



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:38 AM UTC

PDB ID : 5FUO / pdb_00005fu0
Title : Extending the half-life of a Fab fragment through generation of a humanised anti-Human Serum Albumin (HSA) Fv domain: an investigation into the correlation between affinity and serum half-life
Authors : Adams, R.; Ceska, T.
Deposited on : 2016-01-28
Resolution : 3.60 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

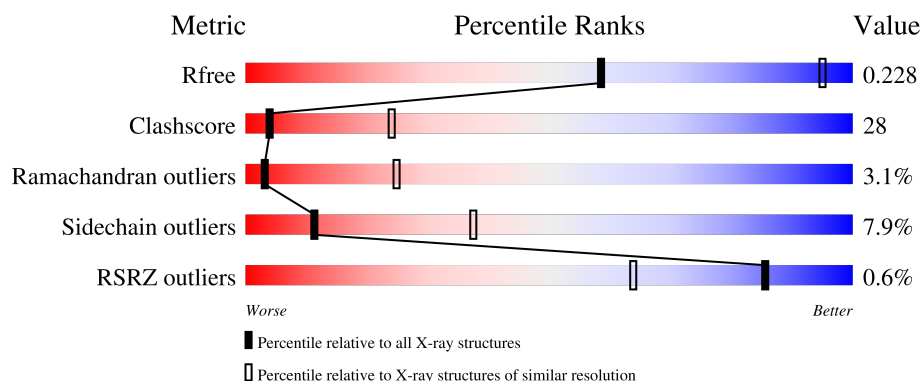
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	585	52% 41% 5%
2	H	233	43% 43% 6% 7%
3	L	217	44% 46% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7869 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 SERUM ALBUMIN.

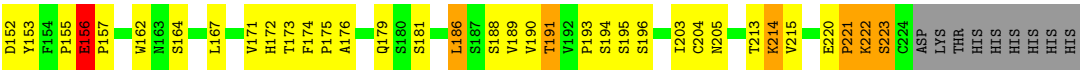
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	579	Total	C	N	O	S	0	0	1
			4600	2903	777	879	41			

- Molecule 2 is a protein called FAB HEAVY CHAIN.

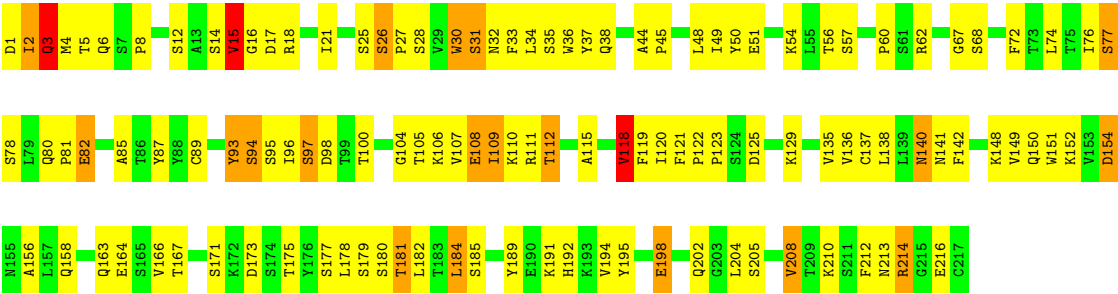
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	1
			1623	1034	271	313	5			

- Molecule 3 is a protein called FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	217	Total	C	N	O	S	0	0	0
			1646	1028	271	341	6			



• Molecule 3: FAB LIGHT CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	217.64Å 217.64Å 78.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.60 30.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (30.00-3.60) 97.4 (30.00-3.60)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 3.65Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.215 , 0.254 (Not available) , 0.228	Depositor DCC
R_{free} test set	2405 reflections (9.85%)	wwPDB-VP
Wilson B-factor (Å ²)	104.4	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.069 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7869	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.62	1/4689 (0.0%)	1.02	12/6326 (0.2%)
2	H	0.65	1/1664 (0.1%)	1.05	10/2275 (0.4%)
3	L	0.62	0/1682	1.09	12/2282 (0.5%)
All	All	0.62	2/8035 (0.0%)	1.04	34/10883 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	144	ALA	CA-CB	6.09	1.62	1.53
1	A	582	ALA	C-N	-5.58	1.25	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	GLU	N-CA-C	-8.70	100.21	112.13
3	L	194	VAL	N-CA-C	8.09	118.28	106.55
1	A	415	VAL	CA-C-N	7.79	128.51	119.47
1	A	415	VAL	C-N-CA	7.79	128.51	119.47
3	L	26	SER	CA-C-N	-7.38	110.61	119.84
3	L	26	SER	C-N-CA	-7.38	110.61	119.84
1	A	544	LEU	N-CA-C	-7.05	103.01	111.69
2	H	60	ALA	N-CA-C	-6.90	101.43	110.53
1	A	566	THR	N-CA-C	6.77	118.55	111.03
1	A	360	CYS	N-CA-C	6.65	118.18	111.07
1	A	178	LEU	N-CA-C	6.42	119.59	111.69
3	L	118	VAL	N-CA-C	6.13	118.81	109.12
1	A	581	ALA	N-CA-C	-6.12	104.88	112.90
3	L	109	ILE	N-CA-C	6.07	117.87	109.80
2	H	152	ASP	N-CA-C	5.90	118.40	111.02
3	L	93	TYR	N-CA-C	5.89	117.97	110.61
3	L	154	ASP	N-CA-C	-5.84	103.35	111.52
1	A	562	ASP	N-CA-C	-5.75	105.34	112.47
2	H	156	GLU	N-CA-C	-5.74	100.58	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	208	VAL	N-CA-C	5.66	116.60	110.21
2	H	133	ALA	CA-C-N	5.61	125.56	119.78
2	H	133	ALA	C-N-CA	5.61	125.56	119.78
2	H	74	SER	N-CA-C	-5.59	106.41	113.18
1	A	578	ALA	N-CA-C	-5.50	104.97	110.97
3	L	185	SER	N-CA-C	-5.45	103.43	110.19
2	H	128	SER	N-CA-C	-5.39	100.91	109.59
1	A	564	LYS	N-CA-C	-5.34	104.03	110.44
2	H	134	PRO	N-CA-C	5.25	119.56	111.21
2	H	144	ALA	N-CA-C	5.24	116.86	110.41
3	L	77	SER	N-CA-C	5.21	116.95	111.28
3	L	140	ASN	N-CA-C	5.17	118.65	109.96
3	L	15	VAL	N-CA-C	-5.12	102.99	109.80
1	A	543	GLN	N-CA-C	-5.07	107.05	113.18
2	H	68	THR	N-CA-C	5.00	117.09	107.44

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	4600	0	4518	217	0
2	H	1623	0	1601	122	0
3	L	1646	0	1590	123	0
All	All	7869	0	7709	437	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 28.

