



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2026 – 01:47 AM UTC

PDB ID : 5A7D / pdb_00005a7d
Title : Tetrameric assembly of LGN with Inscuteable
Authors : Culurgioni, S.; Mari, S.; Bonetto, G.; Gallini, S.; Brennich, M.; Round, A.;
Mapelli, M.
Deposited on : 2015-07-07
Resolution : 3.40 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

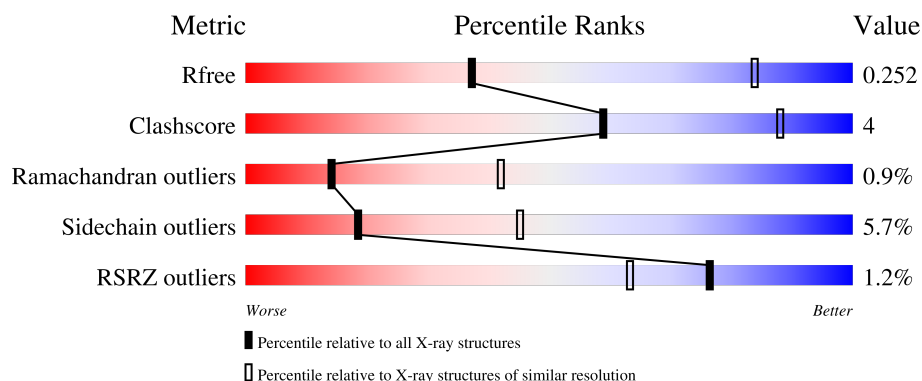
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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.



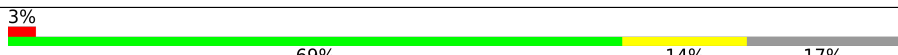
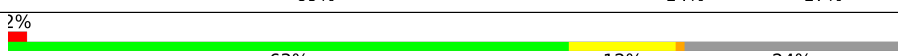
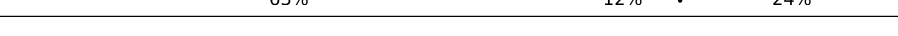
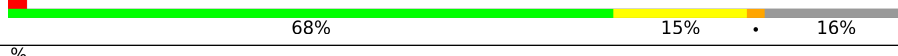
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	B	382	2% 76% 14% • 7%
1	C	382	80% 10% • 9%
1	D	382	79% 11% 10%
1	E	382	2% 77% 15% • 8%
1	F	382	81% 9% 9%

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Mol	Chain	Length	Quality of chain
1	G	382	
1	H	382	
1	I	382	
2	L	341	
2	M	341	
2	N	341	
2	O	341	
2	P	341	
2	Q	341	
2	R	341	
2	S	341	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 38980 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 PINS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	354	Total	C	N	O	S	0	0	0
			2742	1695	513	521	13			
1	C	348	Total	C	N	O	S	0	0	0
			2685	1655	504	513	13			
1	D	345	Total	C	N	O	S	0	0	0
			2643	1635	489	506	13			
1	E	352	Total	C	N	O	S	0	0	0
			2616	1618	489	497	12			
1	F	346	Total	C	N	O	S	0	0	0
			2676	1652	502	509	13			
1	G	346	Total	C	N	O	S	0	0	0
			2679	1655	504	507	13			
1	H	347	Total	C	N	O	S	0	0	0
			2668	1650	499	506	13			
1	I	346	Total	C	N	O	S	0	0	0
			2608	1615	481	499	13			

- Molecule 2 is a protein called INSCUTEABLE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	284	Total	C	N	O	S	0	0	0
			2127	1329	386	402	10			
2	M	259	Total	C	N	O	S	0	0	0
			1977	1237	361	369	10			
2	N	283	Total	C	N	O	S	0	0	0
			2228	1395	407	416	10			
2	O	288	Total	C	N	O	S	0	0	0
			2250	1410	409	421	10			
2	P	288	Total	C	N	O	S	0	0	0
			2233	1396	406	421	10			
2	Q	281	Total	C	N	O	S	0	0	0
			2215	1388	401	416	10			

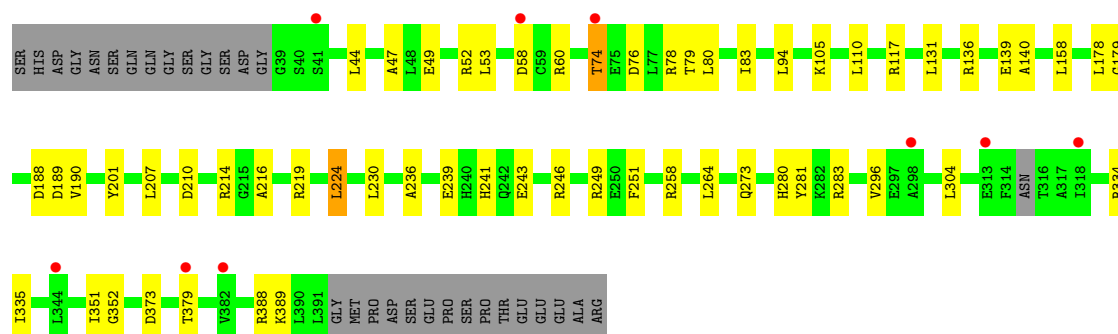
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	311	Total	C	N	O	S	0	0	0
			2386	1490	439	447	10			
2	S	287	Total	C	N	O	S	0	0	0
			2243	1405	408	420	10			

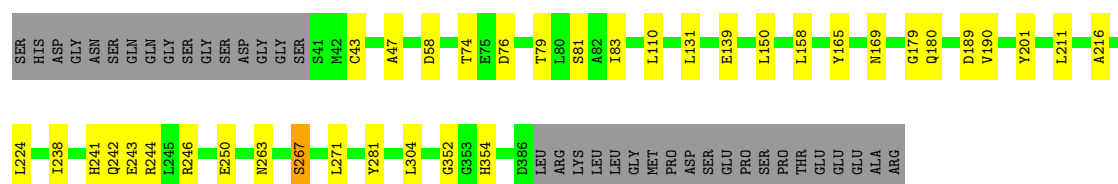
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	O	0	0
			2	2		
3	H	2	Total	O	0	0
			2	2		



