



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 12:55 PM UTC

PDB ID : 3O78 / pdb_00003o78
Title : The structure of Ca²⁺ Sensor (Case-12)
Authors : Leder, L.; Stark, W.; Freuler, F.; Marsh, M.; Meyerhofer, M.; Stettler, T.;
Mayr, L.M.; Britanova, O.V.; Strukova, L.A.; Chudakov, D.M.
Deposited on : 2010-07-30
Resolution : 2.60 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (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

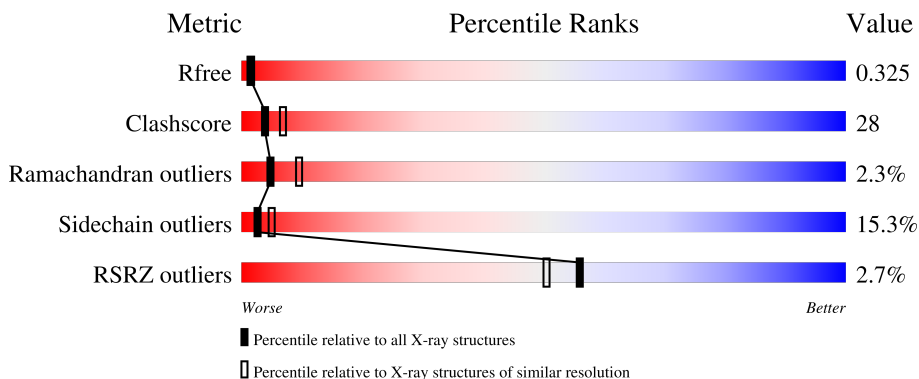
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	415	
1	B	415	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6423 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 Myosin light chain kinase, smooth muscle, Green fluorescent protein, Green fluorescent protein, Calmodulin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	403	3168	1982	540	631	15	0	0	0
1	B	401	3170	1986	538	630	16	0	0	0

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P11799
A	2	PRO	-	expression tag	UNP P11799
A	3	GLY	-	expression tag	UNP P11799
A	4	SER	-	expression tag	UNP P11799
A	5	SER	ALA	engineered mutation	UNP P11799
A	10	ASN	GLN	engineered mutation	UNP P11799
A	25	LEU	SER	engineered mutation	UNP P42212
A	26	GLU	HIS	engineered mutation	UNP P42212
A	41	ALA	VAL	engineered mutation	UNP P42212
A	49	VAL	ILE	engineered mutation	UNP P42212
A	81	PHE	THR	engineered mutation	UNP P42212
A	84	VAL	ALA	engineered mutation	UNP P42212
A	109	LEU	HIS	engineered mutation	UNP P42212
A	116	ASN	LYS	engineered mutation	UNP P42212
A	117	VAL	-	linker	UNP P42212
A	118	ASP	-	linker	UNP P42212
A	119	GLY	-	linker	UNP P42212
A	120	GLY	-	linker	UNP P42212
A	121	SER	-	linker	UNP P42212
A	122	GLY	-	linker	UNP P42212
A	123	GLY	-	linker	UNP P42212
A	124	THR	-	linker	UNP P42212
A	125	GLY	-	linker	UNP P42212
A	170	LEU	PHE	engineered mutation	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
A	188	LEU	PHE	engineered mutation	UNP P42212
A	190	CR2	SER	chromophore	UNP P42212
A	190	CR2	TYR	chromophore	UNP P42212
A	190	CR2	GLY	chromophore	UNP P42212
A	192	LEU	VAL	engineered mutation	UNP P42212
A	193	LYS	GLN	engineered mutation	UNP P42212
A	196	ALA	SER	see sequence details	UNP P42212
A	253	GLY	ASP	engineered mutation	UNP P42212
A	269	THR	TYR	engineered mutation	UNP P42212
A	270	ARG	ASN	engineered mutation	UNP P42212
B	1	GLY	-	expression tag	UNP P11799
B	2	PRO	-	expression tag	UNP P11799
B	3	GLY	-	expression tag	UNP P11799
B	4	SER	-	expression tag	UNP P11799
B	5	SER	ALA	engineered mutation	UNP P11799
B	10	ASN	GLN	engineered mutation	UNP P11799
B	25	LEU	SER	engineered mutation	UNP P42212
B	26	GLU	HIS	engineered mutation	UNP P42212
B	41	ALA	VAL	engineered mutation	UNP P42212
B	49	VAL	ILE	engineered mutation	UNP P42212
B	81	PHE	THR	engineered mutation	UNP P42212
B	84	VAL	ALA	engineered mutation	UNP P42212
B	109	LEU	HIS	engineered mutation	UNP P42212
B	116	ASN	LYS	engineered mutation	UNP P42212
B	117	VAL	-	linker	UNP P42212
B	118	ASP	-	linker	UNP P42212
B	119	GLY	-	linker	UNP P42212
B	120	GLY	-	linker	UNP P42212
B	121	SER	-	linker	UNP P42212
B	122	GLY	-	linker	UNP P42212
B	123	GLY	-	linker	UNP P42212
B	124	THR	-	linker	UNP P42212
B	125	GLY	-	linker	UNP P42212
B	170	LEU	PHE	engineered mutation	UNP P42212
B	188	LEU	PHE	engineered mutation	UNP P42212
B	190	CR2	SER	chromophore	UNP P42212
B	190	CR2	TYR	chromophore	UNP P42212
B	190	CR2	GLY	chromophore	UNP P42212
B	192	LEU	VAL	engineered mutation	UNP P42212
B	193	LYS	GLN	engineered mutation	UNP P42212
B	196	ALA	SER	see sequence details	UNP P42212
B	253	GLY	ASP	engineered mutation	UNP P42212