All (437) 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:A:384:PRO:HB2	1:A:446:MET:HE2	1.42	0.98
1:A:106:LYS:HD2	1:A:148:TYR:CE1	2.00	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.49	0.93
3:L:12:SER:HB3	3:L:110:LYS:HE3	1.49	0.92
3:L:136:VAL:HG22	3:L:181:THR:HG23	1.51	0.91
2:H:214:LYS:HB2	2:H:214:LYS:HZ3	1.41	0.86
1:A:317:LYS:O	1:A:321:GLU:HG2	1.76	0.85
3:L:26:SER:HB3	3:L:27:PRO:HD3	1.56	0.85
2:H:2:VAL:HG13	2:H:27:ILE:HG12	1.59	0.85
1:A:302:LEU:HB3	1:A:337:ARG:NH1	1.93	0.84
3:L:178:LEU:HD23	3:L:179:SER:N	1.93	0.83
2:H:144:ALA:HB1	3:L:119:PHE:HE2	1.43	0.82
2:H:214:LYS:HB2	2:H:214:LYS:NZ	1.93	0.82
2:H:12:VAL:HG11	2:H:85:LEU:HD12	1.61	0.82
1:A:156:PHE:CE1	1:A:285:GLU:HA	2.15	0.81
1:A:120:VAL:HG21	1:A:175:ALA:HA	1.62	0.81
1:A:525:LYS:HD2	1:A:548:MET:HE1	1.62	0.81
3:L:54:LYS:HZ3	3:L:54:LYS:HB3	1.45	0.80
1:A:156:PHE:HE1	1:A:285:GLU:HA	1.46	0.79
3:L:85:ALA:O	3:L:107:VAL:HG22	1.83	0.78
2:H:127:PRO:HB3	2:H:153:TYR:HB3	1.64	0.78
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.66	0.77
2:H:143:THR:HB	2:H:193:PRO:HA	1.66	0.76
1:A:495:GLU:OE1	1:A:538:LYS:HG3	1.85	0.76
1:A:540:THR:HA	1:A:543:GLN:NE2	2.00	0.76
1:A:490:ALA:HA	2:H:143:THR:HG21	1.67	0.76
1:A:222:ARG:HH11	1:A:222:ARG:HG3	1.50	0.76
2:H:24:VAL:HG13	2:H:76:ASN:HD21	1.51	0.75
3:L:4:MET:HE3	3:L:25:SER:HB3	1.69	0.74
1:A:48:GLU:OE1	1:A:48:GLU:HA	1.88	0.74
3:L:2:ILE:HD13	3:L:27:PRO:HG2	1.70	0.73
2:H:82:MET:HB3	2:H:85:LEU:HD21	1.69	0.73
2:H:90:THR:HG23	2:H:118:THR:HA	1.70	0.73
1:A:344:VAL:HG21	1:A:450:GLU:HG2	1.71	0.72
1:A:408:LEU:HD11	1:A:526:GLN:HB3	1.70	0.72
3:L:30:TRP:CG	3:L:31:SER:H	2.08	0.72
1:A:262:LYS:O	1:A:266:GLU:HG3	1.89	0.72
1:A:384:PRO:O	1:A:388:ILE:HG12	1.90	0.72
1:A:31:LEU:HD23	1:A:87:MET:HE3	1.71	0.72
3:L:38:GLN:HB2	3:L:48:LEU:HD11	1.72	0.71
1:A:496:THR:HG22	1:A:497:TYR:N	2.03	0.71
3:L:98:ASP:O	3:L:100:THR:HG23	1.90	0.71
1:A:419:SER:OG	1:A:421:PRO:HD2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:80:GLN:HB3	3:L:82:GLU:OE2	1.91	0.70
1:A:440:HIS:CD2	1:A:444:LYS:HD2	2.26	0.70
1:A:502:PHE:HA	1:A:535:HIS:HD2	1.56	0.70
3:L:12:SER:CB	3:L:110:LYS:HE3	2.21	0.69
1:A:430:LEU:O	1:A:433:VAL:HG12	1.91	0.69
1:A:198:LEU:HD13	1:A:458:ASN:HB2	1.73	0.69
1:A:109:ASN:ND2	1:A:463:LEU:HD21	2.08	0.68
2:H:66:ARG:HG3	2:H:66:ARG:HH11	1.59	0.68
3:L:96:ILE:C	3:L:98:ASP:H	2.00	0.68
3:L:2:ILE:O	3:L:27:PRO:HD3	1.95	0.67
1:A:209:ARG:NH1	1:A:209:ARG:HG2	2.10	0.67
3:L:95:SER:HB2	3:L:98:ASP:HB2	1.77	0.67
3:L:36:TRP:CE2	3:L:74:LEU:HB2	2.30	0.66
2:H:2:VAL:CG2	2:H:27:ILE:HG23	2.25	0.66
2:H:174:PHE:CE2	3:L:179:SER:HB3	2.32	0.65
2:H:150:VAL:HB	2:H:186:LEU:HD13	1.78	0.65
3:L:34:LEU:HG	3:L:72:PHE:CG	2.31	0.65
1:A:303:PRO:O	1:A:337:ARG:NH1	2.30	0.65
1:A:502:PHE:HA	1:A:535:HIS:CD2	2.30	0.65
1:A:90:CYS:O	1:A:98:ARG:HG3	1.96	0.65
1:A:398:LEU:O	1:A:402:LYS:HB2	1.96	0.65
2:H:18:LEU:HD23	2:H:82:MET:HE2	1.79	0.65
1:A:420:THR:O	1:A:424:VAL:HG23	1.97	0.65
2:H:167:LEU:HD21	2:H:190:VAL:HG21	1.78	0.65
3:L:191:LYS:O	3:L:191:LYS:HG3	1.96	0.65
1:A:356:THR:HG21	1:A:376:GLU:OE2	1.97	0.64
2:H:2:VAL:HG22	2:H:27:ILE:HG23	1.79	0.64
3:L:122:PRO:HB3	3:L:212:PHE:CE1	2.33	0.64
1:A:25:ILE:HD13	1:A:154:LEU:HD23	1.78	0.64
2:H:193:PRO:HG2	2:H:196:SER:HB3	1.80	0.64
2:H:24:VAL:HG11	2:H:29:LEU:HB2	1.78	0.64
2:H:132:LEU:HB3	3:L:121:PHE:CD2	2.33	0.64
3:L:122:PRO:HB3	3:L:212:PHE:CZ	2.32	0.64
1:A:159:LYS:NZ	1:A:284:LEU:HB2	2.13	0.63
1:A:215:ALA:HB3	1:A:235:VAL:HG13	1.80	0.63
1:A:501:GLU:HG3	1:A:502:PHE:H	1.63	0.63
1:A:327:LEU:HD11	1:A:354:GLU:HG3	1.80	0.63
3:L:123:PRO:HD3	3:L:135:VAL:HG22	1.81	0.63
1:A:302:LEU:HD13	1:A:337:ARG:HG2	1.80	0.63
1:A:412:THR:OG1	1:A:423:LEU:HD13	1.98	0.63
3:L:164:GLU:HB3	3:L:180:SER:HA	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ARG:NH1	1:A:222:ARG:HH12	1.97	0.63
2:H:222:LYS:O	2:H:223:SER:HB2	1.98	0.63