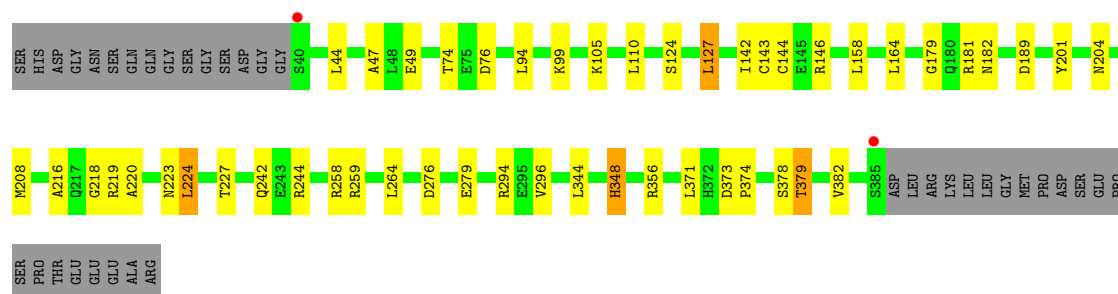
• Molecule 1: PINS

Chain F: 81% 9% 9%



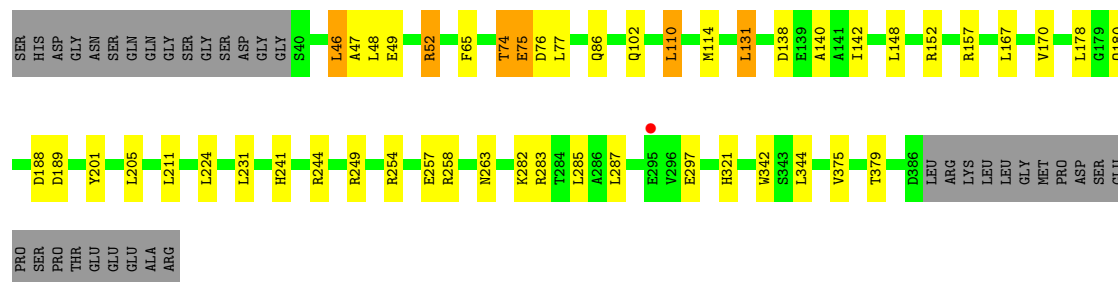
• Molecule 1: PINS

Chain G: 78% 12% 9%



• Molecule 1: PINS

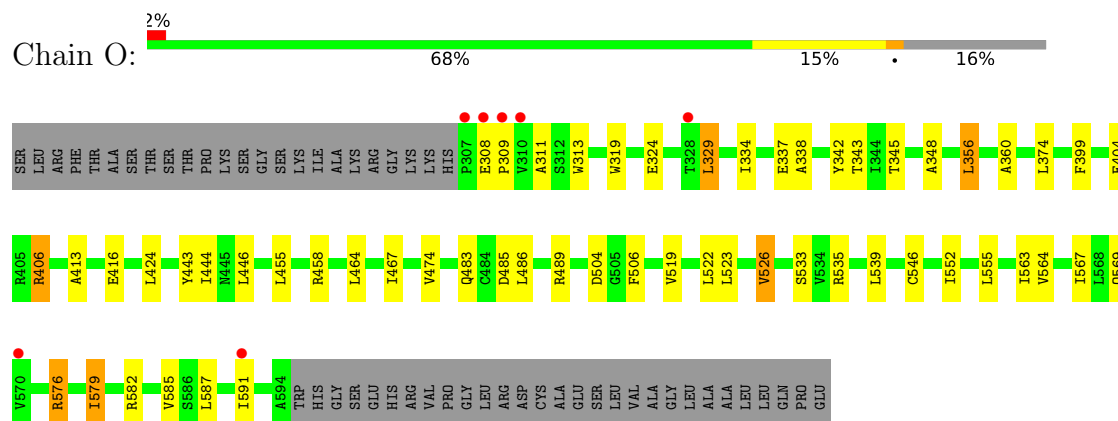
Chain H: 78% 11% 9%



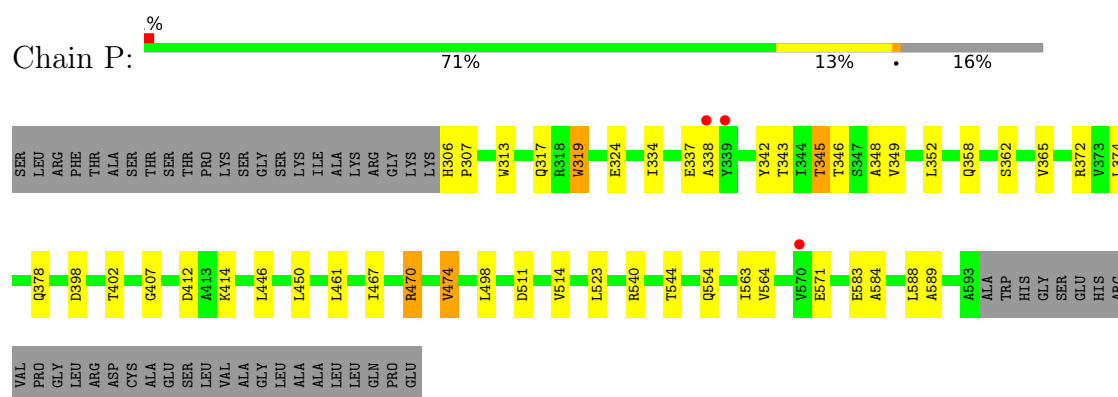
• Molecule 1: PINS

Chain I: 79% 12% 9%

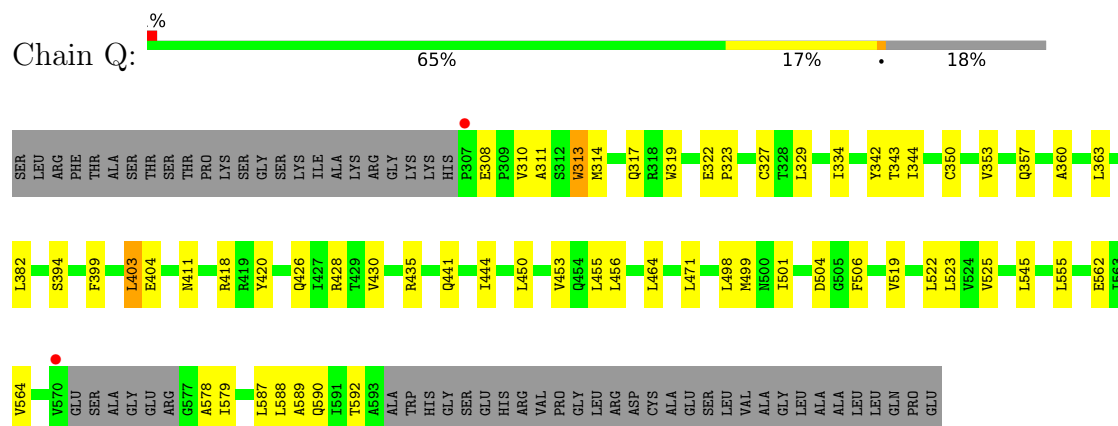
- Molecule 2: INSCUTEABLE



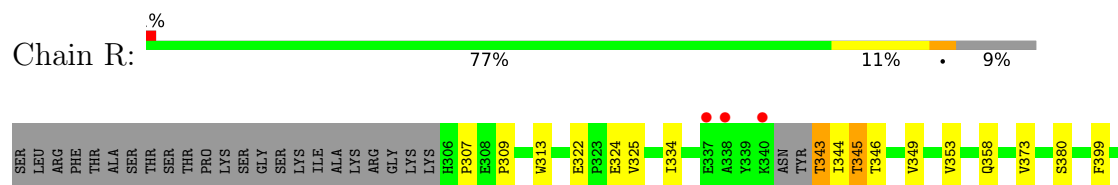
- Molecule 2: INSCUTEABLE

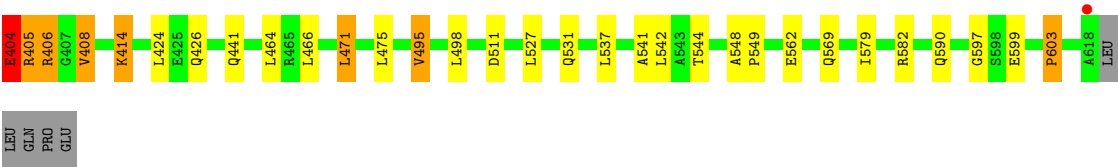


- Molecule 2: INSCUTEABLE

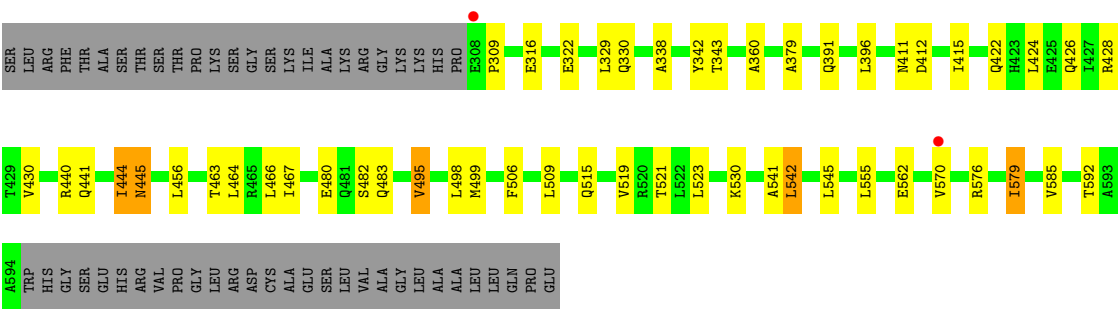


- Molecule 2: INSCUTEABLE





● Molecule 2: INSCUTEABLE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	128.19Å 212.58Å 280.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.58 – 3.40 75.58 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (75.58-3.40) 99.9 (75.58-3.40)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.41Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.209 , 0.250 0.212 , 0.252	Depositor DCC
R_{free} test set	5219 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	84.1	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	38980	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	B	0.26	0/2787	0.65	0/3748
1	C	0.28	0/2729	0.66	0/3673
1	D	0.26	0/2688	0.67	0/3623
1	E	0.26	0/2657	0.67	0/3583
1	F	0.26	0/2721	0.67	0/3662
1	G	0.26	0/2724	0.67	0/3665
1	H	0.27	0/2713	0.68	2/3654 (0.1%)
1	I	0.26	0/2650	0.68	0/3576
2	L	0.28	0/2149	0.72	1/2914 (0.0%)
2	M	0.29	0/1999	0.71	1/2710 (0.0%)
2	N	0.28	0/2254	0.70	0/3049
2	O	0.27	0/2278	0.69	0/3085
2	P	0.28	0/2260	0.70	0/3063
2	Q	0.27	0/2242	0.68	1/3034 (0.0%)
2	R	0.28	0/2416	0.71	1/3273 (0.0%)
2	S	0.28	0/2270	0.69	0/3074
All	All	0.27	0/39537	0.68	6/53386 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	603	PRO	N-CA-CB	7.06	110.67	103.25
2	R	603	PRO	N-CA-CB	6.92	110.52	103.25
1	H	74	THR	CA-C-N	5.91	132.33	121.70
1	H	74	THR	C-N-CA	5.91	132.33	121.70
2	M	581	ARG	CB-CA-C	-5.26	110.53	116.63
2	Q	578	ALA	CB-CA-C	-5.05	110.37	117.23

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	B	2742	0	2647	34	0
1	C	2685	0	2569	25	0
1	D	2643	0	2503	20	0
1	E	2616	0	2438	31	0
1	F	2676	0	2560	20	0
1	G	2679	0	2570	26	0
1	H	2668	0	2545	28	0
1	I	2608	0	2457	22	0
2	L	2127	0	2088	19	0
2	M	1977	0	1958	20	0
2	N	2228	0	2268	20	0
2	O	2250	0	2285	30	0
2	P	2233	0	2253	26	0
2	Q	2215	0	2251	25	0
2	R	2386	0	2372	22	0
2	S	2243	0	2277	20	0
3	B	2	0	0	0	0
3	H	2	0	0	0	0
All	All	38980	0	38041	342	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 4.