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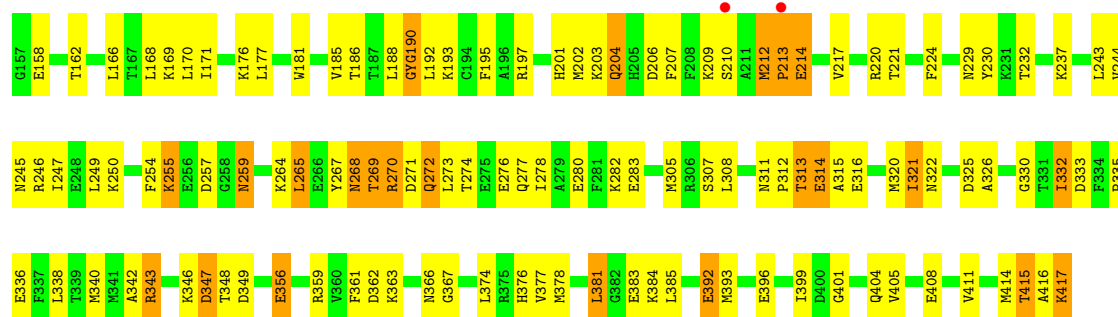
Chain	Residue	Modelled	Actual	Comment	Reference
B	269	THR	TYR	engineered mutation	UNP P42212
B	270	ARG	ASN	engineered mutation	UNP P42212

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Ca 4 4	0	0
2	B	4	Total Ca 4 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	41	Total O 41 41	0	0
3	B	36	Total O 36 36	0	0



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.37Å 101.64Å 82.21Å 90.00° 91.45° 90.00°	Depositor
Resolution (Å)	50.83 – 2.60 50.83 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.83-2.60) 99.8 (50.83-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.242 , 0.316 0.261 , 0.325	Depositor DCC
R_{free} test set	1174 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtrriage
Anisotropy	0.179	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 16.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.052 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6423	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CR2, CA

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	1.43	26/3203 (0.8%)	1.21	17/4311 (0.4%)
1	B	1.04	5/3205 (0.2%)	1.13	11/4312 (0.3%)
All	All	1.25	31/6408 (0.5%)	1.17	28/8623 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	GLU	C-O	-6.27	1.16	1.24
1	A	245	ASN	C-O	-6.25	1.16	1.24
1	A	16	VAL	C-O	-6.23	1.18	1.24
1	B	315	ALA	CA-CB	-6.15	1.43	1.53
1	A	22	LEU	C-O	-5.94	1.16	1.24
1	A	67	GLY	C-O	-5.78	1.16	1.23
1	A	15	ALA	C-O	-5.73	1.16	1.24
1	B	6	ARG	C-O	-5.72	1.16	1.24
1	A	60	TYR	C-O	-5.71	1.17	1.24
1	A	40	LYS	C-O	-5.71	1.16	1.23
1	A	32	ALA	CA-CB	-5.61	1.44	1.53
1	A	10	ASN	C-O	-5.51	1.17	1.24
1	B	315	ALA	C-O	-5.50	1.17	1.24
1	A	6	ARG	C-O	-5.39	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	ALA	CA-CB	-5.38	1.44	1.53
1	A	21	ARG	CZ-NH2	-5.35	1.26	1.33
1	A	128	GLY	C-O	-5.35	1.16	1.23
1	A	28	VAL	C-O	-5.32	1.18	1.24
1	A	12	THR	C-O	-5.31	1.17	1.24
1	A	63	ASN	C-O	-5.30	1.17	1.23
1	A	145	ASP	C-O	-5.28	1.17	1.24
1	A	218	GLN	C-O	-5.24	1.18	1.24
1	A	231	LYS	C-O	-5.24	1.17	1.24
1	A	219	GLU	CA-C	-5.23	1.46	1.52
1	A	223	PHE	C-O	-5.17	1.17	1.24
1	A	136	VAL	CA-CB	5.17	1.58	1.54
1	A	232	THR	C-O	-5.10	1.17	1.23
1	A	105	ALA	C-O	-5.10	1.17	1.23
1	B	106	GLY	C-O	-5.06	1.17	1.24
1	B	312	PRO	C-O	-5.04	1.18	1.23
1	A	141	GLU	C-O	-5.03	1.18	1.23

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	LYS	N-CA-C	-10.08	99.69	112.90
1	A	14	HIS	N-CA-C	-9.54	100.50	113.18
1	A	127	LYS	N-CA-C	-7.83	102.69	111.14
1	B	110	GLY	N-CA-C	7.56	124.91	112.66
1	A	247	ILE	N-CA-C	7.03	120.32	108.86
1	A	212	MET	CB-CA-C	-7.03	104.11	110.44
1	B	71	VAL	N-CA-C	6.92	123.73	109.34
1	A	270	ARG	NE-CZ-NH2	6.90	125.41	119.20
1	A	6	ARG	N-CA-C	-6.87	102.14	112.04
1	A	270	ARG	NE-CZ-NH1	-6.71	114.79	121.50
1	A	36	LYS	N-CA-C	-6.28	104.93	112.59
1	A	16	VAL	N-CA-C	-6.20	105.10	110.74
1	B	3	GLY	N-CA-C	5.92	123.23	115.36
1	B	321	ILE	CB-CA-C	-5.68	104.63	112.24
1	B	405	VAL	N-CA-C	5.59	115.64	107.37
1	A	135	VAL	N-CA-C	5.58	116.25	108.89
1	B	136	VAL	CA-C-N	-5.55	114.25	120.14
1	B	136	VAL	C-N-CA	-5.55	114.25	120.14
1	A	107	ILE	N-CA-C	5.49	115.79	108.11
1	B	4	SER	N-CA-C	5.38	122.25	110.80
1	A	334	PHE	CA-C-N	-5.35	113.22	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	PHE	C-N-CA	-5.35	113.22	119.32
1	A	331	THR	CA-C-N	-5.22	116.72	123.19
1	A	331	THR	C-N-CA	-5.22	116.72	123.19
1	A	61	GLN	N-CA-C	5.21	117.39	108.90
1	B	24	SER	N-CA-C	5.15	116.65	108.67
1	B	111	MET	N-CA-C	-5.14	96.60	111.00
1	A	344	LYS	N-CA-C	-5.12	102.49	110.42

