53
1:A:656:ILE:HG12	1:A:657:VAL:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:SER:HB3	1:A:467:GLN:HG2	1.89	0.53
1:A:478:TRP:CD1	1:A:539:ARG:HG2	2.43	0.53
1:A:780:HIS:HD2	1:A:781:PRO:HD2	1.65	0.53
1:B:502:SER:O	1:B:503:GLU:HB3	2.08	0.53
1:B:595:MET:HG2	1:B:608:GLN:CD	2.34	0.53
1:A:532:LYS:H	1:A:532:LYS:CE	2.20	0.53
1:A:589:LEU:C	1:A:591:GLY:H	2.16	0.53
1:B:589:LEU:C	1:B:591:GLY:H	2.17	0.53
1:B:656:ILE:HG12	1:B:657:VAL:N	2.23	0.53
1:A:662:LEU:O	1:A:663:VAL:CG2	2.44	0.53
1:A:1027:ILE:O	1:A:1030:PHE:HB3	2.08	0.53
1:A:1052:TYR:CE1	1:A:1054:TYR:HD1	2.27	0.53
1:B:654:ILE:HG23	1:B:700:LEU:HD11	1.90	0.53
1:B:616:VAL:HA	1:B:847:ARG:HH12	1.74	0.53
1:B:662:LEU:O	1:B:663:VAL:CG2	2.44	0.53
1:A:392:ALA:HB2	1:A:446:GLY:HA2	1.90	0.53
1:A:424:GLU:HB3	1:A:426:TYR:HE1	1.71	0.53
1:A:1029:ARG:HG3	1:A:1029:ARG:HH11	1.72	0.53
1:A:386:GLU:O	1:A:387:HIS:HB2	2.09	0.53
1:A:995:ALA:O	1:A:999:ILE:HG13	2.08	0.53
1:B:386:GLU:O	1:B:387:HIS:HB2	2.10	0.53
1:B:480:ILE:H	1:B:480:ILE:CD1	1.99	0.53
1:B:583:LEU:HD22	1:B:991:ALA:HA	1.90	0.53
1:B:625:PRO:HG2	1:B:628:PHE:HB3	1.89	0.53
1:A:583:LEU:HD22	1:A:991:ALA:HA	1.90	0.52
1:B:478:TRP:CD1	1:B:539:ARG:HG2	2.43	0.52
1:B:624:LEU:HD23	1:B:625:PRO:HD2	1.90	0.52
1:B:1052:TYR:CE1	1:B:1054:TYR:HD1	2.27	0.52
1:A:644:ASN:HD22	1:A:647:GLU:HG3	1.73	0.52
1:B:583:LEU:HB3	1:B:994:ILE:HG12	1.90	0.52
1:B:400:GLY:HA3	1:B:433:VAL:HG13	1.91	0.52
1:B:701:PHE:HA	1:B:710:MET:O	2.09	0.52
1:A:583:LEU:HB3	1:A:994:ILE:HG12	1.90	0.52
1:B:1044:ARG:HG3	1:B:1044:ARG:HH11	1.74	0.52
1:A:419:GLU:O	1:A:420:ALA:C	2.53	0.52
1:A:627:ASN:HB2	1:A:720:PRO:HD3	1.91	0.52
1:A:1059:ARG:HB3	1:A:1059:ARG:NH1	2.25	0.52
1:A:400:GLY:HA3	1:A:433:VAL:HG13	1.91	0.52
1:A:768:PHE:CE1	1:A:902:VAL:HG11	2.44	0.52
1:A:579:ASP:O	1:A:582:ILE:HG13	2.10	0.52
1:A:616:VAL:HA	1:A:847:ARG:HH12	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:ARG:C	1:B:514:LEU:H	2.18	0.52
1:B:413:TRP:O	1:B:414:PHE:C	2.53	0.52
1:B:579:ASP:O	1:B:582:ILE:HG13	2.10	0.52
1:A:524:ASP:HB2	1:A:827:GLU:HB3	1.92	0.52
1:A:770:LEU:HG	1:A:774:ARG:HD2	1.92	0.52
1:A:874:PHE:CE1	1:A:1027:ILE:HA	2.45	0.52
1:B:627:ASN:HB2	1:B:720:PRO:HD3	1.91	0.52
1:B:768:PHE:CE1	1:B:902:VAL:HG11	2.44	0.52
1:A:413:TRP:O	1:A:414:PHE:C	2.53	0.51
1:A:878:ILE:N	1:A:878:ILE:HD12	2.25	0.51
1:B:524:ASP:HB2	1:B:827:GLU:HB3	1.92	0.51
1:B:874:PHE:CE1	1:B:1027:ILE:HA	2.45	0.51
1:B:1059:ARG:HB3	1:B:1059:ARG:NH1	2.25	0.51
1:A:374:ALA:O	1:A:465:SER:OG	2.29	0.51
1:A:963:VAL:O	1:A:964:LEU:HD23	2.10	0.51
1:B:436:ILE:CD1	1:B:462:ILE:HD11	2.26	0.51
1:A:654:ILE:HG23	1:A:700:LEU:HD11	1.90	0.51
1:A:697:PRO:HB3	1:A:716:ILE:HA	1.93	0.51
1:A:701:PHE:HA	1:A:710:MET:O	2.09	0.51
1:B:374:ALA:O	1:B:465:SER:OG	2.29	0.51
1:B:538:PRO:O	1:B:541:VAL:HG22	2.11	0.51
1:B:839:HIS:HD2	1:B:841:PRO:HD2	1.73	0.51
1:B:569:THR:HG22	1:B:569:THR:O	2.10	0.51
1:B:786:LEU:C	1:B:788:PRO:HD2	2.36	0.51
1:B:878:ILE:HD12	1:B:878:ILE:N	2.25	0.51
1:A:435:ASP:O	1:A:471:TYR:CE2	2.64	0.51
1:A:512:ARG:C	1:A:514:LEU:H	2.18	0.51
1:A:1044:ARG:HH11	1:A:1044:ARG:HG3	1.75	0.51
1:A:505:ARG:C	1:A:507:LYS:N	2.65	0.51
1:A:525:MET:CE	1:A:827:GLU:HA	2.41	0.51
1:A:538:PRO:O	1:A:541:VAL:HG22	2.11	0.51
1:B:525:MET:CE	1:B:827:GLU:HA	2.41	0.51
1:A:784:LYS:HD3	1:A:1017:ALA:HB3	1.93	0.51
1:B:419:GLU:O	1:B:420:ALA:C	2.53	0.51
1:B:729:PRO:HA	1:B:737:TRP:CD2	2.46	0.51
1:A:569:THR:O	1:A:569:THR:HG22	2.10	0.51
1:B:412:LYS:HB2	1:B:415:HIS:HD2	1.75	0.51
1:B:697:PRO:HB3	1:B:716:ILE:HA	1.93	0.51
1:A:559:LEU:HD12	1:A:559:LEU:C	2.36	0.50
1:A:877:GLU:O	1:A:881:ILE:HG13	2.11	0.50
1:A:1041:ILE:O	1:A:1045:ASN:ND2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:ASP:O	1:B:471:TYR:CE2	2.64	0.50
1:B:879:ILE:HD12	1:B:929:LYS:HB2	1.93	0.50
1:B:432:ASP:OD2	1:B:466:THR:HG21	2.11	0.50
1:B:770:LEU:HG	1:B:774:ARG:HD2	1.92	0.50