All (342) 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:M:567:ILE:HG23	2:M:587:LEU:HD21	1.63	0.80
1:B:74:THR:OG1	1:B:75:GLU:N	2.16	0.76
2:O:523:LEU:HD22	2:O:563:ILE:HD11	1.70	0.74
2:P:342:TYR:N	2:P:343:THR:HA	2.04	0.73
1:E:47:ALA:HB1	2:O:334:ILE:HD13	1.71	0.72
2:M:407:GLY:O	2:M:409:PHE:N	2.23	0.71
1:E:258:ARG:HD2	1:E:296:VAL:HG11	1.76	0.68
1:B:335:ILE:HD13	1:B:371:LEU:HD13	1.76	0.68
1:I:318:ILE:O	1:I:322:ASN:ND2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:ALA:HB1	2:M:334:ILE:HD13	1.79	0.65
2:S:523:LEU:HD11	2:S:555:LEU:HD12	1.79	0.65
1:H:249:ARG:HD2	1:H:283:ARG:HH22	1.62	0.64
1:E:243:GLU:OE1	1:E:246:ARG:NH1	2.31	0.64
1:H:379:THR:HG22	2:R:307:PRO:HG2	1.79	0.64
1:C:196:ARG:O	1:C:199:GLU:HG2	1.98	0.64
1:I:258:ARG:HD2	1:I:296:VAL:HG11	1.78	0.64
1:E:201:TYR:HB3	1:E:224:LEU:HG	1.78	0.63
2:M:360:ALA:HB1	2:M:506:PHE:HB3	1.79	0.63
1:D:351:ILE:HD12	1:D:353:GLY:H	1.64	0.62
1:G:201:TYR:HB3	1:G:224:LEU:HG	1.81	0.62
1:B:258:ARG:NH1	2:L:322:GLU:OE1	2.32	0.62
1:E:334:ARG:HH21	2:Q:418:ARG:HD2	1.64	0.62
2:P:342:TYR:H	2:P:343:THR:HA	1.62	0.61
1:G:47:ALA:HB1	2:Q:334:ILE:HD13	1.81	0.61
2:O:585:VAL:HG12	2:Q:589:ALA:HB1	1.83	0.61
2:S:444:ILE:HG13	2:S:445:ASN:H	1.65	0.61
1:F:81:SER:HB2	1:F:110:LEU:HD22	1.83	0.61
1:D:78:ARG:HG3	1:D:114:MET:HE1	1.82	0.60
1:D:224:LEU:HB3	1:D:240:HIS:HD2	1.67	0.60
1:F:201:TYR:HB3	1:F:224:LEU:HG	1.84	0.60
2:N:310:VAL:HG12	2:N:314:MET:HE2	1.84	0.60
1:D:219:ARG:HA	2:N:324:GLU:HG3	1.82	0.59
1:B:152:ARG:NH1	1:B:160:GLU:OE2	2.36	0.59
1:F:43:CYS:HG	1:F:74:THR:HG1	1.48	0.59
1:F:47:ALA:HB1	2:P:334:ILE:HD13	1.84	0.59
2:Q:310:VAL:HG12	2:Q:314:MET:HE2	1.85	0.58
1:H:131:LEU:HB3	1:H:140:ALA:HB2	1.85	0.58
2:Q:523:LEU:HD11	2:Q:555:LEU:HD12	1.84	0.58
1:B:201:TYR:HB3	1:B:224:LEU:HG	1.85	0.58
2:R:414:LYS:H	2:R:414:LYS:HD3	1.69	0.58
1:B:259:ARG:NH2	2:L:324:GLU:OE1	2.37	0.57
1:E:49:GLU:OE2	1:E:52:ARG:NH1	2.37	0.57
1:D:47:ALA:HB1	2:N:334:ILE:HD13	1.85	0.57
1:H:49:GLU:OE2	1:H:52:ARG:NH1	2.36	0.57
2:M:511:ASP:HA	2:M:514:VAL:HG22	1.87	0.57
2:N:364:GLN:HE22	2:N:505:GLY:HA3	1.69	0.57
1:B:223:ASN:O	1:B:227:THR:OG1	2.23	0.56
1:C:352:GLY:O	1:C:354:HIS:ND1	2.37	0.56
1:H:201:TYR:HB3	1:H:224:LEU:HG	1.86	0.56
2:P:337:GLU:N	2:P:338:ALA:HA	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:474:VAL:O	2:N:478:SER:OG	2.19	0.56
1:F:165:TYR:O	1:F:169:ASN:ND2	2.39	0.56
1:G:189:ASP:N	1:G:189:ASP:OD1	2.39	0.55
1:H:189:ASP:OD1	1:H:189:ASP:N	2.40	0.55
1:I:266:ASN:OD1	1:I:281:TYR:OH	2.24	0.55
1:B:189:ASP:OD1	1:B:189:ASP:N	2.29	0.55
1:G:258:ARG:HD2	1:G:296:VAL:HG11	1.87	0.55
1:G:105:LYS:HG3	1:G:127:LEU:HD11	1.89	0.55
1:B:80:LEU:HD13	1:B:110:LEU:HD11	1.88	0.55
2:M:564:VAL:HG13	2:M:587:LEU:HG	1.88	0.54
2:S:396:LEU:HD21	2:S:456:LEU:HD22	1.89	0.54
1:D:242:GLN:HG3	1:D:264:LEU:HD21	1.89	0.54
1:H:74:THR:HB	1:H:76:ASP:N	2.23	0.54
2:O:579:ILE:HG22	2:O:582:ARG:HH22	1.73	0.54
1:E:216:ALA:HA	1:E:219:ARG:HE	1.73	0.54
1:I:56:ALA:N	1:I:57:GLY:HA2	2.22	0.54
2:O:523:LEU:HD11	2:O:555:LEU:HD12	1.89	0.54
1:H:102:GLN:HG3	2:P:446:LEU:HB2	1.89	0.54
2:N:579:ILE:O	2:N:582:ARG:HG2	2.08	0.53
1:C:258:ARG:HD3	1:C:296:VAL:HG11	1.90	0.53
1:E:219:ARG:HA	2:O:324:GLU:HG3	1.89	0.53
1:B:257:GLU:O	1:B:261:ASN:ND2	2.39	0.53
1:E:79:THR:HG22	2:O:337:GLU:HB3	1.90	0.53
1:F:216:ALA:HB2	2:M:340:LYS:HE3	1.89	0.53
2:M:352:LEU:HD13	2:M:406:ARG:HG2	1.91	0.53
1:B:58:ASP:OD1	1:B:58:ASP:N	2.42	0.53
2:L:577:GLY:HA2	2:L:581:ARG:HG3	1.89	0.53
2:N:512:ALA:O	2:N:516:ASN:ND2	2.34	0.53
2:Q:453:VAL:HA	2:Q:456:LEU:HD12	1.90	0.53
1:E:158:LEU:HD11	1:G:158:LEU:HD21	1.90	0.53
2:Q:403:LEU:O	2:Q:420:TYR:OH	2.26	0.52
2:N:360:ALA:HB1	2:N:506:PHE:HB3	1.90	0.52
2:S:495:VAL:HG22	2:S:541:ALA:HB1	1.91	0.52
1:I:59:CYS:H	2:N:358:GLN:HE22	1.58	0.52
2:O:579:ILE:HD13	2:O:579:ILE:H	1.75	0.52
2:R:399:PHE:HZ	2:R:464:LEU:HD21	1.75	0.52
1:H:157:ARG:HE	1:H:211:LEU:HD11	1.75	0.51
1:E:249:ARG:HH12	1:E:283:ARG:HH21	1.57	0.51
2:M:562:GLU:HG3	2:M:565:ARG:HH22	1.76	0.51
2:P:372:ARG:NH1	2:P:378:GLN:OE1	2.43	0.51