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	212	MET	Peptide
1	A	415	THR	Peptide
1	B	212	MET	Peptide
1	B	268	ASN	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3168	0	3061	180	0
1	B	3170	0	3080	206	1
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	41	0	0	23	0
3	B	36	0	0	21	0
All	All	6423	0	6141	353	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (353) 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:6:ARG:NH1	1:B:396:GLU:OE2	1.80	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:GLY:N	1:B:2:PRO:HD2	1.63	1.13
1:B:35:GLN:HB2	3:B:448:HOH:O	1.51	1.10
1:B:6:ARG:HG2	1:B:7:ARG:H	1.13	1.07
1:B:108:THR:O	1:B:109:LEU:HB3	1.54	1.05
1:B:1:GLY:H2	1:B:2:PRO:HD2	1.11	1.04
1:B:1:GLY:N	1:B:2:PRO:CD	2.20	1.03
1:B:8:LYS:N	1:B:8:LYS:HD3	1.74	1.00
1:A:274:THR:HG22	1:A:277:GLN:HG3	1.46	0.98
1:A:213:PRO:HD2	1:A:214:GLU:H	1.25	0.98
1:B:109:LEU:C	1:B:109:LEU:HD23	1.92	0.94
1:A:378:MET:SD	1:A:385:LEU:HD11	2.07	0.94
1:B:6:ARG:H	1:B:8:LYS:NZ	1.63	0.94
1:B:6:ARG:O	1:B:8:LYS:HD3	1.70	0.92
1:A:320:MET:HE3	1:B:23:SER:HA	1.50	0.91
1:A:6:ARG:HH11	1:B:396:GLU:CG	1.84	0.91
1:B:213:PRO:HD2	1:B:214:GLU:H	1.35	0.90
1:B:6:ARG:H	1:B:8:LYS:HZ1	1.18	0.89
1:B:61:GLN:HE22	1:B:193:LYS:HE3	1.40	0.87
1:B:6:ARG:HG2	1:B:7:ARG:N	1.89	0.86
1:B:274:THR:HG22	1:B:277:GLN:HG3	1.57	0.85
1:A:141:GLU:OE1	1:A:246:ARG:NH1	2.11	0.83
1:A:61:GLN:OE1	1:A:220:ARG:NH2	2.12	0.82
1:B:259:ASN:HA	1:B:264:LYS:HB2	1.60	0.81
1:B:6:ARG:O	1:B:8:LYS:CE	2.29	0.81
1:B:138:ILE:HD11	1:B:195:PHE:CE2	2.17	0.80
1:B:6:ARG:O	1:B:8:LYS:CD	2.29	0.80
1:B:6:ARG:N	1:B:8:LYS:NZ	2.29	0.80
1:B:108:THR:O	1:B:109:LEU:CB	2.30	0.80
1:B:417:LYS:H	1:B:417:LYS:HE2	1.45	0.80
1:B:1:GLY:H3	1:B:2:PRO:CD	1.94	0.79
1:A:144:GLY:HA2	1:A:249:LEU:O	1.82	0.79
1:A:213:PRO:CD	1:A:214:GLU:H	1.97	0.78
1:A:6:ARG:HH11	1:B:396:GLU:CD	1.89	0.78
1:B:3:GLY:O	1:B:4:SER:CB	2.30	0.78
1:B:109:LEU:HD23	1:B:109:LEU:O	1.83	0.78
1:A:13:GLY:HA3	1:B:414:MET:CE	2.14	0.78
1:B:109:LEU:O	1:B:109:LEU:CD2	2.33	0.77
1:B:417:LYS:H	1:B:417:LYS:CE	1.97	0.76
1:B:141:GLU:OE1	1:B:246:ARG:NH1	2.19	0.76
1:B:209:LYS:O	1:B:212:MET:HB2	1.85	0.76
1:B:268:ASN:HB3	1:B:269:THR:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:GLY:N	1:B:384:LYS:O	2.19	0.75
1:B:213:PRO:CD	1:B:214:GLU:H	1.99	0.75
1:A:267:TYR:O	1:A:268:ASN:HB2	1.84	0.75
1:B:210:SER:HB3	3:B:440:HOH:O	1.84	0.75
1:B:404:GLN:HG3	3:B:446:HOH:O	1.86	0.74
1:B:110:GLY:O	1:B:111:MET:HB2	1.86	0.74
1:A:6:ARG:HH11	1:B:396:GLU:HG3	1.50	0.74
1:A:259:ASN:HA	1:A:264:LYS:HB2	1.70	0.73
1:A:33:ASP:OD2	1:A:36:LYS:HB2	1.88	0.73
1:A:202:MET:HA	3:A:430:HOH:O	1.88	0.73
1:B:109:LEU:C	1:B:109:LEU:CD2	2.62	0.72
1:A:270:ARG:HD2	1:A:270:ARG:O	1.89	0.72
1:A:209:LYS:O	1:A:212:MET:HB2	1.89	0.72
1:A:320:MET:HE3	1:B:23:SER:CA	2.20	0.72
1:A:415:THR:HG22	1:A:417:LYS:HE3	1.71	0.71
1:B:408:GLU:HG3	3:B:436:HOH:O	1.90	0.71
1:B:6:ARG:N	1:B:8:LYS:HZ1	1.84	0.71
1:B:8:LYS:HD3	1:B:8:LYS:H	1.52	0.71
1:A:356:GLU:OE1	1:A:359:ARG:NH1	2.23	0.71
1:A:23:SER:HA	1:B:320:MET:HE3	1.73	0.70
1:B:267:TYR:O	1:B:268:ASN:HB2	1.90	0.69
1:A:197:ARG:NE	3:A:425:HOH:O	2.26	0.69
1:B:411:VAL:O	1:B:415:THR:HG23	1.93	0.69
1:A:70:PRO:N	3:A:447:HOH:O	2.26	0.69
1:A:70:PRO:CD	3:A:447:HOH:O	2.40	0.69
1:A:203:LYS:HG3	3:A:446:HOH:O	1.91	0.68
1:B:35:GLN:HE21	1:B:35:GLN:HA	1.58	0.68
1:B:35:GLN:O	1:B:36:LYS:HG3	1.92	0.68
1:A:190:CR2:HD1	1:A:190:CR2:N2	2.09	0.67
1:B:6:ARG:C	1:B:7:ARG:CG	2.67	0.67
1:B:313:THR:O	1:B:314:GLU:C	2.35	0.67
1:A:213:PRO:HD2	1:A:214:GLU:N	2.07	0.66
1:B:3:GLY:O	1:B:4:SER:HB3	1.94	0.66
1:B:356:GLU:OE1	1:B:359:ARG:NH1	2.28	0.66
1:B:1:GLY:HA2	1:B:8:LYS:HD2	1.78	0.66
1:B:147:ASN:ND2	1:B:254:PHE:O	2.29	0.66
1:B:270:ARG:CD	3:B:452:HOH:O	2.43	0.66
1:A:274:THR:HG22	1:A:277:GLN:CG	2.24	0.65
1:B:2:PRO:O	1:B:7:ARG:NH1	2.29	0.65
1:A:142:LEU:HD23	1:A:142:LEU:C	2.21	0.65