1:B:784:LYS:HD3	1:B:1017:ALA:HB3	1.93	0.50
1:A:632:ASN:ND2	1:A:645:LEU:HB3	2.27	0.50
1:B:512:ARG:NH1	1:B:773:TRP:O	2.44	0.50
1:B:574:TRP:HE3	1:B:579:ASP:HB3	1.77	0.50
1:B:963:VAL:O	1:B:964:LEU:HD23	2.10	0.50
1:A:663:VAL:O	1:A:663:VAL:CG1	2.59	0.50
1:A:728:THR:C	1:A:730:HIS:H	2.18	0.50
1:B:559:LEU:C	1:B:559:LEU:HD12	2.36	0.50
1:B:814:SER:O	1:B:963:VAL:HG23	2.11	0.50
1:B:877:GLU:O	1:B:881:ILE:HG13	2.11	0.50
1:B:452:ASP:C	1:B:454:ASP:N	2.68	0.50
1:B:774:ARG:HH11	1:B:774:ARG:HB3	1.77	0.50
1:A:529:ILE:HB	1:A:770:LEU:HD13	1.94	0.50
1:B:529:ILE:HB	1:B:770:LEU:HD13	1.94	0.50
1:B:663:VAL:O	1:B:663:VAL:CG1	2.59	0.50
1:B:1053:ILE:HB	1:B:1056:LEU:HD12	1.92	0.50
1:A:729:PRO:HA	1:A:737:TRP:CD2	2.46	0.50
1:A:1053:ILE:HB	1:A:1056:LEU:HD12	1.92	0.50
1:B:554:SER:O	1:B:555:ARG:O	2.30	0.50
1:B:728:THR:C	1:B:730:HIS:H	2.18	0.50
1:B:751:PHE:O	1:B:755:ASN:HB3	2.12	0.50
1:B:922:PHE:HE2	1:B:931:VAL:HG21	1.77	0.50
1:A:432:ASP:OD2	1:A:466:THR:HG21	2.11	0.50
1:B:815:LEU:HD22	1:B:815:LEU:H	1.76	0.50
1:A:554:SER:O	1:A:555:ARG:O	2.30	0.49
1:A:559:LEU:HG	1:A:560:VAL:N	2.27	0.49
1:A:871:ILE:O	1:A:875:ILE:HG13	2.11	0.49
1:A:879:ILE:HD12	1:A:929:LYS:HB2	1.93	0.49
1:B:505:ARG:C	1:B:507:LYS:N	2.65	0.49
1:A:398:ILE:HD13	1:A:462:ILE:HD12	1.94	0.49
1:A:567:LEU:O	1:A:988:SER:HB3	2.12	0.49
1:A:814:SER:O	1:A:963:VAL:HG23	2.11	0.49
1:A:815:LEU:HD22	1:A:815:LEU:H	1.77	0.49
1:B:849:VAL:HG11	1:B:858:PHE:CE2	2.47	0.49
1:B:1041:ILE:O	1:B:1044:ARG:HB3	2.12	0.49
1:B:1041:ILE:O	1:B:1045:ASN:ND2	2.44	0.49
1:A:526:PRO:HG3	1:A:764:THR:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:SER:H	1:A:692:ARG:HB2	1.77	0.49
1:A:751:PHE:O	1:A:755:ASN:HB3	2.12	0.49
1:A:786:LEU:C	1:A:788:PRO:HD2	2.36	0.49
1:B:567:LEU:O	1:B:988:SER:HB3	2.12	0.49
1:B:635:VAL:O	1:B:636:ASN:C	2.56	0.49
1:B:723:GLU:O	1:B:725:PRO:HD3	2.12	0.49
1:A:599:TRP:HB2	1:A:959:ASN:HD22	1.77	0.49
1:B:632:ASN:ND2	1:B:645:LEU:HB3	2.27	0.49
1:B:704:ASN:HB3	1:B:706:LEU:H	1.76	0.49
1:B:871:ILE:O	1:B:875:ILE:HG13	2.12	0.49
1:A:520:TYR:CE2	1:A:908:ARG:HD3	2.48	0.49
1:A:723:GLU:O	1:A:725:PRO:HD3	2.12	0.49
1:A:774:ARG:HH11	1:A:774:ARG:HB3	1.76	0.49
1:A:793:VAL:HG21	1:A:939:PHE:CE2	2.47	0.49
1:A:1041:ILE:O	1:A:1044:ARG:HB3	2.12	0.49
1:B:398:ILE:HD13	1:B:462:ILE:HD12	1.93	0.49
1:B:625:PRO:HG2	1:B:628:PHE:CB	2.42	0.49
1:B:1004:SER:OG	1:B:1006:ASP:OD1	2.29	0.49
1:A:559:LEU:HD13	1:A:568:PHE:CE1	2.48	0.49
1:A:879:ILE:HG23	1:A:928:LEU:HD23	1.94	0.49
1:A:883:TYR:OH	1:A:892:ASP:OD2	2.28	0.49
1:B:559:LEU:HG	1:B:560:VAL:N	2.27	0.49
1:B:649:ILE:O	1:B:650:LYS:CB	2.59	0.49
1:B:879:ILE:HG23	1:B:928:LEU:HD23	1.94	0.49
1:A:625:PRO:HG2	1:A:628:PHE:CB	2.43	0.49
1:B:661:VAL:HG22	1:B:825:PHE:HE1	1.78	0.49
1:B:667:SER:H	1:B:692:ARG:HB2	1.77	0.49
1:A:599:TRP:CG	1:A:600:HIS:N	2.80	0.49
1:B:526:PRO:HG3	1:B:764:THR:HA	1.94	0.49
1:B:574:TRP:HE1	1:B:987:LYS:HA	1.78	0.49
1:B:731:GLU:OE1	1:B:731:GLU:HA	2.13	0.49
1:A:574:TRP:HE3	1:A:579:ASP:HB3	1.77	0.49
1:A:849:VAL:HG11	1:A:858:PHE:CE2	2.47	0.49
1:A:1044:ARG:NH2	1:A:1052:TYR:HB3	2.28	0.49
1:A:449:TRP:CE3	1:A:449:TRP:HA	2.47	0.49
1:A:667:SER:HA	1:A:692:ARG:H	1.78	0.49
1:B:532:LYS:H	1:B:532:LYS:CE	2.20	0.49
1:B:793:VAL:HG21	1:B:939:PHE:CE2	2.47	0.49
1:B:874:PHE:CD1	1:B:1030:PHE:HB2	2.48	0.49
1:A:555:ARG:CG	1:A:556:LYS:N	2.76	0.48
1:A:649:ILE:O	1:A:650:LYS:CB	2.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:TYR:CE2	1:B:908:ARG:HD3	2.48	0.48
1:B:599:TRP:CG	1:B:600:HIS:N	2.80	0.48
1:B:599:TRP:HB2	1:B:959:ASN:HD22	1.77	0.48
1:B:619:THR:HG22	1:B:847:ARG:HB3	1.95	0.48
1:A:464:SER:CB	1:A:467:GLN:HG2	2.44	0.48
1:A:574:TRP:HE1	1:A:987:LYS:HA	1.78	0.48
1:A:614:ASN:C	1:A:616:VAL:H	2.22	0.48
1:A:922:PHE:HE2	1:A:931:VAL:HG21	1.77	0.48
1:A:661:VAL:HG22	1:A:825:PHE:HE1	1.78	0.48
1:A:731:GLU:HA	1:A:731:GLU:OE1	2.13	0.48