2:L:522:LEU:O	2:L:526:VAL:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:148:LEU:HD21	1:H:152:ARG:HH21	1.75	0.50
1:G:379:THR:HA	1:G:382:VAL:HG22	1.93	0.50
2:O:399:PHE:HZ	2:O:464:LEU:HD21	1.76	0.50
1:G:74:THR:C	1:G:76:ASP:H	2.20	0.50
2:Q:430:VAL:HG21	2:Q:455:LEU:HD23	1.94	0.50
2:S:579:ILE:HD13	2:S:579:ILE:H	1.77	0.50
1:B:251:PHE:HE2	1:H:114:MET:HE3	1.77	0.50
1:G:242:GLN:HG3	1:G:264:LEU:HD21	1.94	0.50
1:D:139:GLU:O	1:D:142:ILE:HG13	2.12	0.49
1:E:178:LEU:HB3	1:E:190:VAL:HG22	1.92	0.49
1:F:243:GLU:OE1	1:F:246:ARG:NH1	2.44	0.49
2:N:430:VAL:HG21	2:N:455:LEU:HD23	1.94	0.49
1:F:241:HIS:CE1	1:F:263:ASN:HB3	2.47	0.49
1:B:352:GLY:O	1:B:354:HIS:ND1	2.39	0.49
1:D:201:TYR:HB3	1:D:224:LEU:HG	1.93	0.49
2:M:532:SER:OG	2:M:583:GLU:OE1	2.30	0.49
2:O:535:ARG:HH12	2:O:576:ARG:HE	1.61	0.49
1:H:321:HIS:HB3	1:H:344:LEU:HG	1.95	0.49
2:M:539:LEU:HD13	2:M:587:LEU:HD12	1.93	0.49
2:P:319:TRP:HA	2:P:319:TRP:CE3	2.48	0.49
1:D:302:TYR:HB2	1:D:324:HIS:CD2	2.48	0.49
1:I:44:LEU:HD11	2:S:338:ALA:HB2	1.94	0.49
1:D:80:LEU:HA	1:D:83:ILE:HG12	1.95	0.48
1:F:238:ILE:HG13	1:F:267:SER:HB3	1.95	0.48
2:P:470:ARG:HA	2:P:470:ARG:HH11	1.78	0.48
1:C:243:GLU:O	1:C:247:ILE:HG12	2.13	0.48
1:B:148:LEU:HD21	1:B:152:ARG:HH21	1.78	0.48
1:E:264:LEU:HD13	1:E:280:HIS:CE1	2.48	0.48
1:H:77:LEU:HD22	1:H:110:LEU:HD21	1.96	0.48
2:S:562:GLU:OE1	2:S:562:GLU:N	2.42	0.48
1:D:149:THR:O	1:D:152:ARG:HG2	2.13	0.47
1:C:43:CYS:HB2	1:C:72:ALA:HB3	1.96	0.47
1:F:131:LEU:HD13	1:F:139:GLU:HB2	1.97	0.47
1:G:216:ALA:HA	1:G:219:ARG:HE	1.79	0.47
1:I:102:GLN:HG2	1:I:106:HIS:HE1	1.79	0.47
1:H:74:THR:HA	1:H:75:GLU:CB	2.45	0.47
1:F:352:GLY:O	1:F:354:HIS:ND1	2.48	0.47
1:C:81:SER:OG	1:C:107:ASP:OD1	2.22	0.47
2:S:499:MET:HE3	2:S:509:LEU:HB2	1.95	0.47
1:C:243:GLU:OE1	1:C:246:ARG:NH1	2.48	0.47
1:E:44:LEU:HD11	2:O:338:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:388:ARG:HA	1:E:389:LYS:HA	1.58	0.47
2:P:470:ARG:HA	2:P:470:ARG:HD2	1.71	0.47
1:E:58:ASP:OD1	1:E:58:ASP:N	2.48	0.47
1:I:178:LEU:HA	1:I:179:GLY:HA3	1.67	0.47
2:R:399:PHE:CZ	2:R:464:LEU:HD21	2.50	0.47
2:Q:404:GLU:OE2	2:Q:428:ARG:NH2	2.48	0.46
1:G:142:ILE:HG13	1:G:143:CYS:N	2.29	0.46
1:G:44:LEU:HD22	2:Q:342:TYR:CG	2.51	0.46
1:I:44:LEU:HD22	2:S:342:TYR:CG	2.51	0.46
2:M:584:ALA:O	2:M:587:LEU:HB2	2.15	0.46
2:P:514:VAL:HG13	2:P:554:GLN:HE21	1.79	0.46
2:Q:343:THR:OG1	2:Q:344:ILE:N	2.46	0.46
1:F:189:ASP:OD1	1:F:189:ASP:N	2.48	0.46
1:H:178:LEU:HD13	1:H:189:ASP:HB2	1.98	0.46
2:L:413:ALA:O	2:L:415:ILE:N	2.47	0.46
1:B:234:PHE:HB2	1:B:271:LEU:HD13	1.98	0.46
1:B:295:GLU:HG3	2:R:408:VAL:HG13	1.98	0.46
1:C:220:ALA:O	1:C:224:LEU:HB2	2.15	0.46
1:G:181:ARG:NH1	1:G:182:ASN:OD1	2.49	0.46
1:B:220:ALA:O	1:B:224:LEU:HB2	2.15	0.46
2:Q:363:LEU:HD22	2:Q:399:PHE:CD2	2.50	0.46
2:R:404:GLU:O	2:R:406:ARG:N	2.49	0.46
1:C:294:ARG:HH21	1:C:327:ILE:HG12	1.80	0.46
1:D:281:TYR:HB3	1:D:304:LEU:HG	1.98	0.46
1:C:332:GLY:HA2	2:P:414:LYS:NZ	2.31	0.45
1:B:187:GLY:HA2	2:O:443:TYR:HB3	1.97	0.45
1:C:51:GLU:HG2	1:C:55:LYS:HE2	1.98	0.45
1:C:264:LEU:HD13	1:C:280:HIS:CE1	2.51	0.45
2:L:360:ALA:HB1	2:L:506:PHE:HB3	1.98	0.45
1:D:220:ALA:O	1:D:224:LEU:HB2	2.16	0.45
2:L:563:ILE:O	2:L:567:ILE:HG12	2.16	0.45
2:N:474:VAL:O	2:N:477:ILE:HG13	2.16	0.45
2:Q:394:SER:OG	2:Q:435:ARG:NH2	2.48	0.45
1:B:157:ARG:HD3	1:B:211:LEU:HD21	1.98	0.45
2:M:541:ALA:O	2:M:544:THR:HG22	2.17	0.45
2:R:579:ILE:HD12	2:R:582:ARG:HD2	1.98	0.45
2:S:499:MET:HE2	2:S:499:MET:HA	1.99	0.45
1:E:74:THR:C	1:E:76:ASP:H	2.24	0.45
2:P:345:THR:HG23	2:P:348:ALA:HB3	1.99	0.45
2:R:343:THR:HA	2:R:344:ILE:HA	1.58	0.45
1:G:164:LEU:HB3	1:G:204:ASN:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:346:THR:HG22	2:M:474:VAL:HG12	1.98	0.45
2:N:322:GLU:HA	2:N:323:PRO:HD3	1.81	0.45
2:O:535:ARG:NH1	2:O:576:ARG:HE	2.14	0.45
1:C:118:LEU:HD11	1:F:211:LEU:HD22	1.99	0.45
1:D:44:LEU:HD22	2:N:342:TYR:CG	2.52	0.45
1:F:244:ARG:NH1	2:P:324:GLU:OE1	2.49	0.45
1:I:275:GLU:HG2	1:I:311:LEU:HD11	1.99	0.45
2:R:344:ILE:HG13	2:R:345:THR:H	1.82	0.45