1:B:6:ARG:O	1:B:8:LYS:NZ	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:LEU:HD21	1:B:381:LEU:HD13	1.79	0.65
1:A:71:VAL:N	3:A:447:HOH:O	2.15	0.65
1:A:13:GLY:HA3	1:B:414:MET:HE2	1.79	0.65
1:A:203:LYS:CG	3:A:446:HOH:O	2.43	0.65
1:B:272:GLN:OE1	3:B:419:HOH:O	2.15	0.65
1:B:126:SER:HB3	3:B:440:HOH:O	1.97	0.64
1:A:142:LEU:HD23	1:A:143:ASP:N	2.13	0.64
1:A:221:THR:OG1	1:A:231:LYS:HE3	1.98	0.63
1:A:313:THR:OG1	1:A:316:GLU:HG3	1.97	0.63
1:A:5:SER:HB3	1:B:392:GLU:OE1	1.98	0.63
1:A:13:GLY:HA3	1:B:414:MET:HE1	1.80	0.63
1:A:391:ASP:HA	3:A:458:HOH:O	1.97	0.63
1:B:417:LYS:HE2	1:B:417:LYS:N	2.13	0.63
1:A:287:LEU:HD11	1:B:11:LYS:HE2	1.81	0.63
1:B:313:THR:O	1:B:316:GLU:N	2.31	0.63
1:A:244:VAL:CG1	1:A:246:ARG:HG3	2.29	0.62
1:B:6:ARG:O	1:B:7:ARG:HG3	2.00	0.62
1:B:336:GLU:HG3	3:B:424:HOH:O	1.99	0.62
1:A:192:LEU:HD22	1:A:243:LEU:HD12	1.81	0.62
1:A:274:THR:CG2	1:A:277:GLN:HG3	2.27	0.62
1:A:33:ASP:CG	1:A:36:LYS:HB2	2.24	0.61
1:A:396:GLU:OE1	1:B:5:SER:HB3	2.00	0.61
1:A:82:GLN:NE2	3:A:457:HOH:O	2.33	0.61
1:A:61:GLN:HE22	1:A:193:LYS:HE3	1.66	0.61
1:B:378:MET:SD	1:B:385:LEU:HD11	2.41	0.61
1:B:274:THR:HG22	1:B:277:GLN:HE21	1.67	0.60
1:A:376:HIS:CE1	3:A:453:HOH:O	2.54	0.60
1:A:204:GLN:HG3	3:A:430:HOH:O	2.01	0.60
1:B:177:LEU:HD22	1:B:181:TRP:CE2	2.36	0.60
1:A:129:GLU:OE2	1:A:203:LYS:HE2	2.01	0.59
1:A:11:LYS:HD2	1:B:283:GLU:HB3	1.85	0.59
1:B:33:ASP:HA	3:B:447:HOH:O	2.01	0.59
1:A:346:LYS:O	1:A:348:THR:N	2.36	0.59
1:A:5:SER:CB	1:B:392:GLU:OE1	2.50	0.59
1:B:268:ASN:HA	3:B:431:HOH:O	2.03	0.59
1:A:61:GLN:HG3	1:A:220:ARG:CG	2.33	0.59
1:A:361:PHE:CZ	1:B:12:THR:HG22	2.36	0.59
1:B:84:VAL:HG21	1:B:278:ILE:HD11	1.84	0.59
1:A:374:LEU:HD21	1:A:393:MET:HE2	1.84	0.58
1:B:110:GLY:C	1:B:111:MET:O	2.40	0.58
1:B:272:GLN:OE1	1:B:272:GLN:HA	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ASP:HA	3:B:437:HOH:O	2.03	0.58
1:B:214:GLU:O	1:B:237:LYS:HB2	2.04	0.58
1:B:321:ILE:HG22	1:B:325:ASP:HB2	1.86	0.58
1:A:5:SER:O	1:A:9:TRP:HD1	1.87	0.57
1:A:413:MET:SD	1:B:6:ARG:HG3	2.44	0.57
1:A:127:LYS:O	1:A:129:GLU:N	2.37	0.57
1:B:6:ARG:N	1:B:8:LYS:HZ2	2.00	0.57
1:B:206:ASP:OD2	1:B:209:LYS:HD2	2.04	0.57
1:A:3:GLY:O	1:A:8:LYS:NZ	2.36	0.57
1:B:1:GLY:H3	1:B:2:PRO:HD3	1.68	0.57
1:A:268:ASN:HB3	1:A:269:THR:O	2.05	0.56
1:A:127:LYS:C	1:A:129:GLU:H	2.14	0.56
1:B:1:GLY:H3	1:B:2:PRO:HD2	1.59	0.56
1:B:6:ARG:C	1:B:8:LYS:HZ2	2.13	0.56
1:B:276:GLU:HG2	1:B:417:LYS:HE3	1.88	0.56
1:A:39:ILE:HG13	1:A:63:ASN:HB2	1.88	0.56
1:A:343:ARG:HG3	1:A:343:ARG:HH11	1.71	0.55
1:A:70:PRO:CB	3:A:447:HOH:O	2.54	0.55
1:B:170:LEU:HD13	1:B:188:LEU:HD13	1.87	0.55
1:B:343:ARG:HG3	1:B:343:ARG:HH11	1.72	0.55
1:A:396:GLU:OE1	1:B:5:SER:CB	2.55	0.55
1:A:361:PHE:HA	1:A:377:VAL:HG21	1.89	0.54
1:A:146:VAL:HG23	1:A:151:PHE:HE1	1.72	0.54
1:B:11:LYS:O	1:B:14:HIS:HB2	2.07	0.54
1:B:158:GLU:HG2	3:B:420:HOH:O	2.07	0.54
1:B:8:LYS:N	1:B:8:LYS:CD	2.58	0.54
1:A:10:ASN:OD1	1:B:414:MET:HA	2.08	0.54
1:A:332:ILE:HA	1:A:336:GLU:OE2	2.08	0.54
1:A:36:LYS:O	1:A:37:ASN:C	2.50	0.53
1:A:70:PRO:CA	3:A:447:HOH:O	2.54	0.53
1:B:50:GLU:C	1:B:52:GLY:H	2.15	0.53
1:B:212:MET:CE	1:B:243:LEU:HD21	2.39	0.53
1:B:332:ILE:HA	1:B:336:GLU:OE2	2.07	0.53
1:A:14:HIS:CD2	1:A:17:ARG:NH2	2.77	0.53
1:B:34:LYS:C	1:B:36:LYS:H	2.16	0.53
1:B:55:GLN:OE1	1:B:259:ASN:ND2	2.41	0.53
1:A:274:THR:HG23	1:A:277:GLN:H	1.73	0.53
1:A:45:ILE:O	1:A:56:LEU:HA	2.09	0.53
1:B:316:GLU:O	1:B:320:MET:HG3	2.08	0.53
1:A:42:ASN:HB3	1:A:60:TYR:CD2	2.43	0.52
1:B:72:LEU:CD2	3:B:440:HOH:O	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:CR2:N2	1:B:190:CR2:HD1	2.25	0.52
1:B:6:ARG:O	1:B:7:ARG:CG	2.57	0.52
1:A:247:ILE:HG22	1:A:248:GLU:N	2.25	0.52
1:A:283:GLU:HB3	1:B:11:LYS:HE3	1.92	0.52
1:A:280:GLU:OE2	1:B:14:HIS:HE1	1.91	0.52
1:A:388:GLU:HB3	3:A:454:HOH:O	2.09	0.52
1:B:362:ASP:OD1	1:B:367:GLY:N	2.38	0.52
1:A:25:LEU:HD21	1:B:320:MET:HA	1.92	0.51