2:H:171:VAL:HG22	2:H:190:VAL:HB	1.81	0.62
3:L:8:PRO:O	3:L:105:THR:HG23	1.99	0.62
1:A:225:LYS:HG2	1:A:299:PRO:HG3	1.82	0.62
3:L:34:LEU:HG	3:L:72:PHE:CD2	2.35	0.62
3:L:54:LYS:HB3	3:L:54:LYS:NZ	2.14	0.62
1:A:36:PHE:O	1:A:40:VAL:HG23	1.99	0.62
1:A:151:ALA:HB2	1:A:250:LEU:HD22	1.82	0.62
1:A:504:ALA:O	1:A:508:THR:HG23	1.99	0.61
1:A:222:ARG:HG3	1:A:222:ARG:NH1	2.13	0.61
1:A:378:LYS:HE3	1:A:382:GLU:OE2	1.99	0.61
2:H:24:VAL:HG12	2:H:29:LEU:HD13	1.82	0.61
1:A:485:ARG:HB3	1:A:486:PRO:CD	2.28	0.61
2:H:150:VAL:HB	2:H:186:LEU:CD1	2.30	0.61
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.82	0.61
3:L:30:TRP:CG	3:L:31:SER:N	2.67	0.61
1:A:168:CYS:SG	1:A:177:CYS:C	2.84	0.61
1:A:409:VAL:HG22	1:A:529:LEU:HD21	1.82	0.60
1:A:218:ARG:NH1	1:A:222:ARG:NH1	2.49	0.60
3:L:192:HIS:O	3:L:214:ARG:HD3	2.00	0.60
2:H:144:ALA:CB	3:L:119:PHE:HE2	2.15	0.60
1:A:223:PHE:HB3	1:A:271:ILE:O	2.01	0.60
2:H:59:TYR:O	3:L:97:SER:HB2	2.02	0.60
2:H:124:THR:HG23	2:H:124:THR:O	2.02	0.60
2:H:146:LEU:HD12	2:H:146:LEU:C	2.26	0.59
2:H:82:MET:CB	2:H:85:LEU:HD21	2.31	0.59
3:L:34:LEU:HD13	3:L:34:LEU:C	2.26	0.59
2:H:1:GLU:HG3	2:H:2:VAL:HG23	1.85	0.59
2:H:66:ARG:HD2	2:H:84:SER:HB2	1.85	0.59
1:A:209:ARG:HG2	1:A:209:ARG:HH11	1.68	0.58
1:A:492:GLU:OE1	2:H:143:THR:N	2.36	0.58
2:H:156:GLU:OE1	2:H:157:PRO:HA	2.02	0.58
1:A:221:GLN:HE21	1:A:339:PRO:HA	1.68	0.58
2:H:2:VAL:CG1	2:H:27:ILE:HG12	2.32	0.58
2:H:72:ASP:OD1	2:H:75:LYS:HG3	2.03	0.58
1:A:495:GLU:CB	3:L:115:ALA:HB3	2.33	0.58
3:L:135:VAL:HG12	3:L:151:TRP:CH2	2.39	0.58
1:A:5:SER:HB3	1:A:57:GLU:OE1	2.03	0.58
3:L:18:ARG:HG3	3:L:77:SER:HA	1.83	0.58
1:A:490:ALA:O	1:A:491:LEU:O	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:CYS:O	1:A:571:GLU:HB2	2.04	0.58
2:H:6:GLU:H	2:H:113:GLN:NE2	2.01	0.58
1:A:159:LYS:HZ3	1:A:284:LEU:HB2	1.67	0.57
3:L:173:ASP:O	3:L:175:THR:HG23	2.05	0.57
1:A:249:ASP:HB3	1:A:252:GLU:CD	2.29	0.57
1:A:223:PHE:CD1	1:A:272:SER:HB2	2.40	0.57
1:A:420:THR:HG23	1:A:530:VAL:HB	1.86	0.57
2:H:87:ALA:HB3	2:H:88:GLU:OE2	2.05	0.56
1:A:548:MET:HE3	1:A:548:MET:O	2.04	0.56
2:H:24:VAL:CG1	2:H:29:LEU:HD13	2.36	0.56
2:H:68:THR:HB	2:H:81:GLN:HB3	1.87	0.56
2:H:94:TYR:CD1	2:H:114:GLY:HA3	2.41	0.56
2:H:174:PHE:CD1	3:L:167:THR:HG23	2.40	0.56
3:L:87:TYR:HE1	3:L:107:VAL:HG21	1.70	0.56
2:H:6:GLU:OE2	2:H:95:CYS:HB3	2.06	0.56
2:H:134:PRO:HG2	2:H:221:PRO:HB3	1.86	0.56
3:L:2:ILE:O	3:L:26:SER:HB3	2.05	0.56
3:L:178:LEU:HD23	3:L:178:LEU:C	2.30	0.56
3:L:93:TYR:C	3:L:95:SER:H	2.14	0.56
3:L:154:ASP:OD2	3:L:192:HIS:HB3	2.06	0.56
2:H:90:THR:HA	2:H:117:VAL:O	2.06	0.56
1:A:577:ALA:HA	1:A:580:GLN:HB3	1.89	0.55
3:L:214:ARG:HG3	3:L:214:ARG:HH11	1.69	0.55
1:A:417:GLN:CD	1:A:417:GLN:H	2.15	0.55
3:L:87:TYR:O	3:L:104:GLY:HA2	2.06	0.55
1:A:47:THR:O	1:A:51:LYS:HG3	2.06	0.55
1:A:458:ASN:HA	1:A:484:ARG:NH1	2.22	0.55
2:H:179:GLN:C	2:H:181:SER:H	2.15	0.55
1:A:222:ARG:HD3	1:A:293:VAL:O	2.07	0.55
2:H:147:GLY:HA3	2:H:189:VAL:HA	1.89	0.55
2:H:162:TRP:CH2	2:H:204:CYS:HB3	2.42	0.55
1:A:441:PRO:C	1:A:443:ALA:H	2.15	0.54
1:A:29:GLN:HG2	1:A:147:PRO:HA	1.89	0.54
2:H:11:LEU:HD22	2:H:155:PRO:HD3	1.89	0.54
3:L:109:ILE:HG22	3:L:110:LYS:N	2.22	0.54
1:A:268:GLN:C	1:A:270:SER:H	2.16	0.54
1:A:64:LYS:HG3	1:A:69:LEU:HG	1.90	0.54
2:H:50:ILE:HG12	2:H:51:ILE:N	2.22	0.54
1:A:112:LEU:HD21	1:A:144:ARG:NH2	2.22	0.54
1:A:265:CYS:SG	1:A:286:LYS:HD2	2.48	0.54
2:H:6:GLU:O	2:H:7:SER:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:28:ASP:OD1	2:H:30:SER:HB2	2.08	0.53
3:L:25:SER:HB2	3:L:93:TYR:OH	2.09	0.53
1:A:564:LYS:O	1:A:565:GLU:HB2	2.07	0.53
2:H:12:VAL:HB	2:H:119:VAL:HG22	1.91	0.53
1:A:50:ALA:O	1:A:54:VAL:HG23	2.09	0.53
1:A:387:LEU:HD13	2:H:195:SER:HB3	1.91	0.53
1:A:561:ALA:C	1:A:563:ASP:N	2.62	0.53
2:H:11:LEU:HD12	2:H:118:THR:O	2.08	0.53
1:A:283:LEU:HD23	1:A:284:LEU:N	2.24	0.52