1:B:118:LEU:HG	1:B:154:LEU:HD13	1.99	0.45
1:B:388:ARG:O	1:B:390:LEU:N	2.41	0.45
1:H:47:ALA:HB1	2:R:334:ILE:HD13	1.98	0.45
1:I:43:CYS:HB2	1:I:72:ALA:HB3	1.99	0.45
1:F:281:TYR:HB3	1:F:304:LEU:HG	1.99	0.45
1:F:179:GLY:HA3	2:P:319:TRP:HZ2	1.82	0.45
2:O:399:PHE:CZ	2:O:464:LEU:HD21	2.52	0.45
2:P:306:HIS:HA	2:P:307:PRO:HD3	1.82	0.45
2:L:492:ILE:O	2:L:495:VAL:HG13	2.17	0.44
1:C:78:ARG:HG3	1:C:114:MET:HE1	1.98	0.44
1:H:257:GLU:HB3	1:H:287:LEU:HD13	1.99	0.44
2:L:352:LEU:HG	2:L:406:ARG:HH11	1.82	0.44
2:N:458:ARG:O	2:N:462:ILE:HG12	2.17	0.44
2:O:522:LEU:O	2:O:526:VAL:HG13	2.16	0.44
1:E:236:ALA:HA	1:E:239:GLU:HG2	2.00	0.44
1:G:201:TYR:CZ	1:G:223:ASN:HB3	2.52	0.44
2:Q:350:CYS:HA	2:Q:353:VAL:HG12	1.99	0.44
2:N:364:GLN:NE2	2:N:505:GLY:HA3	2.32	0.44
2:O:486:LEU:HA	2:O:489:ARG:HD2	1.99	0.44
2:R:349:VAL:O	2:R:353:VAL:HG13	2.17	0.44
1:D:190:VAL:HG11	2:N:319:TRP:HH2	1.82	0.44
1:F:79:THR:O	1:F:83:ILE:HG12	2.17	0.44
1:I:233:ASP:OD1	1:I:233:ASP:N	2.50	0.44
2:O:587:LEU:O	2:O:591:ILE:HG12	2.17	0.44
1:H:138:ASP:O	1:H:142:ILE:HG12	2.18	0.44
2:M:463:THR:O	2:M:467:ILE:HG13	2.18	0.44
2:Q:564:VAL:HG21	2:Q:587:LEU:HD23	2.00	0.44
1:B:74:THR:O	1:B:76:ASP:N	2.51	0.44
1:B:281:TYR:HB3	1:B:304:LEU:HG	2.00	0.44
1:E:74:THR:HG21	1:E:80:LEU:HD13	1.99	0.44
1:E:79:THR:O	1:E:83:ILE:HG13	2.17	0.44
1:G:344:LEU:O	1:G:348:HIS:HB2	2.18	0.44
2:Q:426:GLN:O	2:Q:430:VAL:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:335:ILE:HD12	1:E:335:ILE:H	1.83	0.43
2:R:562:GLU:OE1	2:R:562:GLU:N	2.49	0.43
2:S:426:GLN:O	2:S:430:VAL:HG12	2.18	0.43
1:B:304:LEU:HD13	1:B:320:TYR:CE1	2.53	0.43
2:Q:499:MET:HG3	2:Q:545:LEU:HD12	2.00	0.43
2:R:475:LEU:HD21	2:R:495:VAL:HG12	2.01	0.43
1:B:258:ARG:HH12	2:L:322:GLU:CD	2.26	0.43
1:F:74:THR:C	1:F:76:ASP:H	2.25	0.43
2:M:530:LYS:O	2:M:535:ARG:NH1	2.50	0.43
2:R:541:ALA:O	2:R:544:THR:HG22	2.19	0.43
1:C:321:HIS:HB3	1:C:344:LEU:HG	2.00	0.43
1:C:351:ILE:HD12	1:C:353:GLY:H	1.82	0.43
1:G:378:SER:O	1:G:382:VAL:HG13	2.18	0.43
2:L:560:GLY:HA2	2:L:563:ILE:HD12	2.01	0.43
1:B:224:LEU:HD13	1:B:240:HIS:CD2	2.54	0.43
2:Q:308:GLU:HG3	2:Q:311:ALA:H	1.83	0.43
2:P:349:VAL:HG21	2:P:474:VAL:HG21	2.00	0.43
2:Q:313:TRP:O	2:Q:317:GLN:HG2	2.18	0.43
2:S:519:VAL:HG13	2:S:542:LEU:HD21	1.99	0.43
1:H:241:HIS:CE1	1:H:263:ASN:HB3	2.53	0.43
1:I:258:ARG:NH1	2:S:322:GLU:OE1	2.52	0.43
2:L:522:LEU:HA	2:L:525:VAL:HG12	2.00	0.43
2:S:360:ALA:HB1	2:S:506:PHE:HB3	2.00	0.43
1:D:335:ILE:HD12	1:D:335:ILE:H	1.83	0.43
1:H:231:LEU:HD23	1:H:231:LEU:HA	1.89	0.43
2:L:480:GLU:HG3	2:L:481:GLN:HG3	2.01	0.43
2:S:480:GLU:HB3	2:S:521:THR:HG23	2.01	0.43
1:G:179:GLY:HA3	2:Q:319:TRP:CH2	2.54	0.43
2:N:589:ALA:HB1	2:S:585:VAL:HG12	2.00	0.43
1:C:332:GLY:HA2	2:P:414:LYS:HZ1	1.83	0.43
1:E:136:ARG:HB3	1:E:139:GLU:OE1	2.19	0.43
1:G:244:ARG:HH21	1:G:259:ARG:HH21	1.67	0.43
1:B:348:HIS:CD2	1:B:356:ARG:HD2	2.54	0.42
1:C:74:THR:C	1:C:76:ASP:H	2.26	0.42
2:R:353:VAL:HG12	2:R:471:LEU:HD23	2.01	0.42
2:R:404:GLU:HB3	2:R:405:ARG:H	1.61	0.42
1:C:74:THR:OG1	1:C:75:GLU:N	2.52	0.42
1:E:179:GLY:HA3	2:O:319:TRP:CZ2	2.54	0.42
1:G:224:LEU:HA	1:G:227:THR:HG22	2.01	0.42
1:H:342:TRP:CD1	2:R:309:PRO:HG3	2.54	0.42
2:M:492:ILE:O	2:M:495:VAL:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:373:ASP:OD2	1:E:379:THR:OG1	2.37	0.42
2:M:592:THR:HG21	2:P:589:ALA:HB2	2.01	0.42
2:Q:360:ALA:HB1	2:Q:506:PHE:HB3	2.01	0.42
1:C:228:TYR:HD1	1:C:228:TYR:HA	1.79	0.42
1:E:214:ARG:HB3	1:E:251:PHE:HZ	1.83	0.42
1:H:46:LEU:HD12	1:H:65:PHE:CD2	2.55	0.42
1:C:182:ASN:HB2	1:C:183:PRO:HD3	2.01	0.42
1:I:339:ARG:NH2	2:S:316:GLU:OE1	2.53	0.42
2:L:350:CYS:HA	2:L:353:VAL:HG12	2.02	0.42
2:M:536:ALA:HA	2:M:539:LEU:HD12	2.00	0.42
1:F:242:GLN:O	1:F:246:ARG:HG3	2.20	0.42
2:L:322:GLU:HA	2:L:323:PRO:HD3	1.77	0.42
2:O:345:THR:HG23	2:O:348:ALA:H	1.85	0.42
1:B:271:LEU:HD12	1:B:271:LEU:HA	1.80	0.42
1:C:60:ARG:HG3	2:P:358:GLN:HB3	2.02	0.42
1:C:335:ILE:HD12	1:C:335:ILE:H	1.84	0.42
1:I:264:LEU:HD13	1:I:280:HIS:CE1	2.54	0.42