1:A:70:PRO:HD2	3:A:447:HOH:O	2.05	0.51
1:A:298:THR:HG21	1:A:318:GLN:HG2	1.92	0.51
1:B:61:GLN:NE2	1:B:193:LYS:HE3	2.18	0.51
1:B:146:VAL:HG23	1:B:151:PHE:HE1	1.74	0.51
1:B:188:LEU:O	1:B:190:CR2:HA31	2.10	0.51
1:A:274:THR:HG22	1:A:277:GLN:HE21	1.74	0.51
1:B:343:ARG:HH11	1:B:343:ARG:CG	2.24	0.51
1:B:100:GLU:OE1	1:B:166:LEU:HD23	2.10	0.51
1:A:6:ARG:NH1	1:B:396:GLU:HG3	2.23	0.51
1:A:33:ASP:OD2	1:A:36:LYS:CB	2.56	0.51
1:A:127:LYS:O	1:A:130:GLU:HG3	2.11	0.51
1:B:6:ARG:CA	1:B:8:LYS:HZ2	2.24	0.51
1:B:274:THR:HG23	1:B:276:GLU:HB3	1.92	0.51
1:A:11:LYS:CD	1:B:283:GLU:HB3	2.41	0.50
1:A:274:THR:CG2	1:A:276:GLU:HB3	2.42	0.50
1:A:274:THR:HG23	1:A:276:GLU:HB3	1.92	0.50
1:A:147:ASN:ND2	1:A:254:PHE:O	2.39	0.50
1:B:139:LEU:HB3	1:B:244:VAL:HG22	1.93	0.50
1:B:192:LEU:HD22	1:B:243:LEU:HD12	1.94	0.50
1:A:127:LYS:C	1:A:129:GLU:N	2.69	0.50
1:B:88:ASP:CA	3:B:437:HOH:O	2.60	0.50
1:A:4:SER:HB3	1:A:7:ARG:CB	2.42	0.50
1:B:308:LEU:HD21	1:B:381:LEU:CD1	2.41	0.50
1:B:346:LYS:O	1:B:348:THR:N	2.45	0.49
1:A:51:ASP:OD1	1:A:53:SER:OG	2.29	0.49
1:A:70:PRO:O	1:A:71:VAL:O	2.30	0.49
1:B:39:ILE:HG13	1:B:63:ASN:HB2	1.94	0.49
1:B:214:GLU:O	1:B:237:LYS:CB	2.60	0.49
1:B:213:PRO:HD2	1:B:214:GLU:N	2.14	0.49
1:A:376:HIS:HE1	3:A:453:HOH:O	1.95	0.49
1:A:14:HIS:HE1	1:B:280:GLU:OE2	1.96	0.49
1:B:72:LEU:HD22	3:B:440:HOH:O	2.12	0.48
1:B:186:THR:O	1:B:190:CR2:C2	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:HIS:CD2	1:A:222:ILE:HG12	2.49	0.48
1:A:396:GLU:OE1	1:B:5:SER:OG	2.28	0.48
1:A:356:GLU:OE1	1:A:359:ARG:CZ	2.62	0.48
1:A:4:SER:HB3	1:A:7:ARG:H	1.77	0.48
1:B:333:ASP:OD1	1:B:335:PRO:HD2	2.13	0.48
1:B:109:LEU:O	1:B:109:LEU:HD22	2.11	0.48
1:A:153:VAL:HG13	1:A:171:ILE:O	2.13	0.48
1:A:204:GLN:CG	3:A:430:HOH:O	2.60	0.48
1:A:201:HIS:CD2	1:A:329:ASN:CB	2.97	0.47
1:A:343:ARG:HH11	1:A:343:ARG:CG	2.28	0.47
1:B:5:SER:O	1:B:6:ARG:CB	2.61	0.47
1:B:144:GLY:HA2	1:B:249:LEU:O	2.14	0.47
1:A:47:HIS:N	1:A:55:GLN:O	2.39	0.47
1:A:395:ARG:HA	3:A:450:HOH:O	2.15	0.47
1:B:3:GLY:O	1:B:4:SER:HB2	2.10	0.47
1:B:202:MET:C	1:B:204:GLN:H	2.23	0.47
1:B:404:GLN:NE2	3:B:446:HOH:O	2.43	0.47
1:A:46:ARG:NH1	3:A:440:HOH:O	2.32	0.47
1:A:50:GLU:HG3	1:A:264:LYS:O	2.15	0.47
1:A:177:LEU:HD22	1:A:181:TRP:CE2	2.50	0.47
1:B:42:ASN:HB2	1:B:59:HIS:O	2.15	0.46
1:B:88:ASP:HB2	3:B:437:HOH:O	2.14	0.46
1:B:361:PHE:HA	1:B:377:VAL:HG21	1.97	0.46
1:A:61:GLN:HG3	1:A:220:ARG:HG3	1.97	0.46
1:A:213:PRO:CD	1:A:214:GLU:N	2.64	0.46
1:B:155:GLY:HA3	1:B:169:LYS:O	2.15	0.46
1:A:70:PRO:HB2	3:A:447:HOH:O	2.15	0.46
1:A:12:THR:HG23	1:B:381:LEU:CD2	2.46	0.46
1:A:61:GLN:OE1	1:A:220:ARG:NE	2.49	0.46
1:A:378:MET:SD	1:A:385:LEU:CD1	2.94	0.46
1:B:70:PRO:O	1:B:71:VAL:O	2.34	0.46
1:B:212:MET:HE1	1:B:243:LEU:HD21	1.97	0.46
1:B:6:ARG:C	1:B:7:ARG:HG2	2.41	0.45
1:B:399:ILE:C	1:B:401:GLY:H	2.23	0.45
1:B:166:LEU:HD11	1:B:168:LEU:HG	1.99	0.45
1:B:274:THR:CG2	1:B:276:GLU:HB3	2.46	0.45
1:B:37:ASN:HD22	1:B:65:PRO:HG3	1.82	0.45
1:A:13:GLY:CA	1:B:414:MET:HE1	2.44	0.45
1:A:33:ASP:O	1:A:34:LYS:C	2.56	0.45
1:A:61:GLN:OE1	1:A:220:ARG:CZ	2.64	0.45
1:A:396:GLU:CD	1:B:5:SER:HB3	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ILE:O	1:B:201:HIS:HE1	1.99	0.45
1:B:404:GLN:CG	3:B:446:HOH:O	2.56	0.45
1:A:58:ASP:HB3	1:A:223:PHE:HB2	1.99	0.45
1:A:316:GLU:O	1:A:320:MET:HG3	2.17	0.45
1:B:270:ARG:HD2	1:B:270:ARG:HA	1.64	0.45
1:A:33:ASP:O	1:A:36:LYS:N	2.33	0.45
1:A:246:ARG:C	1:A:247:ILE:HG13	2.38	0.44
1:B:5:SER:HA	1:B:8:LYS:HZ1	1.82	0.44
1:B:25:LEU:HD23	1:B:25:LEU:HA	1.83	0.44
1:B:321:ILE:HG23	1:B:332:ILE:HG22	1.99	0.44
1:A:25:LEU:HD23	1:A:25:LEU:HA	1.65	0.44
1:B:274:THR:HG22	1:B:277:GLN:CG	2.37	0.44
1:A:229:ASN:OD1	1:A:229:ASN:C	2.60	0.44
1:A:274:THR:H	1:A:277:GLN:NE2	2.15	0.44
1:B:185:VAL:O	1:B:190:CR2:N1	2.51	0.44
1:A:221:THR:HG23	1:A:231:LYS:HG2	2.00	0.44
1:B:51:ASP:C	1:B:51:ASP:OD1	2.61	0.44
