WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2020 – 04:04 PM BST

PDB ID	:	6EU9
Title	:	Crystal structure of Platynereis dumerilii RAR ligand-binding domain in complex with all-trans retinoic acid
Authors	:	Handberg-Thorsager, M.; Gutierrez-Mazariegos, J.; Arold, S.T.; Nadendla, E.K.; Bertucci, P.Y.; Germain, P.; Tomancak, P.; Pierzchalski, K.; Jones, J.W.; Albalat, R.; Kane, M.A.; Bourguet, W.; Laudet, V.; Arendt, D.; Schubert, M.
Deposited on	:	2017-10-29
Resolution	:	2.69 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 (i) symbol.

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

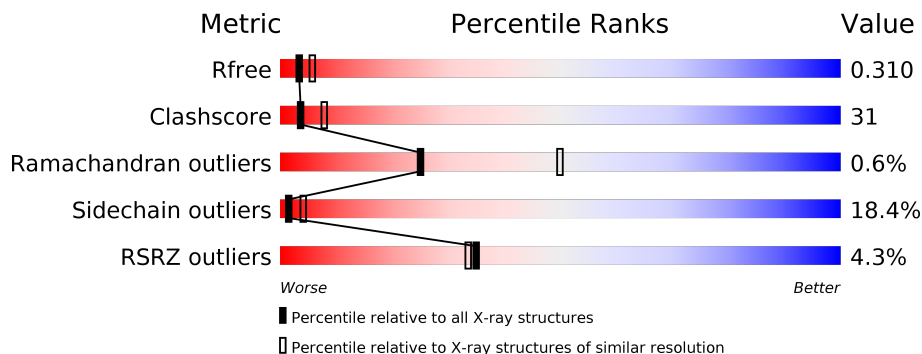|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	Percentile Ranks	Value
Rfree		0.310
Clashscore		31
Ramachandran outliers		0.6%
Sidechain outliers		18.4%
RSRZ outliers		4.3%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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 <=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	241	5% 44% 38% 10% • 6%
1	B	241	2% 52% 35% 7% 6%
1	C	241	3% 48% 33% 9% 10%
1	D	241	6% 35% 46% 12% • 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7157 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 Retinoic acid receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1780	1131	295	346	8			
1	B	227	Total	C	N	O	S	0	0	0
			1786	1137	293	349	7			
1	C	217	Total	C	N	O	S	0	0	0
			1705	1083	283	333	6			
1	D	227	Total	C	N	O	S	0	0	0
			1796	1143	296	349	8			

- Molecule 2 is RETINOIC ACID (three-letter code: REA) (formula: $C_{20}H_{28}O_2$).
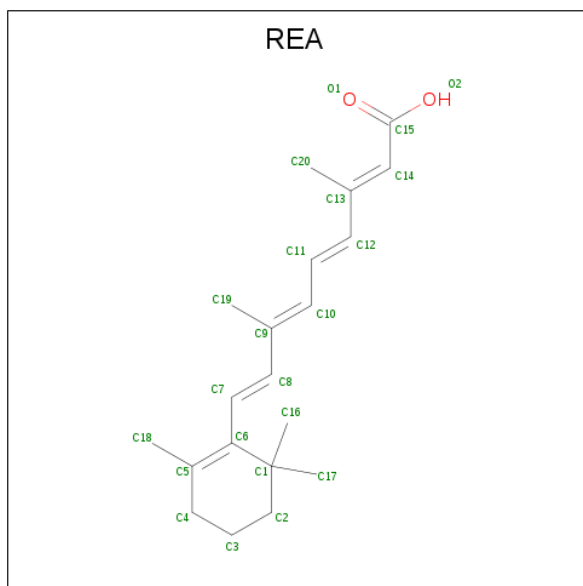
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			22	20	2		
2	D	1	Total	C	O	0	0
			22	20	2		

• Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total 12	O 12	0	0
3	B	14	Total 14	O 14	0	0
3	C	12	Total 12	O 12	0	0
3	D	8	Total 8	O 8	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
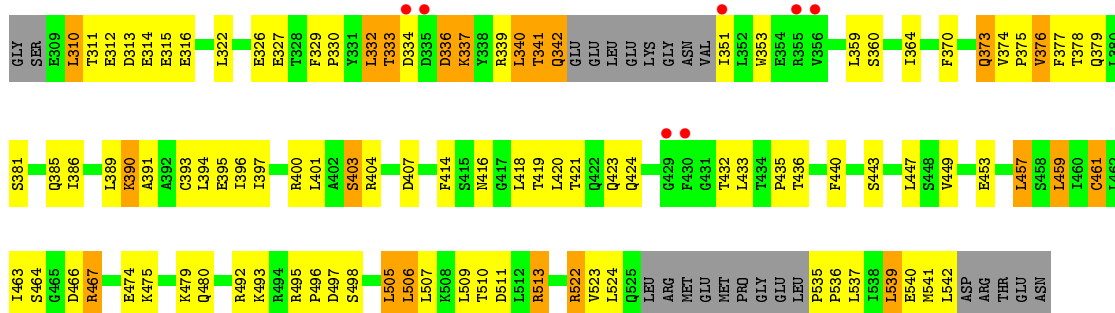
- Molecule 1: Retinoic acid receptor
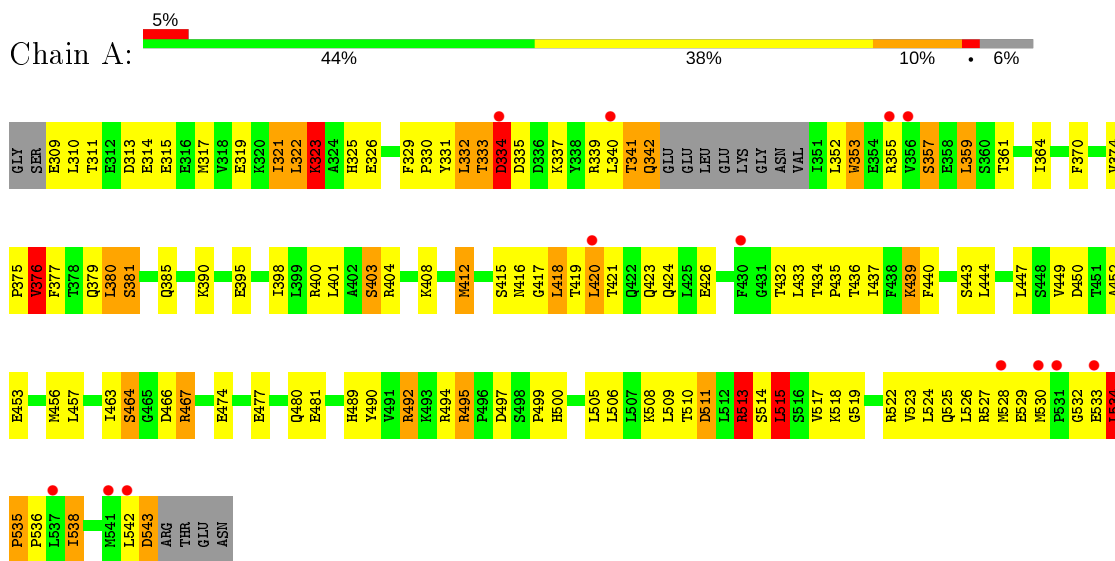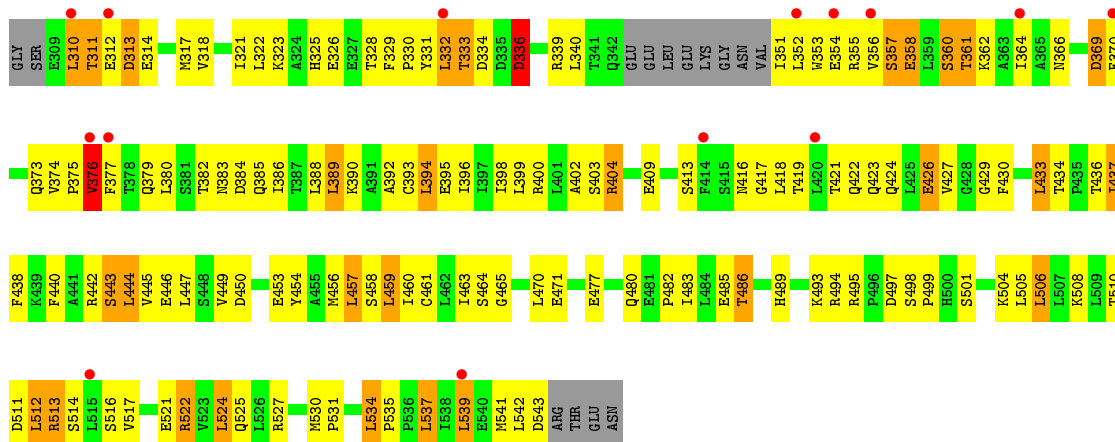