1:B:58:ASP:HA	2:R:358:GLN:NE2	2.35	0.42
2:L:383:PRO:HA	2:L:386:LEU:HD13	2.02	0.42
2:P:313:TRP:O	2:P:317:GLN:HG2	2.20	0.42
1:G:99:LYS:HB2	1:G:99:LYS:HE3	1.83	0.42
1:G:220:ALA:O	1:G:224:LEU:HB2	2.20	0.42
1:G:276:ASP:OD1	1:G:276:ASP:N	2.52	0.42
2:L:382:LEU:H	2:L:383:PRO:HD2	1.85	0.42
2:Q:464:LEU:HD12	2:Q:464:LEU:HA	1.90	0.42
1:H:282:LYS:HA	1:H:282:LYS:HD2	1.91	0.41
2:P:564:VAL:HG13	2:P:584:ALA:HB1	2.02	0.41
1:E:189:ASP:N	1:E:189:ASP:OD1	2.53	0.41
1:H:244:ARG:NH2	2:R:324:GLU:OE1	2.53	0.41
2:P:511:ASP:HA	2:P:514:VAL:HB	2.02	0.41
2:R:527:LEU:HD23	2:R:527:LEU:HA	1.92	0.41
1:E:131:LEU:HB2	1:E:140:ALA:HB2	2.02	0.41
1:E:281:TYR:HB3	1:E:304:LEU:HG	2.02	0.41
2:O:309:PRO:O	2:O:311:ALA:N	2.45	0.41
2:O:406:ARG:HB3	2:O:467:ILE:HD11	2.01	0.41
2:O:455:LEU:HA	2:O:458:ARG:HD2	2.03	0.41
2:S:440:ARG:HB3	2:S:441:GLN:H	1.47	0.41
1:B:187:GLY:HA3	1:B:188:ASP:HA	1.87	0.41
1:G:348:HIS:CD2	1:G:356:ARG:HB3	2.56	0.41
2:P:398:ASP:O	2:P:402:THR:HG23	2.21	0.41
1:B:336:GLY:HA2	1:B:339:ARG:HE	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:ARG:HG2	2:O:337:GLU:CD	2.45	0.41
1:G:373:ASP:HA	1:G:374:PRO:HD2	1.92	0.41
2:O:360:ALA:HB1	2:O:506:PHE:HB3	2.02	0.41
2:Q:522:LEU:HA	2:Q:525:VAL:HG12	2.02	0.41
1:B:167:LEU:HD13	1:B:200:PHE:CE1	2.56	0.41
1:G:218:GLY:HA3	1:G:244:ARG:HH11	1.86	0.41
1:H:285:LEU:HD11	1:H:297:GLU:HG3	2.02	0.41
1:I:194:LEU:O	1:I:198:VAL:HG23	2.21	0.41
2:N:423:HIS:O	2:N:427:ILE:HG13	2.20	0.41
1:D:304:LEU:HD13	1:D:320:TYR:CE1	2.55	0.41
1:I:42:MET:HE2	2:S:483:GLN:HG3	2.03	0.41
1:I:338:ALA:HA	1:I:367:LEU:HD13	2.02	0.41
2:O:374:LEU:HD22	2:O:446:LEU:HD22	2.03	0.41
2:O:564:VAL:HA	2:O:567:ILE:HG12	2.03	0.41
1:C:337:GLU:HG2	1:C:367:LEU:HD11	2.02	0.41
1:H:375:VAL:O	1:H:379:THR:HG23	2.21	0.41
1:I:121:ALA:HB1	1:I:147:HIS:HD2	1.86	0.41
2:R:548:ALA:HA	2:R:549:PRO:HD3	1.90	0.41
1:D:196:ARG:O	1:D:199:GLU:HG2	2.21	0.41
1:D:243:GLU:HA	1:D:246:ARG:HG2	2.03	0.41
1:H:254:ARG:HA	1:H:257:GLU:HB2	2.03	0.41
1:I:53:LEU:O	1:I:58:ASP:N	2.50	0.41
1:I:242:GLN:HG3	1:I:264:LEU:HD11	2.03	0.41
2:L:339:TYR:HE1	2:L:348:ALA:HB2	1.86	0.41
2:O:464:LEU:HD23	2:O:464:LEU:HA	1.96	0.41
1:E:241:HIS:HB3	1:E:264:LEU:HG	2.02	0.40
1:I:102:GLN:HG2	1:I:106:HIS:CE1	2.55	0.40
2:M:343:THR:OG1	2:M:344:ILE:N	2.54	0.40
2:Q:322:GLU:HA	2:Q:323:PRO:HD3	1.86	0.40
2:S:424:LEU:O	2:S:428:ARG:HG3	2.21	0.40
1:B:87:LEU:HD13	1:B:103:TYR:CE2	2.57	0.40
1:B:372:HIS:C	1:B:374:PRO:HD3	2.46	0.40
1:E:44:LEU:HD22	2:O:342:TYR:CG	2.57	0.40
1:H:167:LEU:HA	1:H:170:VAL:HG12	2.03	0.40
2:P:540:ARG:O	2:P:544:THR:HG23	2.21	0.40
2:N:468:PHE:HD1	2:N:468:PHE:HA	1.80	0.40
2:Q:353:VAL:O	2:Q:357:GLN:HB2	2.21	0.40
1:F:246:ARG:O	1:F:250:GLU:HG3	2.21	0.40
2:N:325:VAL:HG12	2:N:327:CYS:H	1.87	0.40
2:O:356:LEU:HD22	2:O:356:LEU:HA	1.91	0.40
2:P:362:SER:O	2:P:365:VAL:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:523:LEU:HD22	2:P:563:ILE:HD12	2.03	0.40
2:R:373:VAL:HG13	2:R:380:SER:HB3	2.03	0.40
1:D:352:GLY:O	1:D:354:HIS:ND1	2.54	0.40
2:L:523:LEU:HA	2:L:526:VAL:HG22	2.04	0.40
2:O:546:CYS:HB3	2:O:552:ILE:HD13	2.03	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	B	352/382 (92%)	329 (94%)	17 (5%)	6 (2%)	7	28
1	C	346/382 (91%)	334 (96%)	11 (3%)	1 (0%)	36	65
1	D	343/382 (90%)	332 (97%)	10 (3%)	1 (0%)	36	65
1	E	348/382 (91%)	330 (95%)	16 (5%)	2 (1%)	21	50
1	F	344/382 (90%)	334 (97%)	9 (3%)	1 (0%)	36	65
1	G	344/382 (90%)	331 (96%)	13 (4%)	0	100	100
1	H	345/382 (90%)	337 (98%)	7 (2%)	1 (0%)	36	65
1	I	344/382 (90%)	330 (96%)	9 (3%)	5 (2%)	8	30
2	L	278/341 (82%)	255 (92%)	20 (7%)	3 (1%)	11	38
2	M	251/341 (74%)	236 (94%)	13 (5%)	2 (1%)	16	44
2	N	279/341 (82%)	263 (94%)	16 (6%)	0	100	100
2	O	286/341 (84%)	270 (94%)	12 (4%)	4 (1%)	9	31
2	P	286/341 (84%)	273 (96%)	12 (4%)	1 (0%)	36	65
2	Q	277/341 (81%)	269 (97%)	6 (2%)	2 (1%)	18	47
2	R	307/341 (90%)	283 (92%)	17 (6%)	7 (2%)	5	23
2	S	285/341 (84%)	266 (93%)	10 (4%)	9 (3%)	3	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5015/5784 (87%)	4772 (95%)	198 (4%)	45 (1%)	14	42