1:A:839:HIS:HD2	1:A:841:PRO:HD2	1.73	0.48
1:B:1044:ARG:NH2	1:B:1052:TYR:HB3	2.28	0.48
1:A:390:THR:HG22	1:A:453:PRO:HA	1.95	0.48
1:A:654:ILE:HG23	1:A:700:LEU:CD1	2.43	0.48
1:A:693:TYR:CE2	1:A:967:PRO:HG3	2.49	0.48
1:A:704:ASN:HB3	1:A:706:LEU:H	1.76	0.48
1:A:859:TYR:CZ	1:A:1048:LEU:HD12	2.49	0.48
1:B:375:ILE:HA	1:B:428:VAL:O	2.14	0.48
1:B:617:ILE:HB	1:B:657:VAL:HG13	1.96	0.48
1:A:874:PHE:O	1:A:875:ILE:C	2.57	0.48
1:B:464:SER:CB	1:B:467:GLN:HG2	2.43	0.48
1:B:614:ASN:C	1:B:616:VAL:H	2.21	0.48
1:B:693:TYR:CE2	1:B:967:PRO:HG3	2.49	0.48
1:B:830:PHE:C	1:B:832:GLU:N	2.71	0.48
1:A:386:GLU:O	1:A:387:HIS:CB	2.61	0.48
1:A:406:ASP:O	1:A:408:LEU:CD2	2.62	0.48
1:A:554:SER:OG	1:A:1002:LYS:HG2	2.14	0.48
1:A:619:THR:HG22	1:A:847:ARG:HB3	1.95	0.48
1:B:554:SER:OG	1:B:1002:LYS:HG2	2.14	0.48
1:B:604:TRP:O	1:B:608:GLN:HG3	2.14	0.48
1:B:874:PHE:HE1	1:B:1027:ILE:HA	1.78	0.48
1:A:436:ILE:CD1	1:A:462:ILE:HD11	2.26	0.48
1:A:498:PRO:HG2	1:A:501:VAL:HG23	1.95	0.48
1:A:604:TRP:O	1:A:608:GLN:HG3	2.14	0.48
1:A:616:VAL:O	1:A:618:LEU:N	2.47	0.48
1:A:635:VAL:O	1:A:636:ASN:C	2.56	0.48
1:A:780:HIS:CD2	1:A:781:PRO:CD	2.95	0.48
1:A:1050:VAL:HA	1:A:1051:PRO:HD2	1.65	0.48
1:B:616:VAL:O	1:B:618:LEU:N	2.47	0.48
1:B:654:ILE:HG23	1:B:700:LEU:CD1	2.43	0.48
1:B:667:SER:HA	1:B:692:ARG:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:830:PHE:C	1:A:832:GLU:N	2.71	0.48
1:A:874:PHE:HE1	1:A:1027:ILE:HA	1.78	0.48
1:B:525:MET:HE3	1:B:827:GLU:HG2	1.96	0.48
1:B:555:ARG:CG	1:B:556:LYS:H	2.27	0.48
1:A:874:PHE:CD1	1:A:1030:PHE:HB2	2.48	0.48
1:B:390:THR:HG22	1:B:453:PRO:HA	1.95	0.48
1:B:559:LEU:HD13	1:B:568:PHE:CE1	2.48	0.48
1:A:488:GLY:CA	1:A:1019:GLU:HG3	2.40	0.47
1:B:438:LEU:C	1:B:438:LEU:CD1	2.87	0.47
1:B:780:HIS:CD2	1:B:781:PRO:CD	2.95	0.47
1:A:554:SER:C	1:A:555:ARG:O	2.57	0.47
1:A:727:TRP:CH2	1:A:972:LYS:HG2	2.49	0.47
1:B:620:ARG:HB2	1:B:848:GLY:O	2.14	0.47
1:B:727:TRP:CH2	1:B:972:LYS:HG2	2.49	0.47
1:B:874:PHE:O	1:B:875:ILE:C	2.57	0.47
1:B:964:LEU:HD22	1:B:983:THR:HG22	1.97	0.47
1:A:375:ILE:HA	1:A:428:VAL:O	2.14	0.47
1:A:964:LEU:HD22	1:A:983:THR:HG22	1.96	0.47
1:B:386:GLU:O	1:B:387:HIS:CB	2.61	0.47
1:B:449:TRP:HA	1:B:449:TRP:CE3	2.48	0.47
1:B:498:PRO:HG2	1:B:501:VAL:HG23	1.95	0.47
1:B:879:ILE:HD11	1:B:929:LYS:HA	1.96	0.47
1:A:498:PRO:O	1:A:499:ALA:C	2.57	0.47
1:B:406:ASP:O	1:B:408:LEU:CD2	2.62	0.47
1:A:512:ARG:NH1	1:A:773:TRP:O	2.44	0.47
1:A:617:ILE:HB	1:A:657:VAL:HG13	1.96	0.47
1:A:648:GLU:HG3	1:A:653:HIS:HB2	1.97	0.47
1:A:667:SER:OG	1:A:668:TYR:N	2.48	0.47
1:A:750:ASN:HD21	1:A:816:SER:H	1.63	0.47
1:B:555:ARG:CG	1:B:556:LYS:N	2.76	0.47
1:B:667:SER:OG	1:B:668:TYR:N	2.48	0.47
1:B:859:TYR:CZ	1:B:1048:LEU:HD12	2.49	0.47
1:B:902:VAL:HA	1:B:906:GLY:HA3	1.96	0.47
1:B:954:TYR:HD2	1:B:960:ALA:HB3	1.80	0.47
1:A:555:ARG:CG	1:A:556:LYS:H	2.27	0.47
1:A:443:SER:OG	1:A:444:ASP:N	2.48	0.47
1:A:760:ARG:O	1:A:838:TYR:HE2	1.98	0.47
1:B:758:LEU:O	1:B:762:HIS:HB2	2.15	0.47
1:B:883:TYR:OH	1:B:892:ASP:OD2	2.28	0.47
1:A:520:TYR:CD2	1:A:908:ARG:CZ	2.98	0.47
1:A:879:ILE:HD11	1:A:929:LYS:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:993:ALA:O	1:B:994:ILE:C	2.57	0.47
1:B:443:SER:OG	1:B:444:ASP:N	2.48	0.46
1:A:620:ARG:HB2	1:A:848:GLY:O	2.14	0.46
1:A:810:ILE:HD12	1:A:811:VAL:N	2.31	0.46
1:A:886:ASP:OD2	1:A:924:SER:HB2	2.16	0.46
1:A:913:HIS:CD2	1:A:913:HIS:N	2.83	0.46
1:B:516:TYR:O	1:B:774:ARG:NE	2.49	0.46
1:B:644:ASN:HD22	1:B:647:GLU:HG3	1.73	0.46
1:B:733:ASN:O	1:B:734:GLU:C	2.58	0.46
1:A:954:TYR:HD2	1:A:960:ALA:HB3	1.80	0.46
1:B:532:LYS:N	1:B:532:LYS:CD	2.79	0.46
1:A:902:VAL:HA	1:A:906:GLY:HA3	1.96	0.46
1:B:444:ASP:C	1:B:446:GLY:H	2.24	0.46
1:B:520:TYR:CD2	1:B:908:ARG:CZ	2.98	0.46
1:A:516:TYR:O	1:A:774:ARG:NE	2.49	0.46
1:A:525:MET:HE3	1:A:827:GLU:HG2	1.96	0.46