- Molecule 1: Retinoic acid receptor

- Molecule 1: Retinoic acid receptor

• Molecule 1: Retinoic acid receptor

Chain D:
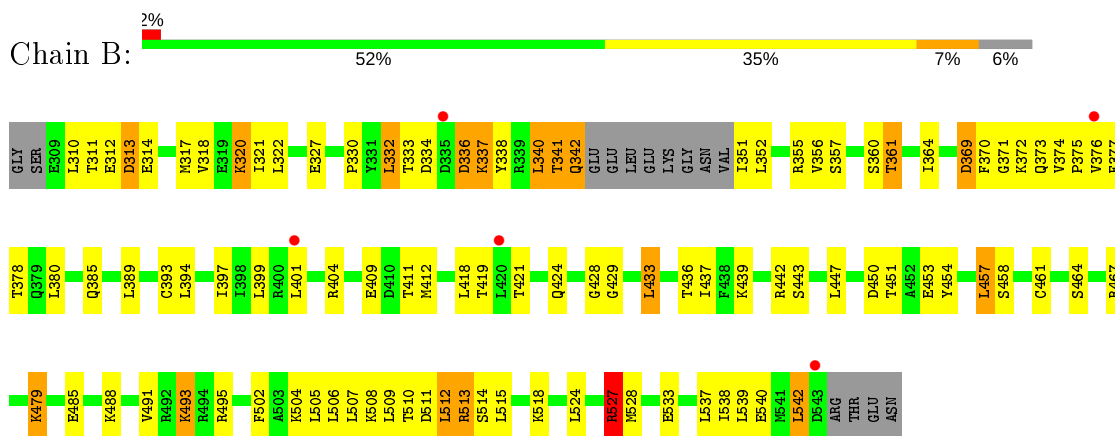
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	187.41Å 68.15Å 95.08Å 90.00° 100.75° 90.00°	Depositor
Resolution (Å)	50.00 – 2.69 54.42 – 2.69	Depositor EDS
% Data completeness (in resolution range)	98.6 (50.00-2.69) 98.6 (54.42-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.255 , 0.300 0.263 , 0.310	Depositor DCC
R_{free} test set	1634 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	70.6	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 57.5	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7157	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: REA

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	1.00	2/1807 (0.1%)	1.20	12/2445 (0.5%)
1	B	0.92	1/1813 (0.1%)	1.12	10/2456 (0.4%)
1	C	0.95	0/1729	1.11	6/2340 (0.3%)
1	D	0.91	0/1823	1.13	10/2467 (0.4%)
All	All	0.95	3/7172 (0.0%)	1.14	38/9708 (0.4%)

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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	464	SER	CB-OG	-7.71	1.32	1.42
1	A	439	LYS	CG-CD	7.45	1.77	1.52
1	B	502	PHE	CG-CD1	5.13	1.46	1.38

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	534	LEU	C-N-CD	-11.62	95.03	120.60
1	A	511	ASP	CB-CG-OD2	-9.21	110.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	515	LEU	CB-CG-CD1	-8.40	96.72	111.00
1	C	457	LEU	CA-CB-CG	8.28	134.34	115.30
1	D	404	ARG	NE-CZ-NH2	8.07	124.33	120.30
1	D	534	LEU	CB-CG-CD1	-7.83	97.69	111.00
1	D	506	LEU	CB-CG-CD1	-7.61	98.07	111.00
1	D	336	ASP	CB-CG-OD2	7.20	124.78	118.30
1	B	467	ARG	NE-CZ-NH2	6.73	123.66	120.30
1	D	512	LEU	CB-CG-CD2	-6.54	99.88	111.00
1	C	457	LEU	CB-CG-CD2	-6.44	100.05	111.00
1	B	369	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	D	537	LEU	CB-CG-CD1	-5.96	100.86	111.00
1	A	467	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	B	513	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	B	442	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	D	426	GLU	OE1-CD-OE2	-5.81	116.33	123.30
1	B	450	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	B	515	LEU	CB-CG-CD2	-5.72	101.28	111.00
1	D	313	ASP	CB-CG-OD2	5.54	123.28	118.30
1	C	461	CYS	CA-CB-SG	-5.51	104.07	114.00
1	A	323	LYS	CD-CE-NZ	5.49	124.34	111.70
1	A	420	LEU	CB-CG-CD2	5.48	120.32	111.00
1	A	313	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	C	334	ASP	N-CA-C	-5.46	96.25	111.00
1	A	513	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	B	369	ASP	CB-CG-OD1	5.33	123.10	118.30
1	C	524	LEU	CB-CG-CD1	5.32	120.04	111.00
1	A	492	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	C	492	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	513	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	D	495	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	A	359	LEU	CB-CG-CD1	-5.10	102.33	111.00
1	D	336	ASP	CB-CG-OD1	-5.09	113.72	118.30
1	A	447	LEU	CA-CB-CG	5.07	126.97	115.30
1	B	332	LEU	CA-CB-CG	5.06	126.94	115.30
1	A	543	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	527	ARG	CG-CD-NE	5.01	122.32	111.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	334	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	B	334	ASP	Peptide
1	C	333	THR	Peptide
1	D	334	ASP	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	1780	0	1781	123	0
1	B	1786	0	1793	93	0
1	C	1705	0	1714	76	0
1	D	1796	0	1813	172	0
2	B	22	0	27	5	0
2	D	22	0	27	1	0
3	A	12	0	0	0	0
3	B	14	0	0	1	0
3	C	12	0	0	1	0
3	D	8	0	0	0	0
All	All	7157	0	7155	449	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 31.