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	183	PRO
1	E	351	ILE
2	M	408	VAL
2	S	343	THR
1	B	75	GLU
1	B	376	GLY
2	O	308	GLU
2	Q	411	ASN
2	R	405	ARG
2	R	603	PRO
2	S	411	ASN
1	B	390	LEU
1	D	183	PRO
1	E	352	GLY
1	H	75	GLU
1	I	74	THR
2	L	329	LEU
2	M	409	PHE
2	O	569	GLN
2	Q	329	LEU
2	R	345	THR
2	R	404	GLU
2	S	309	PRO
2	S	576	ARG
1	B	388	ARG
1	F	58	ASP
2	L	597	GLY
2	R	441	GLN
2	R	599	GLU
2	S	329	LEU
2	S	379	ALA
1	I	193	ALA
1	I	273	GLN
2	L	346	THR
2	O	329	LEU
2	O	413	ALA
2	S	570	VAL

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Mol	Chain	Res	Type
1	B	74	THR
2	P	407	GLY
2	S	445	ASN
1	C	353	GLY
1	I	73	GLY
1	I	353	GLY
2	R	597	GLY
2	S	444	ILE

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	B	271/298 (91%)	250 (92%)	21 (8%)	12	37
1	C	263/298 (88%)	255 (97%)	8 (3%)	36	59
1	D	256/298 (86%)	244 (95%)	12 (5%)	23	50
1	E	241/298 (81%)	228 (95%)	13 (5%)	20	47
1	F	262/298 (88%)	256 (98%)	6 (2%)	44	63
1	G	262/298 (88%)	248 (95%)	14 (5%)	20	47
1	H	259/298 (87%)	249 (96%)	10 (4%)	28	53
1	I	247/298 (83%)	236 (96%)	11 (4%)	24	51
2	L	216/292 (74%)	200 (93%)	16 (7%)	13	38
2	M	206/292 (70%)	194 (94%)	12 (6%)	18	45
2	N	242/292 (83%)	230 (95%)	12 (5%)	22	49
2	O	243/292 (83%)	224 (92%)	19 (8%)	11	37
2	P	241/292 (82%)	226 (94%)	15 (6%)	16	43
2	Q	242/292 (83%)	225 (93%)	17 (7%)	14	40
2	R	248/292 (85%)	227 (92%)	21 (8%)	10	33
2	S	242/292 (83%)	224 (93%)	18 (7%)	13	38
All	All	3941/4720 (84%)	3716 (94%)	225 (6%)	18	45

All (225) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	74	THR
1	B	78	ARG
1	B	80	LEU
1	B	86	GLN
1	B	109	THR
1	B	110	LEU
1	B	129	ASN
1	B	189	ASP
1	B	190	VAL
1	B	224	LEU
1	B	227	THR
1	B	257	GLU
1	B	282	LYS
1	B	291	LEU
1	B	294	ARG
1	B	315	ASN
1	B	316	THR
1	B	356	ARG
1	B	369	LYS
1	B	378	SER
1	B	379	THR
1	C	74	THR
1	C	118	LEU
1	C	129	ASN
1	C	224	LEU
1	C	228	TYR
1	C	295	GLU
1	C	299	GLN
1	C	316	THR
1	D	108	LEU
1	D	110	LEU
1	D	138	ASP
1	D	150	LEU
1	D	180	GLN
1	D	211	LEU
1	D	224	LEU
1	D	239	GLU
1	D	244	ARG
1	D	291	LEU
1	D	295	GLU
1	D	311	LEU
1	E	53	LEU

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Mol	Chain	Res	Type
1	E	60	ARG
1	E	74	THR
1	E	94	LEU
1	E	105	LYS
1	E	110	LEU
1	E	117	ARG
1	E	188	ASP
1	E	207	LEU
1	E	210	ASP
1	E	224	LEU
1	E	230	LEU
1	E	273	GLN
1	F	150	LEU
1	F	158	LEU
1	F	180	GLN
1	F	190	VAL
1	F	267	SER
1	F	271	LEU
1	G	49	GLU
1	G	94	LEU
1	G	110	LEU
1	G	124	SER
1	G	127	LEU
1	G	144	CYS
1	G	146	ARG
1	G	208	MET
1	G	224	LEU
1	G	279	GLU
1	G	294	ARG
1	G	348	HIS
1	G	371	LEU
1	G	379	THR
1	H	46	LEU
1	H	48	LEU
1	H	52	ARG
1	H	86	GLN
1	H	110	LEU
1	H	131	LEU
1	H	180	GLN
1	H	188	ASP
1	H	205	LEU
1	H	258	ARG

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Mol	Chain	Res	Type
1	I	60	ARG
1	I	129	ASN
1	I	180	GLN
1	I	231	LEU
1	I	238	ILE
1	I	264	LEU
1	I	271	LEU
1	I	291	LEU
1	I	310	LEU
1	I	311	LEU
1	I	325	LEU
2	L	313	TRP
2	L	325	VAL
2	L	334	ILE
2	L	336	GLN
2	L	342	TYR
2	L	344	ILE
2	L	361	LEU
2	L	391	GLN
2	L	410	PHE
2	L	414	LYS
2	L	456	LEU
2	L	495	VAL
2	L	530	LYS
2	L	562	GLU
2	L	579	ILE
2	L	588	LEU
2	M	310	VAL
2	M	330	GLN
2	M	354	ARG
2	M	361	LEU
2	M	456	LEU
2	M	464	LEU
2	M	483	GLN
2	M	495	VAL
2	M	526	VAL
2	M	544	THR
2	M	567	ILE
2	M	579	ILE
2	N	313	TRP
2	N	378	GLN
2	N	406	ARG