1:A:33:ASP:O	1:A:35:GLN:N	2.51	0.44
1:A:84:VAL:HG12	3:A:451:HOH:O	2.18	0.44
1:A:30:ILE:CD1	1:A:79:LEU:HG	2.48	0.44
1:A:49:VAL:HG12	1:A:50:GLU:N	2.32	0.44
1:B:245:ASN:ND2	1:B:247:ILE:HD11	2.33	0.43
1:A:397:ALA:HB2	1:A:413:MET:HG2	2.00	0.43
1:B:6:ARG:C	1:B:7:ARG:HG3	2.40	0.43
1:B:138:ILE:CD1	1:B:195:PHE:CE2	2.96	0.43
1:B:265:LEU:HD12	1:B:265:LEU:HA	1.84	0.43
1:A:42:ASN:HB3	1:A:60:TYR:CE2	2.53	0.43
1:B:153:VAL:HG13	1:B:171:ILE:O	2.19	0.43
1:A:255:LYS:C	1:A:257:ASP:H	2.26	0.43
1:B:142:LEU:C	1:B:142:LEU:HD23	2.44	0.43
1:A:73:LEU:HD12	1:A:73:LEU:HA	1.59	0.43
1:B:192:LEU:HD21	1:B:245:ASN:HB2	2.01	0.43
1:A:244:VAL:HG11	1:A:246:ARG:HG3	2.00	0.43
1:A:155:GLY:HA3	1:A:169:LYS:O	2.19	0.43
1:A:340:MET:HE2	1:A:340:MET:HB3	1.97	0.43
1:A:356:GLU:CD	1:A:359:ARG:NH1	2.77	0.43
1:B:326:ALA:HA	3:B:450:HOH:O	2.19	0.43
1:A:105:ALA:CB	1:A:327:ASP:HB3	2.49	0.43
1:A:188:LEU:O	1:A:190:CR2:HA31	2.19	0.42
1:A:204:GLN:HE21	1:A:204:GLN:HB2	1.64	0.42
1:A:325:ASP:OD1	1:A:330:GLY:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:THR:HA	1:B:230:TYR:O	2.19	0.42
1:A:302:GLY:O	1:A:303:THR:C	2.62	0.42
1:B:36:LYS:O	1:B:37:ASN:C	2.63	0.42
1:A:201:HIS:NE2	1:A:329:ASN:HB3	2.35	0.42
1:B:72:LEU:HD12	1:B:72:LEU:HA	1.82	0.42
1:B:91:GLU:HG2	1:B:169:LYS:HZ3	1.84	0.42
1:B:96:MET:HE3	1:B:98:LEU:HB2	2.01	0.42
1:B:220:ARG:HB2	1:B:232:THR:OG1	2.19	0.42
1:A:192:LEU:HB3	1:A:195:PHE:HD2	1.83	0.42
1:A:217:VAL:HA	1:A:234:ALA:O	2.18	0.42
1:B:305:MET:SD	1:B:320:MET:HE1	2.60	0.42
1:A:64:THR:O	1:A:216:TYR:HA	2.20	0.42
1:B:63:ASN:HA	1:B:217:VAL:O	2.20	0.42
1:B:366:ASN:OD1	1:B:366:ASN:C	2.62	0.42
1:A:14:HIS:HD2	1:A:17:ARG:HH21	1.68	0.42
1:A:101:PHE:CE1	1:A:165:LYS:HD2	2.54	0.42
1:B:207:PHE:CD2	1:B:207:PHE:C	2.97	0.42
1:A:51:ASP:OD1	1:A:51:ASP:C	2.58	0.42
1:A:280:GLU:HB3	1:B:14:HIS:CE1	2.55	0.42
1:A:327:ASP:O	1:A:328:GLY:C	2.62	0.42
1:A:361:PHE:HZ	1:B:12:THR:HG22	1.83	0.42
1:B:356:GLU:OE1	1:B:359:ARG:CZ	2.67	0.42
1:B:274:THR:CG2	1:B:277:GLN:HG3	2.39	0.42
1:A:14:HIS:CD2	1:A:17:ARG:HH21	2.37	0.42
1:A:221:THR:OG1	1:A:231:LYS:CE	2.65	0.42
1:B:325:ASP:OD1	1:B:330:GLY:N	2.47	0.42
1:A:12:THR:HG22	1:B:361:PHE:CZ	2.55	0.41
1:A:43:PHE:O	1:A:59:HIS:HB2	2.20	0.41
1:A:201:HIS:CD2	1:A:329:ASN:HB2	2.55	0.41
1:A:202:MET:C	1:A:204:GLN:H	2.29	0.41
1:B:255:LYS:C	1:B:257:ASP:H	2.28	0.41
1:B:274:THR:H	1:B:277:GLN:NE2	2.18	0.41
1:B:374:LEU:HD21	1:B:393:MET:HE2	2.02	0.41
1:A:142:LEU:C	1:A:142:LEU:CD2	2.89	0.41
1:A:180:PRO:HB3	3:A:428:HOH:O	2.20	0.41
1:A:272:GLN:OE1	1:A:272:GLN:HA	2.20	0.41
1:B:50:GLU:C	1:B:52:GLY:N	2.77	0.41
1:B:340:MET:HE2	1:B:340:MET:HB3	1.95	0.41
1:A:33:ASP:HB3	1:A:38:GLY:C	2.44	0.41
1:B:55:GLN:NE2	1:B:224:PHE:HB3	2.36	0.41
1:B:204:GLN:HE21	1:B:204:GLN:HB2	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:HD22	1:A:210:SER:HB3	2.02	0.41
1:A:303:THR:N	1:A:306:ARG:HH11	2.18	0.41
1:A:386:THR:HG23	1:A:389:GLU:OE1	2.21	0.41
1:A:61:GLN:HG3	1:A:220:ARG:HG2	2.03	0.41
1:A:206:ASP:OD2	1:A:209:LYS:HD2	2.21	0.41
1:A:246:ARG:HH11	1:A:246:ARG:HG2	1.86	0.41
1:B:72:LEU:HD23	3:B:440:HOH:O	2.21	0.41
1:B:416:ALA:HA	1:B:417:LYS:NZ	2.36	0.41
1:A:64:THR:O	1:A:217:VAL:N	2.49	0.41
1:B:81:PHE:CE2	1:B:102:VAL:HG22	2.56	0.41
1:A:81:PHE:CE2	1:A:102:VAL:HG22	2.56	0.40
1:B:313:THR:H	1:B:316:GLU:HG3	1.86	0.40
1:A:274:THR:CG2	1:A:277:GLN:H	2.33	0.40
1:A:363:LYS:HD2	3:A:452:HOH:O	2.21	0.40
1:B:346:LYS:O	1:B:349:ASP:N	2.42	0.40
1:A:180:PRO:HD3	1:A:260:ILE:O	2.21	0.40
1:A:192:LEU:CD2	1:A:243:LEU:HD12	2.50	0.40
1:A:212:MET:CE	1:A:243:LEU:HD21	2.51	0.40
1:B:80:SER:O	1:B:102:VAL:HA	2.21	0.40
1:B:342:ALA:O	1:B:343:ARG:C	2.64	0.40
1:B:250:LYS:HG2	3:B:435:HOH:O	2.21	0.40
1:B:269:THR:HB	1:B:271:ASP:OD1	2.22	0.40
1:B:274:THR:HG23	1:B:277:GLN:H	1.86	0.40
1:B:276:GLU:CG	1:B:417:LYS:HE3	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:ASN:OD1	1:B:50:GLU:OE1[1_455]	2.15	0.05