2:H:127:PRO:CB	2:H:153:TYR:HB3	2.38	0.52
2:H:143:THR:CB	2:H:193:PRO:HA	2.38	0.52
1:A:60:GLU:O	1:A:61:ASN:HB2	2.09	0.52
1:A:81:ARG:HA	1:A:85:GLY:H	1.73	0.52
1:A:495:GLU:HB2	3:L:115:ALA:HB3	1.90	0.52
3:L:60:PRO:HB3	3:L:62:ARG:NH1	2.24	0.52
3:L:96:ILE:C	3:L:98:ASP:N	2.67	0.52
2:H:144:ALA:HB1	3:L:119:PHE:CE2	2.35	0.52
1:A:383:GLU:HG3	1:A:384:PRO:N	2.24	0.52
1:A:575:LEU:HD12	1:A:578:ALA:CB	2.39	0.52
3:L:125:ASP:O	3:L:129:LYS:HG3	2.10	0.52
2:H:66:ARG:HG3	2:H:66:ARG:NH1	2.24	0.52
3:L:164:GLU:HB2	3:L:178:LEU:HD21	1.92	0.52
1:A:70:PHE:HZ	1:A:251:LEU:HD11	1.75	0.52
1:A:111:ASN:OD1	1:A:111:ASN:N	2.42	0.52
1:A:318:ASN:HB3	1:A:326:PHE:CD1	2.45	0.52
1:A:156:PHE:CE2	1:A:288:HIS:CG	2.97	0.51
3:L:135:VAL:HG12	3:L:151:TRP:HH2	1.75	0.51
1:A:510:HIS:O	1:A:513:ILE:HG22	2.11	0.51
1:A:537:PRO:O	1:A:539:ALA:N	2.44	0.51
1:A:570:GLU:C	1:A:572:GLY:H	2.18	0.51
1:A:274:LYS:NZ	1:A:297:GLU:OE2	2.39	0.51
2:H:111:TRP:CE3	3:L:45:PRO:HD2	2.45	0.51
1:A:56:ASP:OD2	1:A:59:ALA:HB2	2.11	0.51
3:L:3:GLN:N	3:L:3:GLN:OE1	2.44	0.51
1:A:21:ALA:O	1:A:25:ILE:HG13	2.10	0.51
2:H:174:PHE:CD2	3:L:179:SER:HB3	2.46	0.51
1:A:405:ASN:HA	1:A:408:LEU:HD12	1.91	0.51
1:A:425:GLU:HA	1:A:425:GLU:OE1	2.11	0.51
1:A:490:ALA:O	1:A:491:LEU:C	2.54	0.51
1:A:505:GLU:O	1:A:505:GLU:HG2	2.11	0.51
1:A:500:LYS:O	1:A:501:GLU:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:82:MET:HE1	2:H:117:VAL:HG11	1.93	0.50
1:A:39:HIS:O	1:A:43:VAL:HG23	2.11	0.50
2:H:94:TYR:CE1	2:H:114:GLY:HA3	2.46	0.50
1:A:401:TYR:OH	1:A:525:LYS:HE3	2.10	0.50
3:L:111:ARG:O	3:L:112:THR:C	2.53	0.50
1:A:194:ALA:HB1	1:A:455:VAL:CG1	2.41	0.50
1:A:496:THR:CG2	1:A:497:TYR:N	2.71	0.50
1:A:576:VAL:O	1:A:580:GLN:HB2	2.11	0.50
2:H:104:THR:HB	3:L:96:ILE:HG13	1.93	0.50
2:H:186:LEU:C	2:H:186:LEU:HD22	2.37	0.50
2:H:174:PHE:HE1	3:L:177:SER:O	1.95	0.50
2:H:179:GLN:C	2:H:181:SER:N	2.68	0.50
3:L:2:ILE:HG22	3:L:3:GLN:N	2.26	0.50
2:H:107:TYR:CD1	3:L:35:SER:HB3	2.47	0.50
1:A:197:ARG:HH11	1:A:197:ARG:HG3	1.77	0.50
1:A:490:ALA:HA	2:H:143:THR:CG2	2.37	0.50
2:H:12:VAL:HG11	2:H:85:LEU:CD1	2.36	0.50
3:L:14:SER:HA	3:L:110:LYS:HB2	1.92	0.50
1:A:408:LEU:HD11	1:A:526:GLN:CB	2.40	0.49
1:A:420:THR:HB	1:A:421:PRO:HD3	1.93	0.49
1:A:537:PRO:O	1:A:538:LYS:C	2.55	0.49
2:H:5:LEU:HG	2:H:113:GLN:OE1	2.13	0.49
1:A:383:GLU:CG	1:A:384:PRO:HD3	2.43	0.49
1:A:571:GLU:HG3	1:A:575:LEU:HD22	1.94	0.49
2:H:127:PRO:HB2	2:H:150:VAL:HG12	1.95	0.49
1:A:135:LEU:O	1:A:138:TYR:HB3	2.13	0.49
2:H:48:ILE:HG12	2:H:62:TRP:HH2	1.77	0.49
2:H:203:ILE:HG22	2:H:205:ASN:ND2	2.28	0.49
3:L:120:ILE:CD1	3:L:137:CYS:HB2	2.43	0.48
3:L:204:LEU:HD13	3:L:208:VAL:HG22	1.94	0.48
1:A:32:GLN:NE2	1:A:110:PRO:HG3	2.28	0.48
3:L:48:LEU:C	3:L:49:ILE:HG13	2.37	0.48
3:L:189:TYR:HA	3:L:195:TYR:OH	2.14	0.48
3:L:142:PHE:N	3:L:175:THR:HB	2.28	0.48
1:A:356:THR:HG21	1:A:376:GLU:CD	2.39	0.48
1:A:209:ARG:HH11	1:A:209:ARG:CG	2.25	0.48
1:A:302:LEU:HD13	1:A:337:ARG:CG	2.42	0.48
3:L:95:SER:O	3:L:97:SER:N	2.46	0.48
1:A:25:ILE:HG22	1:A:29:GLN:NE2	2.28	0.48
1:A:127:PHE:CE1	1:A:131:GLU:HG3	2.49	0.48
2:H:28:ASP:O	2:H:29:LEU:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:6:GLN:HG3	3:L:89:CYS:SG	2.54	0.48
1:A:22:LEU:HD21	1:A:155:LEU:HD11	1.95	0.47
1:A:283:LEU:HD23	1:A:284:LEU:H	1.79	0.47
1:A:495:GLU:HB3	3:L:115:ALA:HB3	1.95	0.47
1:A:561:ALA:C	1:A:563:ASP:H	2.21	0.47
1:A:464:HIS:CG	1:A:473:VAL:HG11	2.49	0.47
1:A:319:TYR:OH	1:A:358:GLU:HG2	2.14	0.47
1:A:538:LYS:HE3	3:L:204:LEU:HD22	1.96	0.47
2:H:173:THR:HA	2:H:188:SER:HA	1.95	0.47
1:A:95:GLU:OE1	1:A:99:ASN:HB2	2.14	0.47
1:A:223:PHE:HD1	1:A:272:SER:HB2	1.78	0.47
1:A:496:THR:O	1:A:497:TYR:C	2.58	0.47
3:L:32:ASN:O	3:L:34:LEU:N	2.48	0.47
3:L:93:TYR:C	3:L:95:SER:N	2.73	0.47
1:A:167:GLU:O	1:A:167:GLU:HG2	2.14	0.47
1:A:249:ASP:HB3	1:A:252:GLU:CG	2.45	0.47
1:A:314:ASP:HB3	1:A:318:ASN:ND2	2.30	0.47