1:B:648:GLU:HG3	1:B:653:HIS:HB2	1.96	0.46
1:B:730:HIS:O	1:B:731:GLU:C	2.58	0.46
1:A:385:ARG:HB2	1:A:388:ALA:HB2	1.97	0.46
1:A:532:LYS:N	1:A:532:LYS:CD	2.79	0.46
1:B:986:SER:OG	1:B:989:GLN:HG3	2.16	0.46
1:A:799:ILE:HG22	1:A:803:GLU:HG3	1.97	0.46
1:A:758:LEU:O	1:A:762:HIS:HB2	2.15	0.46
1:A:775:ASN:O	1:A:894:GLU:HG2	2.16	0.46
1:B:400:GLY:N	1:B:433:VAL:HG13	2.30	0.46
1:B:810:ILE:HD12	1:B:811:VAL:N	2.31	0.46
1:A:584:TYR:C	1:A:584:TYR:CD1	2.94	0.46
1:A:993:ALA:O	1:A:994:ILE:C	2.57	0.46
1:B:760:ARG:O	1:B:838:TYR:HE2	1.98	0.46
1:B:851:ASP:HA	1:B:852:PRO:HD3	1.68	0.46
1:B:1044:ARG:HD2	1:B:1048:LEU:HD13	1.97	0.46
1:A:411:ASP:CA	1:A:426:TYR:HE2	2.29	0.46
1:A:417:ASP:HB3	1:A:426:TYR:HH	1.81	0.46
1:A:444:ASP:C	1:A:446:GLY:H	2.24	0.46
1:A:631:THR:N	1:A:634:HIS:CD2	2.64	0.46
1:B:872:GLU:HG3	1:B:929:LYS:HE2	1.98	0.46
1:B:886:ASP:OD2	1:B:924:SER:HB2	2.16	0.46
1:B:1045:ASN:HB3	1:B:1051:PRO:HB3	1.98	0.46
1:A:400:GLY:N	1:A:433:VAL:HG13	2.30	0.45
1:A:412:LYS:HB2	1:A:415:HIS:HD2	1.75	0.45
1:A:733:ASN:O	1:A:734:GLU:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:922:PHE:CE2	1:B:931:VAL:HG21	2.51	0.45
1:B:1018:TRP:HA	1:B:1018:TRP:CE3	2.51	0.45
1:A:504:GLN:C	1:A:507:LYS:HB3	2.41	0.45
1:A:552:GLN:HE21	1:A:552:GLN:HB2	1.54	0.45
1:A:654:ILE:CG2	1:A:700:LEU:HD11	2.46	0.45
1:A:872:GLU:HG3	1:A:929:LYS:HE2	1.98	0.45
1:B:574:TRP:CE2	1:B:987:LYS:HA	2.51	0.45
1:B:584:TYR:CD1	1:B:584:TYR:C	2.94	0.45
1:A:834:ASN:HD21	1:A:836:GLN:HG3	1.80	0.45
1:A:922:PHE:CE2	1:A:931:VAL:HG21	2.51	0.45
1:A:1020:ASP:OD1	1:A:1022:ASP:HB2	2.17	0.45
1:A:1044:ARG:HD2	1:A:1048:LEU:HD13	1.97	0.45
1:B:631:THR:N	1:B:634:HIS:CD2	2.64	0.45
1:B:799:ILE:HG22	1:B:803:GLU:HG3	1.97	0.45
1:B:994:ILE:HD12	1:B:994:ILE:N	2.30	0.45
1:A:444:ASP:O	1:A:444:ASP:CG	2.59	0.45
1:A:743:TRP:O	1:A:746:VAL:HG12	2.17	0.45
1:B:444:ASP:O	1:B:444:ASP:CG	2.59	0.45
1:B:1020:ASP:OD1	1:B:1022:ASP:HB2	2.17	0.45
1:A:397:ARG:HD3	1:A:407:TYR:CE1	2.51	0.45
1:A:452:ASP:C	1:A:454:ASP:N	2.67	0.45
1:A:730:HIS:O	1:A:731:GLU:C	2.58	0.45
1:A:1018:TRP:HA	1:A:1018:TRP:CE3	2.51	0.45
1:B:411:ASP:CA	1:B:426:TYR:HE2	2.29	0.45
1:B:750:ASN:HD21	1:B:816:SER:H	1.63	0.45
1:A:986:SER:OG	1:A:989:GLN:HG3	2.16	0.45
1:A:1045:ASN:HB3	1:A:1051:PRO:HB3	1.98	0.45
1:B:390:THR:HB	1:B:392:ALA:H	1.82	0.45
1:B:610:LEU:HB3	1:B:858:PHE:CD1	2.52	0.45
1:A:400:GLY:CA	1:A:437:GLN:HG3	2.43	0.45
1:A:753:GLN:NE2	1:A:950:GLN:NE2	2.63	0.45
1:A:851:ASP:HA	1:A:852:PRO:HD3	1.68	0.45
1:B:397:ARG:HD3	1:B:407:TYR:CE1	2.51	0.45
1:B:498:PRO:O	1:B:499:ALA:C	2.58	0.45
1:B:628:PHE:HB2	1:B:698:LEU:HD11	1.99	0.45
1:A:390:THR:HB	1:A:392:ALA:H	1.82	0.45
1:B:504:GLN:C	1:B:507:LYS:HB3	2.41	0.45
1:B:743:TRP:CE3	1:B:964:LEU:HD12	2.52	0.45
1:B:996:THR:HG22	1:B:1000:LEU:HD23	1.98	0.45
1:A:822:HIS:O	1:A:826:MET:HG3	2.17	0.45
1:A:990:ALA:O	1:A:994:ILE:HD13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:ARG:HB2	1:B:388:ALA:HB2	1.97	0.45
1:B:743:TRP:O	1:B:746:VAL:HG12	2.17	0.45
1:B:834:ASN:HD21	1:B:836:GLN:HG3	1.80	0.45
1:A:438:LEU:HD12	1:A:438:LEU:O	2.17	0.44
1:A:743:TRP:CE3	1:A:964:LEU:HD12	2.52	0.44
1:B:775:ASN:O	1:B:894:GLU:HG2	2.16	0.44
1:B:994:ILE:H	1:B:994:ILE:CD1	2.30	0.44
1:A:610:LEU:HB3	1:A:858:PHE:CD1	2.52	0.44
1:B:807:SER:C	1:B:809:GLY:N	2.74	0.44
1:A:878:ILE:HD12	1:A:878:ILE:H	1.83	0.44
1:A:1009:TYR:N	1:A:1009:TYR:CD1	2.86	0.44
1:B:554:SER:C	1:B:555:ARG:O	2.57	0.44
1:A:587:TRP:CZ3	1:A:994:ILE:HG23	2.52	0.44
1:A:787:GLN:N	1:A:788:PRO:HD2	2.33	0.44
1:A:994:ILE:H	1:A:994:ILE:CD1	2.30	0.44
1:B:594:ASN:HB2	1:B:595:MET:HE1	1.99	0.44
1:B:883:TYR:HE2	1:B:889:VAL:HA	1.83	0.44
1:B:1009:TYR:N	1:B:1009:TYR:CD1	2.86	0.44
1:A:598:ARG:NH1	1:A:1049:GLU:HG2	2.31	0.44
1:A:614:ASN:HD22	1:A:614:ASN:HA	1.62	0.44
1:A:994:ILE:HD12	1:A:994:ILE:N	2.30	0.44
1:A:1029:ARG:O	1:A:1032:ASP:HB2	2.18	0.44