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Mol	Chain	Res	Type
2	N	463	THR
2	N	464	LEU
2	N	467	ILE
2	N	494	MET
2	N	527	LEU
2	N	545	LEU
2	N	565	ARG
2	N	587	LEU
2	N	590	GLN
2	O	313	TRP
2	O	329	LEU
2	O	343	THR
2	O	356	LEU
2	O	404	GLU
2	O	406	ARG
2	O	416	GLU
2	O	424	LEU
2	O	444	ILE
2	O	474	VAL
2	O	483	GLN
2	O	485	ASP
2	O	504	ASP
2	O	519	VAL
2	O	526	VAL
2	O	533	SER
2	O	539	LEU
2	O	576	ARG
2	O	579	ILE
2	P	319	TRP
2	P	345	THR
2	P	346	THR
2	P	352	LEU
2	P	374	LEU
2	P	412	ASP
2	P	450	LEU
2	P	461	LEU
2	P	467	ILE
2	P	470	ARG
2	P	474	VAL
2	P	498	LEU
2	P	571	GLU
2	P	583	GLU

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Mol	Chain	Res	Type
2	P	588	LEU
2	Q	313	TRP
2	Q	327	CYS
2	Q	382	LEU
2	Q	403	LEU
2	Q	441	GLN
2	Q	444	ILE
2	Q	450	LEU
2	Q	471	LEU
2	Q	498	LEU
2	Q	501	ILE
2	Q	504	ASP
2	Q	519	VAL
2	Q	562	GLU
2	Q	579	ILE
2	Q	588	LEU
2	Q	590	GLN
2	Q	592	THR
2	R	313	TRP
2	R	322	GLU
2	R	325	VAL
2	R	343	THR
2	R	346	THR
2	R	404	GLU
2	R	406	ARG
2	R	408	VAL
2	R	414	LYS
2	R	424	LEU
2	R	426	GLN
2	R	466	LEU
2	R	471	LEU
2	R	495	VAL
2	R	498	LEU
2	R	511	ASP
2	R	531	GLN
2	R	537	LEU
2	R	542	LEU
2	R	569	GLN
2	R	590	GLN
2	S	330	GLN
2	S	391	GLN
2	S	412	ASP

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Mol	Chain	Res	Type
2	S	415	ILE
2	S	422	GLN
2	S	463	THR
2	S	464	LEU
2	S	466	LEU
2	S	467	ILE
2	S	482	SER
2	S	495	VAL
2	S	498	LEU
2	S	515	GLN
2	S	530	LYS
2	S	542	LEU
2	S	545	LEU
2	S	579	ILE
2	S	592	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	177	HIS
1	B	226	ASN
1	B	348	HIS
1	C	202	GLN
1	C	273	GLN
1	C	348	HIS
1	D	177	HIS
1	D	202	GLN
1	D	240	HIS
1	D	324	HIS
1	E	129	ASN
1	E	166	ASN
1	E	261	ASN
1	E	280	HIS
1	F	180	GLN
1	F	268	HIS
1	F	324	HIS
1	F	372	HIS
1	F	383	ASN
1	G	204	ASN
1	G	329	GLN
1	G	348	HIS
1	G	364	HIS

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Mol	Chain	Res	Type
1	H	217	GLN
1	H	273	GLN
1	H	383	ASN
1	I	240	HIS
1	I	312	HIS
1	I	346	ASN
2	L	317	GLN
2	L	445	ASN
2	L	481	GLN
2	L	553	ASN
2	M	366	HIS
2	N	359	GLN
2	N	442	HIS
2	N	515	GLN
2	N	590	GLN
2	O	516	ASN
2	O	550	GLN
2	O	553	ASN
2	P	306	HIS
2	P	411	ASN
2	P	441	GLN
2	Q	391	GLN
2	R	317	GLN
2	R	422	GLN
2	R	441	GLN
2	S	454	GLN
2	S	516	ASN
2	S	529	HIS
2	S	554	GLN
2	S	569	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	B	354/382 (92%)	-0.14	3 (0%) 82 71	35, 56, 99, 127	0
1	C	348/382 (91%)	0.07	2 (0%) 85 75	46, 79, 126, 152	0
1	D	345/382 (90%)	-0.04	1 (0%) 90 84	51, 89, 121, 166	0
1	E	352/382 (92%)	0.33	9 (2%) 57 42	46, 104, 147, 191	0
1	F	346/382 (90%)	-0.11	0 100 100	31, 70, 132, 150	0
1	G	346/382 (90%)	-0.07	2 (0%) 85 75	50, 84, 113, 154	0
1	H	347/382 (90%)	-0.14	1 (0%) 90 84	31, 64, 119, 132	0
1	I	346/382 (90%)	0.31	5 (1%) 73 59	50, 103, 147, 161	0
2	L	284/341 (83%)	0.13	9 (3%) 50 37	43, 75, 125, 150	0
2	M	259/341 (75%)	0.19	8 (3%) 51 38	45, 82, 115, 132	0
2	N	283/341 (82%)	-0.12	1 (0%) 88 81	42, 69, 109, 135	0
2	O	288/341 (84%)	-0.09	7 (2%) 59 45	33, 62, 124, 161	0
2	P	288/341 (84%)	-0.13	3 (1%) 79 66	28, 55, 115, 176	0
2	Q	281/341 (82%)	-0.04	2 (0%) 84 73	43, 68, 99, 117	0
2	R	311/341 (91%)	-0.13	4 (1%) 75 61	28, 52, 134, 153	0
2	S	287/341 (84%)	-0.08	2 (0%) 84 73	36, 67, 128, 153	0
All	All	5065/5784 (87%)	-0.00	59 (1%) 76 63	28, 74, 130, 191	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	345	THR	4.0
1	E	379	THR	3.6
2	N	570	VAL	3.6
1	E	344	LEU	3.5
1	G	40	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	I	347	ALA	3.4
1	E	318	ILE	3.3
1	C	40	SER	3.2
2	R	340	LYS	3.2
1	E	41	SER	3.1
1	B	390	LEU	3.1
2	S	570	VAL	3.1
2	M	397	ASP	2.8
1	I	307	THR	2.7
2	P	338	ALA	2.6
1	I	41	SER	2.6
2	Q	307	PRO	2.6
1	B	392	GLY	2.5
2	M	383	PRO	2.5
2	M	427	ILE	2.5
2	L	608	CYS	2.5
2	Q	570	VAL	2.5
2	M	598	SER	2.5
2	O	310	VAL	2.5
2	R	338	ALA	2.4
2	S	308	GLU	2.4
2	L	427	ILE	2.4
2	M	569	GLN	2.4
1	E	74	THR	2.3
1	E	298	ALA	2.3
1	I	56	ALA	2.3
2	L	338	ALA	2.3
2	L	599	GLU	2.3
2	O	570	VAL	2.3
2	L	594	ALA	2.3
2	L	342	TYR	2.2
2	P	339	TYR	2.2
2	O	308	GLU	2.2
2	M	345	THR	2.2
2	M	579	ILE	2.2
1	E	313	GLU	2.2
2	P	570	VAL	2.2
2	M	567	ILE	2.2
1	B	391	LEU	2.2
1	H	295	GLU	2.2
2	R	337	GLU	2.2
1	E	58	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	385	SER	2.1
1	G	385	SER	2.1
2	L	423	HIS	2.1
2	R	618	ALA	2.1
2	L	382	LEU	2.1
2	O	591	ILE	2.1
1	C	365	LEU	2.1
2	O	307	PRO	2.1
1	I	236	ALA	2.1
2	O	328	THR	2.0
2	O	309	PRO	2.0
1	E	382	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.