1:A:364:ALA:O	1:A:366:PRO:HD3	2.14	0.47
2:H:67:PHE:HA	2:H:81:GLN:O	2.14	0.47
2:H:113:GLN:HE21	2:H:113:GLN:HB2	1.49	0.47
3:L:213:ASN:O	3:L:214:ARG:C	2.58	0.47
1:A:319:TYR:CE1	1:A:323:LYS:HD3	2.50	0.47
1:A:420:THR:HG23	1:A:530:VAL:CG1	2.45	0.47
1:A:563:ASP:OD1	1:A:564:LYS:N	2.48	0.47
1:A:71:GLY:HA3	1:A:98:ARG:NH2	2.30	0.47
1:A:441:PRO:O	1:A:443:ALA:N	2.48	0.47
2:H:143:THR:CG2	2:H:193:PRO:HA	2.44	0.47
3:L:44:ALA:HB1	3:L:45:PRO:CD	2.45	0.47
1:A:474:THR:O	1:A:478:THR:OG1	2.25	0.46
2:H:48:ILE:HG12	2:H:62:TRP:CH2	2.50	0.46
3:L:182:LEU:HD21	3:L:184:LEU:HD21	1.97	0.46
1:A:120:VAL:HG21	1:A:175:ALA:CA	2.39	0.46
1:A:183:ASP:O	1:A:186:ARG:HB3	2.16	0.46
2:H:127:PRO:HD2	2:H:213:THR:HG21	1.98	0.46
1:A:76:THR:OG1	1:A:77:VAL:HG23	2.15	0.46
1:A:206:PHE:CE2	1:A:481:LEU:HB2	2.51	0.46
1:A:571:GLU:HB3	1:A:575:LEU:CD2	2.46	0.46
1:A:159:LYS:HD3	1:A:285:GLU:OE2	2.15	0.46
3:L:95:SER:HB2	3:L:98:ASP:CB	2.44	0.46
1:A:24:LEU:HA	1:A:43:VAL:HG21	1.96	0.46
2:H:6:GLU:OE2	2:H:95:CYS:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:36:TRP:HD1	2:H:69:ILE:CD1	2.29	0.46
3:L:85:ALA:H	3:L:107:VAL:HG23	1.79	0.46
1:A:420:THR:HG23	1:A:530:VAL:CB	2.46	0.46
3:L:118:VAL:HB	3:L:210:LYS:HG3	1.97	0.46
1:A:11:PHE:CD1	1:A:54:VAL:HG21	2.51	0.45
2:H:14:PRO:HD3	2:H:120:SER:C	2.41	0.45
1:A:156:PHE:CE2	1:A:160:ARG:NE	2.84	0.45
1:A:492:GLU:HG3	1:A:493:VAL:H	1.81	0.45
3:L:179:SER:O	3:L:179:SER:OG	2.33	0.45
1:A:106:LYS:HD2	1:A:148:TYR:HE1	1.66	0.45
1:A:306:ALA:O	1:A:311:GLU:HG3	2.17	0.45
1:A:525:LYS:HD2	1:A:548:MET:CE	2.39	0.45
2:H:127:PRO:HB3	2:H:153:TYR:CB	2.39	0.45
1:A:457:LEU:CD1	1:A:485:ARG:HA	2.46	0.45
2:H:51:ILE:HG23	2:H:51:ILE:O	2.17	0.45
2:H:189:VAL:HG21	3:L:138:LEU:HD22	1.98	0.45
3:L:6:GLN:OE1	3:L:104:GLY:HA2	2.15	0.45
3:L:50:TYR:HD2	3:L:51:GLU:HG2	1.80	0.45
2:H:146:LEU:C	2:H:146:LEU:CD1	2.88	0.45
3:L:120:ILE:HD12	3:L:137:CYS:HA	1.97	0.45
1:A:106:LYS:HD3	1:A:147:PRO:HB2	1.98	0.45
1:A:34:CYS:SG	1:A:84:TYR:CE1	3.08	0.45
1:A:496:THR:O	1:A:497:TYR:O	2.35	0.45
1:A:260:LEU:O	1:A:260:LEU:HD12	2.16	0.45
1:A:496:THR:HG22	1:A:497:TYR:H	1.81	0.45
2:H:164:SER:HA	2:H:205:ASN:OD1	2.17	0.45
1:A:221:GLN:NE2	1:A:339:PRO:HA	2.31	0.44
1:A:433:VAL:HG11	1:A:453:LEU:HD21	1.99	0.44
2:H:24:VAL:HG11	2:H:29:LEU:CB	2.45	0.44
2:H:143:THR:HG22	2:H:194:SER:H	1.82	0.44
3:L:16:GLY:O	3:L:78:SER:HA	2.17	0.44
1:A:381:VAL:O	1:A:385:GLN:HG3	2.17	0.44
3:L:18:ARG:HG3	3:L:76:ILE:O	2.16	0.44
3:L:111:ARG:O	3:L:112:THR:O	2.35	0.44
2:H:102:TYR:N	2:H:102:TYR:CD1	2.84	0.44
3:L:120:ILE:HD11	3:L:151:TRP:CH2	2.52	0.44
3:L:120:ILE:HD13	3:L:137:CYS:SG	2.57	0.44
2:H:20:LEU:HD12	2:H:80:LEU:HD23	1.98	0.44
2:H:97:ARG:NH2	2:H:109:ASP:OD2	2.48	0.44
3:L:30:TRP:CD1	3:L:31:SER:H	2.35	0.44
1:A:48:GLU:O	1:A:51:LYS:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:PRO:C	1:A:443:ALA:N	2.75	0.44
3:L:136:VAL:HG22	3:L:181:THR:CG2	2.35	0.44
3:L:152:LYS:NZ	3:L:198:GLU:CD	2.75	0.44
1:A:94:GLN:O	1:A:97:GLU:HB2	2.17	0.44
1:A:225:LYS:CG	1:A:299:PRO:HG3	2.46	0.44
3:L:120:ILE:O	3:L:120:ILE:CG2	2.66	0.44
1:A:71:GLY:HA3	1:A:98:ARG:CZ	2.48	0.44
1:A:378:LYS:HE2	1:A:378:LYS:HB3	1.70	0.44
1:A:538:LYS:HE3	3:L:204:LEU:CD2	2.47	0.44
1:A:541:LYS:C	1:A:543:GLN:H	2.26	0.44
1:A:416:PRO:HB2	1:A:497:TYR:CD1	2.52	0.44
2:H:20:LEU:HD22	2:H:115:THR:HG21	2.00	0.44
3:L:156:ALA:O	3:L:158:GLN:NE2	2.50	0.44
1:A:118:PRO:HG2	1:A:123:MET:CG	2.47	0.44
1:A:414:LYS:O	1:A:472:ARG:NH1	2.51	0.44
1:A:393:GLU:O	1:A:397:GLN:HG3	2.17	0.43
2:H:97:ARG:O	2:H:108:PHE:HA	2.18	0.43
1:A:173:ASP:HB3	1:A:176:ALA:HB3	2.00	0.43
1:A:300:ALA:O	1:A:302:LEU:N	2.52	0.43
2:H:22:CYS:O	2:H:77:THR:HG23	2.18	0.43
3:L:18:ARG:HA	3:L:76:ILE:O	2.18	0.43
3:L:178:LEU:C	3:L:178:LEU:CD2	2.91	0.43
1:A:113:PRO:O	1:A:114:ARG:C	2.60	0.43
1:A:189:GLY:O	1:A:190:LYS:C	2.61	0.43
1:A:197:ARG:HG3	1:A:197:ARG:NH1	2.33	0.43