1:B:587:TRP:CZ3	1:B:994:ILE:HG23	2.53	0.44
1:B:654:ILE:CG2	1:B:700:LEU:HD11	2.47	0.44
1:B:757:HIS:CE1	1:B:947:ASN:ND2	2.84	0.44
1:B:822:HIS:O	1:B:826:MET:HG3	2.17	0.44
1:A:398:ILE:HG21	1:A:436:ILE:CD1	2.47	0.44
1:A:574:TRP:CE2	1:A:987:LYS:HA	2.51	0.44
1:B:627:ASN:ND2	1:B:627:ASN:H	2.16	0.44
1:B:787:GLN:N	1:B:788:PRO:HD2	2.33	0.44
1:A:533:THR:CG2	1:A:534:HIS:N	2.81	0.44
1:A:628:PHE:HB2	1:A:698:LEU:HD11	1.99	0.44
1:A:807:SER:C	1:A:809:GLY:N	2.74	0.44
1:A:996:THR:HG22	1:A:1000:LEU:HD23	1.98	0.44
1:A:1004:SER:OG	1:A:1006:ASP:OD1	2.29	0.44
1:B:849:VAL:HG13	1:B:855:LEU:HD23	2.00	0.44
1:A:807:SER:C	1:A:809:GLY:H	2.26	0.44
1:B:777:ALA:O	1:B:779:ALA:N	2.51	0.44
1:B:990:ALA:O	1:B:994:ILE:HD13	2.17	0.44
1:A:662:LEU:HD13	1:A:825:PHE:CE1	2.53	0.44
1:A:777:ALA:O	1:A:779:ALA:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:849:VAL:O	1:B:849:VAL:HG12	2.18	0.44
1:B:1029:ARG:O	1:B:1032:ASP:HB2	2.18	0.44
1:A:757:HIS:CE1	1:A:947:ASN:ND2	2.84	0.43
1:B:1013:TYR:O	1:B:1016:THR:OG1	2.22	0.43
1:A:780:HIS:HA	1:A:781:PRO:HD3	1.90	0.43
1:A:849:VAL:O	1:A:849:VAL:HG12	2.18	0.43
1:A:945:ALA:HB2	1:A:1055:LEU:HD21	2.00	0.43
1:B:566:SER:O	1:B:570:MET:HG3	2.19	0.43
1:A:889:VAL:HG11	1:A:924:SER:O	2.18	0.43
1:B:617:ILE:HG13	1:B:618:LEU:H	1.84	0.43
1:B:753:GLN:NE2	1:B:950:GLN:NE2	2.63	0.43
1:B:878:ILE:HD12	1:B:878:ILE:H	1.83	0.43
1:A:739:MET:HE1	1:A:983:THR:HG21	2.00	0.43
1:A:883:TYR:HE2	1:A:889:VAL:HA	1.83	0.43
1:B:398:ILE:HG21	1:B:436:ILE:CD1	2.47	0.43
1:B:739:MET:HE1	1:B:983:THR:HG21	2.00	0.43
1:A:627:ASN:H	1:A:627:ASN:ND2	2.15	0.43
1:B:593:PRO:HB2	1:B:596:ALA:HB2	2.01	0.43
1:B:830:PHE:C	1:B:832:GLU:H	2.27	0.43
1:B:889:VAL:HG11	1:B:924:SER:O	2.18	0.43
1:B:945:ALA:HB2	1:B:1055:LEU:HD21	2.00	0.43
1:A:849:VAL:CG1	1:A:858:PHE:HE2	2.31	0.43
1:A:849:VAL:HG13	1:A:855:LEU:HD23	2.00	0.43
1:B:474:PRO:HB2	1:B:1017:ALA:HA	2.01	0.43
1:B:1009:TYR:O	1:B:1010:LEU:C	2.61	0.43
1:A:617:ILE:HG13	1:A:618:LEU:H	1.84	0.43
1:B:656:ILE:HG13	1:B:699:ALA:O	2.18	0.43
1:B:858:PHE:HB3	1:B:861:ARG:CZ	2.49	0.43
1:A:534:HIS:NE2	1:A:543:PHE:HB2	2.34	0.43
1:A:548:SER:O	1:A:552:GLN:NE2	2.52	0.43
1:A:777:ALA:C	1:A:779:ALA:N	2.77	0.43
1:B:400:GLY:CA	1:B:437:GLN:HG3	2.43	0.43
1:A:408:LEU:HB3	1:A:428:VAL:CG2	2.42	0.43
1:A:497:VAL:CG1	1:A:501:VAL:HB	2.49	0.43
1:A:544:THR:O	1:A:545:ASP:C	2.62	0.43
1:B:544:THR:O	1:B:545:ASP:C	2.62	0.43
1:A:877:GLU:O	1:A:880:ALA:HB3	2.18	0.42
1:B:406:ASP:O	1:B:407:TYR:C	2.62	0.42
1:B:438:LEU:HD12	1:B:438:LEU:O	2.17	0.42
1:B:614:ASN:N	1:B:615:PRO:HD3	2.34	0.42
1:B:662:LEU:HD13	1:B:825:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:777:ALA:C	1:B:779:ALA:N	2.77	0.42
1:A:830:PHE:C	1:A:832:GLU:H	2.27	0.42
1:B:533:THR:O	1:B:536:ASP:HB3	2.19	0.42
1:B:534:HIS:NE2	1:B:543:PHE:HB2	2.34	0.42
1:A:753:GLN:OE1	1:A:758:LEU:HD11	2.20	0.42
1:A:858:PHE:HB3	1:A:861:ARG:CZ	2.49	0.42
1:A:1009:TYR:O	1:A:1010:LEU:C	2.61	0.42
1:B:517:GLN:HA	1:B:774:ARG:HE	1.84	0.42
1:B:807:SER:C	1:B:809:GLY:H	2.26	0.42
1:A:661:VAL:HG22	1:A:661:VAL:O	2.19	0.42
1:A:699:ALA:HA	1:A:713:ALA:O	2.20	0.42
1:A:750:ASN:ND2	1:A:817:LEU:HG	2.35	0.42
1:B:750:ASN:ND2	1:B:817:LEU:HG	2.35	0.42
1:B:883:TYR:CE2	1:B:889:VAL:HA	2.54	0.42
1:A:520:TYR:CD1	1:A:520:TYR:N	2.87	0.42
1:A:614:ASN:N	1:A:615:PRO:HD3	2.34	0.42
1:A:661:VAL:HG22	1:A:825:PHE:CE1	2.55	0.42
1:A:803:GLU:H	1:A:803:GLU:HG2	1.60	0.42
1:A:1013:TYR:O	1:A:1016:THR:OG1	2.22	0.42
1:B:520:TYR:CD1	1:B:520:TYR:N	2.87	0.42
1:A:953:HIS:HD2	1:A:954:TYR:CE2	2.38	0.42
1:B:497:VAL:CG1	1:B:501:VAL:HB	2.49	0.42
1:A:474:PRO:HG3	1:A:1019:GLU:HG2	2.01	0.42
1:A:517:GLN:HA	1:A:774:ARG:HE	1.84	0.42
1:A:883:TYR:CE2	1:A:889:VAL:HA	2.54	0.42
1:A:976:THR:O	1:A:980:ILE:HG23	2.19	0.42
1:B:548:SER:O	1:B:552:GLN:NE2	2.52	0.42
1:B:661:VAL:HG22	1:B:661:VAL:O	2.19	0.42