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	396/415 (95%)	364 (92%)	23 (6%)	9 (2%)	5	9
1	B	394/415 (95%)	357 (91%)	28 (7%)	9 (2%)	5	9
All	All	790/830 (95%)	721 (91%)	51 (6%)	18 (2%)	5	9

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	VAL
1	A	124	THR
1	A	213	PRO
1	B	4	SER
1	B	6	ARG
1	B	71	VAL
1	B	109	LEU
1	B	213	PRO
1	A	347	ASP
1	A	53	SER
1	A	128	GLY
1	A	133	THR
1	B	35	GLN
1	B	347	ASP
1	A	34	LYS
1	B	36	LYS
1	A	123	GLY
1	B	69	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	339/351 (97%)	290 (86%)	49 (14%)	3	6
1	B	342/351 (97%)	287 (84%)	55 (16%)	2	4
All	All	681/702 (97%)	577 (85%)	104 (15%)	3	5

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

Mol	Chain	Res	Type
1	A	5	SER
1	A	11	LYS
1	A	19	ILE
1	A	21	ARG
1	A	30	ILE
1	A	34	LYS
1	A	36	LYS
1	A	39	ILE
1	A	40	LYS
1	A	42	ASN
1	A	53	SER
1	A	56	LEU
1	A	62	GLN
1	A	64	THR
1	A	72	LEU
1	A	73	LEU
1	A	92	LYS
1	A	127	LYS
1	A	129	GLU
1	A	133	THR
1	A	141	GLU
1	A	162	THR
1	A	166	LEU
1	A	176	LYS
1	A	197	ARG
1	A	203	LYS
1	A	204	GLN
1	A	214	GLU
1	A	229	ASN
1	A	231	LYS
1	A	247	ILE
1	A	255	LYS
1	A	259	ASN
1	A	264	LYS
1	A	265	LEU
1	A	269	THR
1	A	270	ARG
1	A	272	GLN
1	A	282	LYS
1	A	307	SER
1	A	314	GLU
1	A	332	ILE