1:A:110:PRO:C	1:A:112:LEU:H	2.26	0.43
2:H:36:TRP:CE2	2:H:80:LEU:HB2	2.54	0.43
1:A:500:LYS:O	1:A:501:GLU:CB	2.66	0.43
2:H:36:TRP:CD1	2:H:69:ILE:HG12	2.54	0.43
1:A:151:ALA:CB	1:A:250:LEU:HD22	2.46	0.43
1:A:268:GLN:C	1:A:270:SER:N	2.75	0.43
1:A:571:GLU:HB3	1:A:575:LEU:HD23	2.00	0.43
3:L:26:SER:HB3	3:L:27:PRO:CD	2.39	0.43
3:L:67:GLY:HA3	3:L:72:PHE:HA	2.01	0.43
2:H:24:VAL:O	2:H:76:ASN:ND2	2.52	0.43
3:L:6:GLN:HE21	3:L:21:ILE:CG2	2.32	0.43
3:L:26:SER:CB	3:L:27:PRO:HD3	2.38	0.43
3:L:150:GLN:HB2	3:L:198:GLU:HB3	1.99	0.43
1:A:108:ASP:O	1:A:110:PRO:HD3	2.19	0.43
1:A:485:ARG:NH2	1:A:486:PRO:HG3	2.34	0.43
1:A:30:TYR:HE1	1:A:103:LEU:HD23	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:24:VAL:CG1	2:H:76:ASN:HD21	2.25	0.42
3:L:152:LYS:HZ1	3:L:198:GLU:CD	2.27	0.42
3:L:87:TYR:HE1	3:L:107:VAL:CG2	2.31	0.42
2:H:4:LEU:HD23	2:H:24:VAL:HB	2.01	0.42
1:A:165:PHE:CE1	1:A:178:LEU:HD21	2.54	0.42
1:A:495:GLU:OE1	1:A:538:LYS:CG	2.64	0.42
2:H:5:LEU:HA	2:H:113:GLN:OE1	2.19	0.42
3:L:2:ILE:O	3:L:27:PRO:CD	2.67	0.42
3:L:107:VAL:HG23	3:L:107:VAL:O	2.19	0.42
1:A:22:LEU:CD2	1:A:155:LEU:HD11	2.50	0.42
1:A:118:PRO:HG2	1:A:123:MET:HG3	2.02	0.42
1:A:141:GLU:OE1	1:A:145:ARG:NH1	2.49	0.42
1:A:342:SER:HA	1:A:447:PRO:HA	2.02	0.42
1:A:457:LEU:O	1:A:460:LEU:HB3	2.19	0.42
1:A:537:PRO:HB2	1:A:538:LYS:H	1.68	0.42
1:A:382:GLU:O	1:A:383:GLU:C	2.63	0.42
3:L:109:ILE:CG2	3:L:110:LYS:N	2.83	0.42
1:A:340:ASP:O	1:A:447:PRO:HD3	2.20	0.42
2:H:19:ARG:HG3	2:H:81:GLN:OE1	2.20	0.42
2:H:147:GLY:HA3	2:H:189:VAL:HG12	2.02	0.42
2:H:156:GLU:CD	2:H:157:PRO:HA	2.45	0.42
3:L:50:TYR:OH	3:L:54:LYS:NZ	2.38	0.42
2:H:12:VAL:HG21	2:H:18:LEU:HD22	2.02	0.41
2:H:145:ALA:HB2	2:H:191:THR:HA	2.02	0.41
1:A:133:THR:O	1:A:137:LYS:HB2	2.20	0.41
2:H:85:LEU:HA	2:H:89:ASP:OD2	2.21	0.41
2:H:172:HIS:CD2	3:L:140:ASN:OD1	2.73	0.41
2:H:175:PRO:HG2	3:L:166:VAL:O	2.20	0.41
3:L:56:THR:HG22	3:L:57:SER:N	2.35	0.41
1:A:9:HIS:HE1	1:A:10:ARG:NH1	2.18	0.41
2:H:39:GLN:C	2:H:91:ALA:HB1	2.45	0.41
2:H:174:PHE:CE1	3:L:167:THR:HG23	2.54	0.41
2:H:129:VAL:HG21	2:H:215:VAL:HB	2.02	0.41
2:H:153:TYR:OH	2:H:176:ALA:HB2	2.19	0.41
1:A:219:LEU:HD22	1:A:223:PHE:CE2	2.56	0.41
1:A:551:PHE:HD1	1:A:551:PHE:HA	1.77	0.41
2:H:35:ASN:OD1	2:H:50:ILE:HB	2.20	0.41
2:H:85:LEU:HB3	2:H:119:VAL:HG21	2.01	0.41
3:L:15:VAL:CG1	3:L:81:PRO:HD3	2.50	0.41
3:L:35:SER:OG	3:L:37:TYR:HE1	2.04	0.41
1:A:42:LEU:H	1:A:42:LEU:HG	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:35:SER:O	3:L:89:CYS:HA	2.21	0.41
1:A:25:ILE:HD11	1:A:139:LEU:HD22	2.02	0.41
2:H:97:ARG:CZ	2:H:110:LEU:HD12	2.51	0.41
2:H:222:LYS:O	2:H:223:SER:CB	2.68	0.41
1:A:132:GLU:OE1	1:A:136:LYS:HE3	2.21	0.41
1:A:140:TYR:O	1:A:144:ARG:HG2	2.21	0.41
1:A:433:VAL:HG21	1:A:453:LEU:HG	2.02	0.41
1:A:543:GLN:H	1:A:543:GLN:HG2	1.63	0.41
2:H:96:ALA:HB1	2:H:108:PHE:HB3	2.02	0.41
3:L:166:VAL:CG2	3:L:178:LEU:HG	2.50	0.41
3:L:27:PRO:O	3:L:28:SER:C	2.64	0.41
1:A:281:LYS:HB3	1:A:285:GLU:CB	2.51	0.40
3:L:12:SER:HA	3:L:108:GLU:O	2.21	0.40
3:L:120:ILE:CD1	3:L:137:CYS:CB	2.99	0.40
1:A:70:PHE:HZ	1:A:251:LEU:CD1	2.33	0.40
1:A:233:LYS:NZ	1:A:237:ASP:OD2	2.46	0.40
1:A:458:ASN:CB	1:A:484:ARG:HH12	2.35	0.40
1:A:543:GLN:O	1:A:547:VAL:HG23	2.20	0.40
2:H:88:GLU:CD	2:H:88:GLU:N	2.79	0.40
1:A:410:ARG:O	1:A:414:LYS:HG3	2.22	0.40
2:H:11:LEU:HB2	2:H:155:PRO:HG3	2.03	0.40
1:A:186:ARG:NH1	1:A:187:ASP:OD1	2.55	0.40
1:A:343:VAL:HG23	1:A:451:ASP:OD2	2.21	0.40
3:L:95:SER:HB2	3:L:98:ASP:CG	2.46	0.40
3:L:149:VAL:HG11	3:L:180:SER:CB	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	577/585 (99%)	503 (87%)	57 (10%)	17 (3%)	3 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	213/233 (91%)	191 (90%)	20 (9%)	2 (1%)	14	46
3	L	215/217 (99%)	182 (85%)	21 (10%)	12 (6%)	1	14
All	All	1005/1035 (97%)	876 (87%)	98 (10%)	31 (3%)	3	25