1:B:849:VAL:CG1	1:B:858:PHE:HE2	2.31	0.42
1:A:400:GLY:CA	1:A:433:VAL:CG1	2.94	0.42
1:A:474:PRO:HB2	1:A:1017:ALA:HA	2.00	0.42
1:A:656:ILE:HG13	1:A:699:ALA:O	2.18	0.42
1:A:723:GLU:O	1:A:725:PRO:CD	2.68	0.42
1:B:488:GLY:CA	1:B:1019:GLU:HG3	2.40	0.42
1:B:723:GLU:O	1:B:725:PRO:CD	2.68	0.42
1:B:799:ILE:CG2	1:B:803:GLU:HG3	2.50	0.42
1:B:877:GLU:O	1:B:880:ALA:HB3	2.18	0.42
1:B:913:HIS:CD2	1:B:913:HIS:N	2.83	0.42
1:A:533:THR:O	1:A:536:ASP:HB3	2.19	0.42
1:A:692:ARG:C	1:A:693:TYR:CD1	2.97	0.42
1:A:839:HIS:HD2	1:A:842:ASN:H	1.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:PRO:HG3	1:B:1019:GLU:HG2	2.01	0.42
1:B:661:VAL:HG22	1:B:825:PHE:CE1	2.55	0.42
1:B:699:ALA:HA	1:B:713:ALA:O	2.20	0.42
1:B:780:HIS:HD2	1:B:781:PRO:CD	2.30	0.42
1:A:799:ILE:CG2	1:A:803:GLU:HG3	2.50	0.42
1:A:881:ILE:HD13	1:A:1022:ASP:CB	2.50	0.42
1:B:458:ASN:HD22	1:B:458:ASN:HA	1.59	0.42
1:B:692:ARG:C	1:B:693:TYR:CD1	2.97	0.42
1:B:839:HIS:CD2	1:B:841:PRO:CD	2.98	0.42
1:B:881:ILE:HD13	1:B:1022:ASP:CB	2.50	0.42
1:B:953:HIS:HD2	1:B:954:TYR:CE2	2.38	0.42
1:A:594:ASN:HB2	1:A:595:MET:HE1	2.00	0.41
1:A:610:LEU:O	1:A:858:PHE:CE1	2.73	0.41
1:A:644:ASN:HD22	1:A:647:GLU:CB	2.33	0.41
1:A:736:ASP:OD2	1:A:973:GLY:HA2	2.20	0.41
1:B:647:GLU:O	1:B:651:ASP:HB2	2.20	0.41
1:B:1033:LYS:O	1:B:1037:ILE:HG13	2.20	0.41
1:A:566:SER:O	1:A:570:MET:HG3	2.19	0.41
1:A:800:GLY:O	1:A:804:LEU:HB2	2.20	0.41
1:B:506:GLN:HG3	1:B:507:LYS:N	2.29	0.41
1:B:610:LEU:O	1:B:858:PHE:CE1	2.73	0.41
1:B:624:LEU:HD23	1:B:624:LEU:HA	1.86	0.41
1:B:648:GLU:HG2	1:B:702:TYR:CE1	2.55	0.41
1:B:736:ASP:OD2	1:B:973:GLY:HA2	2.20	0.41
1:B:976:THR:O	1:B:980:ILE:HG23	2.19	0.41
1:A:483:MET:HE2	1:A:483:MET:HA	2.02	0.41
1:A:506:GLN:HG3	1:A:507:LYS:N	2.29	0.41
1:A:976:THR:HB	1:A:979:SER:H	1.85	0.41
1:A:979:SER:C	1:A:981:LEU:H	2.29	0.41
1:A:1033:LYS:O	1:A:1037:ILE:HG13	2.19	0.41
1:A:593:PRO:HB2	1:A:596:ALA:HB2	2.01	0.41
1:B:534:HIS:C	1:B:536:ASP:H	2.28	0.41
1:B:552:GLN:HE21	1:B:552:GLN:HB2	1.54	0.41
1:B:555:ARG:HA	1:B:999:ILE:HD13	2.03	0.41
1:B:610:LEU:O	1:B:858:PHE:HE1	2.03	0.41
1:B:644:ASN:HD22	1:B:647:GLU:CB	2.33	0.41
1:A:399:THR:HA	1:A:404:ARG:HA	2.02	0.41
1:A:554:SER:O	1:A:558:ALA:HB3	2.21	0.41
1:A:555:ARG:HA	1:A:999:ILE:HD13	2.03	0.41
1:A:647:GLU:O	1:A:651:ASP:HB2	2.21	0.41
1:A:648:GLU:HG2	1:A:702:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:635:VAL:CG1	1:B:712:ILE:HD12	2.48	0.41
1:B:753:GLN:OE1	1:B:758:LEU:HD11	2.20	0.41
1:B:757:HIS:HE1	1:B:1000:LEU:HD12	1.85	0.41
1:B:868:TRP:CZ3	1:B:934:SER:HA	2.55	0.41
1:A:406:ASP:O	1:A:407:TYR:C	2.62	0.41
1:A:610:LEU:HD21	1:A:618:LEU:HD22	2.03	0.41
1:A:652:GLY:O	1:A:854:LYS:HB3	2.21	0.41
1:A:770:LEU:O	1:A:774:ARG:HG3	2.21	0.41
1:B:598:ARG:NH1	1:B:1049:GLU:HG2	2.31	0.41
1:A:524:ASP:CB	1:A:827:GLU:HB3	2.51	0.41
1:A:534:HIS:C	1:A:536:ASP:H	2.28	0.41
1:A:715:GLN:HB2	1:A:726:ILE:HD13	2.03	0.41
1:A:933:THR:O	1:A:934:SER:C	2.62	0.41
1:B:483:MET:SD	1:B:485:LEU:HD21	2.61	0.41
1:B:594:ASN:OD1	1:B:952:ASP:CG	2.63	0.41
1:B:599:TRP:CD2	1:B:600:HIS:N	2.89	0.41
1:B:770:LEU:O	1:B:774:ARG:HG3	2.21	0.41
1:B:800:GLY:O	1:B:804:LEU:HB2	2.21	0.41
1:B:933:THR:O	1:B:934:SER:C	2.62	0.41
1:A:830:PHE:CD1	1:A:833:VAL:HG11	2.56	0.41
1:B:834:ASN:ND2	1:B:836:GLN:N	2.45	0.41
1:B:950:GLN:HE21	1:B:954:TYR:HE1	1.69	0.41
1:A:438:LEU:C	1:A:438:LEU:CD1	2.87	0.41
1:A:757:HIS:HE1	1:A:1000:LEU:HD12	1.85	0.41
1:A:762:HIS:CE1	1:A:1064:THR:CG2	3.04	0.41
1:A:834:ASN:ND2	1:A:836:GLN:N	2.45	0.41
1:B:379:GLU:OE1	1:B:423:LYS:CE	2.69	0.41
1:B:417:ASP:HB3	1:B:426:TYR:HH	1.85	0.41
1:B:483:MET:HA	1:B:483:MET:HE2	2.02	0.41
1:B:554:SER:O	1:B:558:ALA:HB3	2.21	0.41
1:B:706:LEU:O	1:B:708:HIS:N	2.54	0.41
1:B:762:HIS:CE1	1:B:1064:THR:CG2	3.04	0.41
1:B:788:PRO:HG2	1:B:789:HIS:CD2	2.56	0.41
1:B:976:THR:HB	1:B:979:SER:H	1.85	0.41