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Mol	Chain	Res	Type
1	A	338	LEU
1	A	343	ARG
1	A	347	ASP
1	A	356	GLU
1	A	381	LEU
1	A	383	GLU
1	A	392	GLU
1	B	5	SER
1	B	7	ARG
1	B	8	LYS
1	B	19	ILE
1	B	30	ILE
1	B	34	LYS
1	B	35	GLN
1	B	39	ILE
1	B	42	ASN
1	B	44	LYS
1	B	48	ASN
1	B	54	VAL
1	B	56	LEU
1	B	62	GLN
1	B	64	THR
1	B	71	VAL
1	B	72	LEU
1	B	73	LEU
1	B	92	LYS
1	B	109	LEU
1	B	129	GLU
1	B	154	SER
1	B	156	GLU
1	B	162	THR
1	B	176	LYS
1	B	197	ARG
1	B	203	LYS
1	B	204	GLN
1	B	214	GLU
1	B	229	ASN
1	B	255	LYS
1	B	259	ASN
1	B	265	LEU
1	B	269	THR
1	B	270	ARG

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Mol	Chain	Res	Type
1	B	272	GLN
1	B	273	LEU
1	B	282	LYS
1	B	307	SER
1	B	311	ASN
1	B	313	THR
1	B	314	GLU
1	B	322	ASN
1	B	332	ILE
1	B	338	LEU
1	B	343	ARG
1	B	347	ASP
1	B	356	GLU
1	B	363	LYS
1	B	376	HIS
1	B	381	LEU
1	B	383	GLU
1	B	392	GLU
1	B	415	THR
1	B	417	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	27	ASN
1	A	47	HIS
1	A	48	ASN
1	A	82	GLN
1	A	90	ASN
1	A	201	HIS
1	A	204	GLN
1	A	259	ASN
1	A	277	GLN
1	A	310	GLN
1	A	318	GLN
1	A	376	HIS
1	A	412	GLN
1	B	14	HIS
1	B	35	GLN
1	B	37	ASN
1	B	42	ASN

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Mol	Chain	Res	Type
1	B	47	HIS
1	B	48	ASN
1	B	55	GLN
1	B	82	GLN
1	B	90	ASN
1	B	201	HIS
1	B	204	GLN
1	B	259	ASN
1	B	268	ASN
1	B	272	GLN
1	B	277	GLN
1	B	412	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](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CR2	A	190	1	20,20,21	3.31	6 (30%)	25,27,29	2.64	7 (28%)
1	CR2	B	190	1	20,20,21	3.21	4 (20%)	25,27,29	3.40	6 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CR2	A	190	1	-	1/6/25/26	0/2/2/2
1	CR2	B	190	1	-	1/6/25/26	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	CR2	CB2-CA2	12.60	1.47	1.35
1	B	190	CR2	CB2-CA2	12.41	1.47	1.35
1	B	190	CR2	C1-N2	4.00	1.39	1.32
1	B	190	CR2	C2-N3	-3.81	1.31	1.40
1	A	190	CR2	CA2-C2	-3.78	1.44	1.48
1	B	190	CR2	CA2-C2	-3.65	1.44	1.48
1	A	190	CR2	C2-N3	-3.59	1.31	1.40
1	A	190	CR2	O2-C2	3.44	1.30	1.23
1	A	190	CR2	C1-N2	3.18	1.38	1.32
1	A	190	CR2	CA1-C1	2.48	1.52	1.49

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	190	CR2	O2-C2-CA2	-9.55	124.93	131.02
1	B	190	CR2	CA2-C2-N3	9.21	111.23	103.50
1	A	190	CR2	O2-C2-CA2	-8.64	125.51	131.02
1	B	190	CR2	C2-N3-C1	-8.16	104.41	108.08
1	A	190	CR2	CG2-CB2-CA2	-5.39	123.46	129.87
1	A	190	CR2	CA2-C2-N3	5.30	107.95	103.50
1	B	190	CR2	C2-CA2-N2	-3.50	106.44	108.95
1	B	190	CR2	CB2-CA2-C2	3.27	126.33	122.36
1	A	190	CR2	C1-CA1-N1	-3.00	106.22	112.85
1	A	190	CR2	CB2-CA2-C2	2.86	125.82	122.36
1	A	190	CR2	CD2-CG2-CD1	2.28	121.04	117.65
1	A	190	CR2	CE1-CD1-CG2	-2.23	118.34	121.22
1	B	190	CR2	CD2-CG2-CD1	2.14	120.82	117.65

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	190	CR2	C3-CA3-N3-C2
1	B	190	CR2	C3-CA3-N3-C2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	190	CR2	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	190	CR2	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	188:LEU	C	190:CR2	N1	1.20

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	402/415 (96%)	0.18	6 (1%) 72 68	2, 19, 35, 51	0
1	B	400/415 (96%)	0.27	16 (4%) 42 37	6, 24, 43, 55	0
All	All	802/830 (96%)	0.23	22 (2%) 56 50	2, 22, 40, 55	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	SER	5.8
1	B	3	GLY	4.0
1	A	387	ASP	3.7
1	B	5	SER	3.5
1	B	73	LEU	3.3
1	A	399	ILE	3.0
1	B	72	LEU	2.8
1	B	8	LYS	2.8
1	B	26	GLU	2.4
1	B	34	LYS	2.4
1	B	139	LEU	2.4
1	A	388	GLU	2.4
1	A	270	ARG	2.3
1	B	213	PRO	2.2
1	A	367	GLY	2.2
1	B	210	SER	2.2
1	B	111	MET	2.1
1	B	71	VAL	2.1
1	A	70	PRO	2.1
1	B	6	ARG	2.0
1	B	69	GLY	2.0
1	B	25	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CR2	B	190	19/20	0.89	0.14	19,28,32,32	0
1	CR2	A	190	19/20	0.91	0.09	2,2,2,5	0

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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	A	502	1/1	0.87	0.07	47,47,47,47	0
2	CA	A	504	1/1	0.89	0.04	39,39,39,39	0
2	CA	A	503	1/1	0.91	0.09	32,32,32,32	0
2	CA	B	504	1/1	0.93	0.06	30,30,30,30	0
2	CA	B	502	1/1	0.94	0.04	18,18,18,18	0
2	CA	A	501	1/1	0.95	0.04	20,20,20,20	0
2	CA	B	501	1/1	0.98	0.05	18,18,18,18	0
2	CA	B	503	1/1	0.99	0.02	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.