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	300	ALA
1	A	491	LEU
1	A	497	TYR
1	A	538	LYS
2	H	223	SER
3	L	17	ASP
1	A	301	ASP
1	A	442	GLU
1	A	479	GLU
1	A	537	PRO
1	A	540	THR
3	L	3	GLN
3	L	30	TRP
3	L	33	PHE
3	L	112	THR
3	L	141	ASN
3	L	214	ARG
1	A	56	ASP
1	A	129	ASP
1	A	269	ASP
1	A	281	LYS
1	A	502	PHE
1	A	512	ASP
3	L	31	SER
3	L	97	SER
3	L	216	GLU
1	A	118	PRO
3	L	94	SER
2	H	221	PRO
3	L	2	ILE
1	A	388	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	A	506/511 (99%)	472 (93%)	34 (7%)	15	42
2	H	180/195 (92%)	163 (91%)	17 (9%)	8	32
3	L	190/190 (100%)	172 (90%)	18 (10%)	8	32
All	All	876/896 (98%)	807 (92%)	69 (8%)	11	37

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	37	GLU
1	A	77	VAL
1	A	97	GLU
1	A	111	ASN
1	A	114	ARG
1	A	132	GLU
1	A	218	ARG
1	A	222	ARG
1	A	269	ASP
1	A	283	LEU
1	A	292	GLU
1	A	299	PRO
1	A	305	LEU
1	A	308	ASP
1	A	323	LYS
1	A	324	ASP
1	A	383	GLU
1	A	389	LYS
1	A	435	SER
1	A	444	LYS
1	A	466	LYS
1	A	469	VAL
1	A	478	THR
1	A	496	THR
1	A	505	GLU