1:B:1025:ASP:O	1:B:1026:ALA:C	2.63	0.41
1:B:1050:VAL:HA	1:B:1051:PRO:HD2	1.65	0.41
1:A:379:GLU:OE1	1:A:423:LYS:CE	2.69	0.41
1:A:610:LEU:O	1:A:858:PHE:HE1	2.03	0.41
1:A:635:VAL:CG1	1:A:712:ILE:HD12	2.48	0.41
1:A:788:PRO:HG2	1:A:789:HIS:CD2	2.56	0.41
1:A:842:ASN:HD22	1:A:842:ASN:HA	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:ARG:O	1:B:506:GLN:C	2.63	0.41
1:B:652:GLY:O	1:B:854:LYS:HB3	2.21	0.41
1:B:715:GLN:HB2	1:B:726:ILE:HD13	2.03	0.41
1:B:1023:ALA:O	1:B:1024:LEU:C	2.63	0.41
1:B:1035:GLU:O	1:B:1038:SER:HB3	2.20	0.41
1:A:483:MET:SD	1:A:485:LEU:HD21	2.61	0.40
1:A:582:ILE:HG13	1:A:582:ILE:H	1.51	0.40
1:A:706:LEU:O	1:A:708:HIS:N	2.54	0.40
1:B:400:GLY:CA	1:B:433:VAL:CG1	2.94	0.40
1:B:704:ASN:HB2	1:B:708:HIS:H	1.86	0.40
1:B:723:GLU:C	1:B:725:PRO:HD3	2.46	0.40
1:A:594:ASN:OD1	1:A:952:ASP:CG	2.63	0.40
1:A:599:TRP:CD2	1:A:600:HIS:N	2.89	0.40
1:A:653:HIS:O	1:A:702:TYR:HA	2.21	0.40
1:A:723:GLU:C	1:A:725:PRO:HD3	2.46	0.40
1:A:780:HIS:HD2	1:A:781:PRO:CD	2.30	0.40
1:B:610:LEU:HD21	1:B:618:LEU:HD22	2.03	0.40
1:B:727:TRP:CZ3	1:B:736:ASP:HB3	2.56	0.40
1:B:830:PHE:CD1	1:B:833:VAL:HG11	2.56	0.40
1:A:581:HIS:HE1	1:A:596:ALA:O	2.03	0.40
1:A:645:LEU:HD13	1:A:654:ILE:CD1	2.52	0.40
1:A:868:TRP:CZ3	1:A:934:SER:HA	2.55	0.40
1:A:895:ILE:HG12	1:A:928:LEU:HD13	2.03	0.40
1:A:970:LYS:HD2	1:A:971:LYS:H	1.87	0.40
1:A:1035:GLU:O	1:A:1038:SER:HB3	2.20	0.40
1:B:375:ILE:H	1:B:429:GLN:HA	1.87	0.40
1:B:399:THR:HA	1:B:404:ARG:HA	2.02	0.40
1:B:834:ASN:CG	1:B:917:GLY:HA3	2.46	0.40
1:B:895:ILE:HG12	1:B:928:LEU:HD13	2.02	0.40
1:B:524:ASP:CB	1:B:827:GLU:HB3	2.51	0.40
1:B:575:ASP:HB2	1:B:579:ASP:OD1	2.22	0.40
1:B:581:HIS:HE1	1:B:596:ALA:O	2.03	0.40
1:B:979:SER:C	1:B:981:LEU:H	2.29	0.40
1:B:1044:ARG:HG3	1:B:1044:ARG:NH1	2.37	0.40
1:A:811:VAL:O	1:A:812:ASP:C	2.65	0.40
1:A:1025:ASP:O	1:A:1026:ALA:C	2.62	0.40
1:B:435:ASP:O	1:B:435:ASP:CG	2.65	0.40
1:B:592:THR:HG22	1:B:593:PRO:HD2	2.02	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:ILE:CD1	1:B:633:GLU:CB[1_545]	1.96	0.24
1:A:448:TYR:CE2	1:A:911:PRO:CD[2_655]	1.98	0.22
1:B:413:TRP:CH2	1:B:819:GLY:O[2_544]	2.19	0.01

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	661/699 (95%)	510 (77%)	112 (17%)	39 (6%)	1	10
1	B	661/699 (95%)	511 (77%)	111 (17%)	39 (6%)	1	10
All	All	1322/1398 (95%)	1021 (77%)	223 (17%)	78 (6%)	1	10

All (78) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	420	ALA
1	A	445	GLY
1	A	555	ARG
1	A	583	LEU
1	A	616	VAL
1	A	617	ILE
1	A	636	ASN
1	A	663	VAL
1	A	704	ASN
1	A	707	GLY
1	A	734	GLU
1	A	911	PRO
1	A	1018	TRP
1	B	420	ALA
1	B	445	GLY
1	B	555	ARG
1	B	583	LEU
1	B	616	VAL

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Mol	Chain	Res	Type
1	B	617	ILE
1	B	636	ASN
1	B	663	VAL
1	B	704	ASN
1	B	707	GLY
1	B	734	GLU
1	B	911	PRO
1	B	1018	TRP
1	A	434	GLY
1	A	480	ILE
1	A	487	PRO
1	A	488	GLY
1	A	531	ALA
1	A	556	LYS
1	A	778	SER
1	A	892	ASP
1	A	1017	ALA
1	B	434	GLY
1	B	480	ILE
1	B	487	PRO
1	B	488	GLY
1	B	531	ALA
1	B	556	LYS
1	B	892	ASP
1	B	1017	ALA
1	A	401	ALA
1	A	448	TYR
1	A	581	HIS
1	A	626	SER
1	A	919	PRO
1	A	957	THR
1	A	1046	GLU
1	B	401	ALA
1	B	448	TYR
1	B	581	HIS
1	B	626	SER
1	B	778	SER
1	B	919	PRO
1	B	957	THR
1	B	1046	GLU
1	A	453	PRO
1	A	565	GLY

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Mol	Chain	Res	Type
1	A	762	HIS
1	A	898	TRP
1	A	1010	LEU
1	B	453	PRO
1	B	565	GLY
1	B	762	HIS
1	B	898	TRP
1	B	1010	LEU
1	A	375	ILE
1	A	436	ILE
1	B	375	ILE
1	B	436	ILE
1	A	590	GLY
1	A	731	GLU
1	B	590	GLY
1	B	731	GLU
1	A	909	VAL
1	B	909	VAL

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	533/606 (88%)	488 (92%)	45 (8%)	10	38
1	B	533/606 (88%)	488 (92%)	45 (8%)	10	38
All	All	1066/1212 (88%)	976 (92%)	90 (8%)	10	38

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	411	ASP
1	A	438	LEU
1	A	458	ASN
1	A	462	ILE