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Mol	Chain	Res	Type
1	A	532	LEU
1	A	536	LYS
1	A	538	LYS
1	A	540	THR
1	A	542	GLU
1	A	551	PHE
1	A	557	LYS
1	A	576	VAL
2	H	3	GLN
2	H	30	SER
2	H	50	ILE
2	H	54	SER
2	H	61	THR
2	H	66	ARG
2	H	71	ARG
2	H	99	VAL
2	H	113	GLN
2	H	129	VAL
2	H	150	VAL
2	H	156	GLU
2	H	186	LEU
2	H	191	THR
2	H	214	LYS
2	H	220	GLU
2	H	222	LYS
3	L	1	ASP
3	L	3	GLN
3	L	5	THR
3	L	15	VAL
3	L	68	SER
3	L	82	GLU
3	L	94	SER
3	L	106	LYS
3	L	108	GLU
3	L	118	VAL
3	L	148	LYS
3	L	163	GLN
3	L	171	SER
3	L	181	THR
3	L	184	LEU
3	L	198	GLU
3	L	202	GLN

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Mol	Chain	Res	Type
3	L	205	SER

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

Mol	Chain	Res	Type
1	A	9	HIS
1	A	29	GLN
1	A	61	ASN
1	A	67	HIS
1	A	109	ASN
1	A	221	GLN
1	A	247	HIS
1	A	440	HIS
1	A	483	ASN
1	A	543	GLN
2	H	3	GLN
2	H	13	GLN
2	H	76	ASN
2	H	113	GLN
3	L	155	ASN
3	L	163	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	579/585 (98%)	-0.21	5 (0%) 81 56	75, 111, 185, 211	0
2	H	217/233 (93%)	-0.35	1 (0%) 87 66	81, 103, 131, 151	0
3	L	217/217 (100%)	-0.31	0 100 100	70, 103, 131, 163	0
All	All	1013/1035 (97%)	-0.26	6 (0%) 85 64	70, 107, 177, 211	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	87	MET	2.8
1	A	538	LYS	2.6
2	H	135	SER	2.5
1	A	552	ALA	2.2
1	A	30	TYR	2.2
1	A	78	ALA	2.1

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.