1	A	470	VAL

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Mol	Chain	Res	Type
1	A	480	ILE
1	A	483	MET
1	A	506	GLN
1	A	532	LYS
1	A	537	LEU
1	A	543	PHE
1	A	552	GLN
1	A	559	LEU
1	A	579	ASP
1	A	582	ILE
1	A	594	ASN
1	A	614	ASN
1	A	617	ILE
1	A	627	ASN
1	A	638	SER
1	A	645	LEU
1	A	666	LYS
1	A	698	LEU
1	A	700	LEU
1	A	703	VAL
1	A	704	ASN
1	A	706	LEU
1	A	732	GLU
1	A	738	MET
1	A	796	ILE
1	A	803	GLU
1	A	810	ILE
1	A	815	LEU
1	A	824	THR
1	A	826	MET
1	A	834	ASN
1	A	893	ASN
1	A	909	VAL
1	A	911	PRO
1	A	919	PRO
1	A	936	VAL
1	A	942	GLN
1	A	970	LYS
1	A	1036	ASP
1	A	1048	LEU
1	B	411	ASP
1	B	438	LEU

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Mol	Chain	Res	Type
1	B	458	ASN
1	B	462	ILE
1	B	470	VAL
1	B	480	ILE
1	B	483	MET
1	B	506	GLN
1	B	532	LYS
1	B	537	LEU
1	B	543	PHE
1	B	552	GLN
1	B	559	LEU
1	B	579	ASP
1	B	582	ILE
1	B	594	ASN
1	B	614	ASN
1	B	617	ILE
1	B	627	ASN
1	B	638	SER
1	B	645	LEU
1	B	666	LYS
1	B	698	LEU
1	B	700	LEU
1	B	703	VAL
1	B	704	ASN
1	B	706	LEU
1	B	732	GLU
1	B	738	MET
1	B	796	ILE
1	B	803	GLU
1	B	810	ILE
1	B	815	LEU
1	B	824	THR
1	B	826	MET
1	B	834	ASN
1	B	893	ASN
1	B	909	VAL
1	B	911	PRO
1	B	919	PRO
1	B	936	VAL
1	B	942	GLN
1	B	970	LYS
1	B	1036	ASP

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Mol	Chain	Res	Type
1	B	1048	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	377	ASN
1	A	387	HIS
1	A	415	HIS
1	A	425	GLN
1	A	458	ASN
1	A	467	GLN
1	A	552	GLN
1	A	594	ASN
1	A	608	GLN
1	A	614	ASN
1	A	627	ASN
1	A	632	ASN
1	A	634	HIS
1	A	644	ASN
1	A	653	HIS
1	A	704	ASN
1	A	750	ASN
1	A	780	HIS
1	A	787	GLN
1	A	834	ASN
1	A	839	HIS
1	A	842	ASN
1	A	943	HIS
1	A	947	ASN
1	A	950	GLN
1	A	953	HIS
1	A	959	ASN
1	A	966	HIS
1	A	1031	GLN
1	B	377	ASN
1	B	387	HIS
1	B	415	HIS
1	B	425	GLN
1	B	458	ASN
1	B	467	GLN
1	B	552	GLN
1	B	573	ASN

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Mol	Chain	Res	Type
1	B	594	ASN
1	B	608	GLN
1	B	614	ASN
1	B	627	ASN
1	B	632	ASN
1	B	634	HIS
1	B	644	ASN
1	B	653	HIS
1	B	704	ASN
1	B	750	ASN
1	B	780	HIS
1	B	787	GLN
1	B	834	ASN
1	B	839	HIS
1	B	842	ASN
1	B	943	HIS
1	B	950	GLN
1	B	953	HIS
1	B	959	ASN
1	B	1031	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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, 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	669/699 (95%)	0.46	26 (3%)	43 27	17, 42, 64, 95	0
1	B	669/699 (95%)	0.45	21 (3%)	51 32	17, 42, 64, 95	0
All	All	1338/1398 (95%)	0.45	47 (3%)	47 29	17, 42, 64, 95	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	558	ALA	3.6
1	A	480	ILE	3.5
1	A	503	GLU	3.5
1	B	644	ASN	3.4
1	A	597	ASP	3.2
1	B	1047	ASN	3.0
1	B	449	TRP	2.9
1	A	448	TYR	2.8
1	A	433	VAL	2.7
1	B	471	TYR	2.7
1	B	434	GLY	2.6
1	B	430	GLY	2.6
1	A	414	PHE	2.6
1	A	464	SER	2.5
1	A	449	TRP	2.5
1	A	413	TRP	2.5
1	B	724	ASN	2.4
1	A	435	ASP	2.4
1	B	454	ASP	2.4
1	A	506	GLN	2.4
1	A	384	ASP	2.4
1	A	420	ALA	2.3
1	B	945	ALA	2.3
1	B	818	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	374	ALA	2.3
1	A	644	ASN	2.3
1	A	572	GLU	2.3
1	B	475	CYS	2.3
1	A	374	ALA	2.2
1	A	630	VAL	2.2
1	B	640	ASP	2.2
1	B	433	VAL	2.2
1	A	1004	SER	2.2
1	B	452	ASP	2.2
1	A	808	GLY	2.2
1	A	406	ASP	2.2
1	B	448	TYR	2.1
1	A	561	ASN	2.1
1	A	787	GLN	2.1
1	A	1047	ASN	2.0
1	B	539	ARG	2.0
1	B	392	ALA	2.0
1	B	406	ASP	2.0
1	A	914	GLN	2.0
1	B	926	GLU	2.0
1	B	554	SER	2.0
1	A	690	ASP	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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	B	2401	1/1	0.87	0.12	41,41,41,41	0
3	CA	B	2201	1/1	0.94	0.05	41,41,41,41	0
3	CA	A	2200	1/1	0.96	0.06	41,41,41,41	0
3	CA	A	2300	1/1	0.96	0.09	41,41,41,41	0
3	CA	A	2400	1/1	0.97	0.07	41,41,41,41	0
2	FE2	B	2100	1/1	0.98	0.05	41,41,41,41	0
3	CA	B	2301	1/1	0.99	0.03	41,41,41,41	0
2	FE2	A	2100	1/1	0.99	0.07	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.