All (449) 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:439:LYS:CG	1:A:439:LYS:CD	1.77	1.59
1:C:375:PRO:O	1:C:376:VAL:HG23	1.28	1.26
1:D:326:GLU:CG	1:D:331:TYR:CE2	2.19	1.25
1:C:375:PRO:HA	1:C:378:THR:OG1	1.38	1.23
1:D:326:GLU:HG2	1:D:331:TYR:CE2	1.72	1.22
1:B:443:SER:O	1:B:447:LEU:CD1	1.91	1.19
1:A:453:GLU:OE1	1:A:495:ARG:NH1	1.77	1.18
1:C:310:LEU:CD2	1:C:314:GLU:OE1	1.92	1.18
1:D:444:LEU:HD23	1:D:454:TYR:OH	1.46	1.14
1:D:443:SER:O	1:D:447:LEU:CD1	1.95	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LEU:HD13	1:A:492:ARG:NH2	1.61	1.13
1:D:326:GLU:CG	1:D:331:TYR:HE2	1.60	1.11
1:D:333:THR:HA	1:D:336:ASP:HA	1.30	1.11
1:A:418:LEU:HD11	1:A:420:LEU:HD21	1.32	1.11
1:D:326:GLU:CD	1:D:331:TYR:OH	1.90	1.09
1:D:383:ASN:HA	1:D:386:ILE:HD13	1.15	1.09
1:B:333:THR:OG1	1:B:336:ASP:OD1	1.70	1.09
1:A:370:PHE:O	1:A:374:VAL:HG23	1.51	1.08
1:D:311:THR:HB	1:D:314:GLU:HG3	1.35	1.08
1:A:330:PRO:O	1:A:404:ARG:NH2	1.86	1.08
1:D:385:GLN:O	1:D:389:LEU:HD12	1.52	1.08
1:D:421:THR:OG1	1:D:424:GLN:HG3	1.51	1.07
1:D:422:GLN:HB2	1:D:438:PHE:CE2	1.88	1.07
1:D:314:GLU:OE1	1:D:489:HIS:ND1	1.87	1.07
1:D:522:ARG:NH1	1:D:525:GLN:OE1	1.89	1.06
1:D:326:GLU:HG2	1:D:331:TYR:HE2	0.92	1.05
1:D:383:ASN:CA	1:D:386:ILE:HD13	1.86	1.04
1:D:333:THR:CA	1:D:336:ASP:HA	1.88	1.02
1:A:370:PHE:O	1:A:374:VAL:CG2	2.08	1.02
1:A:416:ASN:OD1	1:A:418:LEU:N	1.92	1.02
1:A:463:ILE:O	1:A:480:GLN:HG3	1.58	1.02
1:A:421:THR:OG1	1:A:424:GLN:HG3	1.57	1.02
1:D:339:ARG:NH1	1:D:409:GLU:OE1	1.93	1.02
1:A:440:PHE:O	1:A:443:SER:OG	1.77	1.00
1:D:386:ILE:H	1:D:386:ILE:HD12	1.27	1.00
1:A:310:LEU:CD1	1:A:492:ARG:HH22	1.74	1.00
1:A:342:GLN:HA	1:A:342:GLN:HE21	1.25	0.99
1:D:326:GLU:CG	1:D:331:TYR:CZ	2.46	0.98
1:D:310:LEU:HD12	1:D:314:GLU:HB2	1.43	0.98
1:D:326:GLU:OE2	1:D:331:TYR:CZ	2.17	0.97
1:C:310:LEU:HD21	1:C:314:GLU:OE1	1.64	0.97
1:C:416:ASN:OD1	1:C:418:LEU:N	1.97	0.97
1:C:359:LEU:HD11	1:C:416:ASN:HD22	1.30	0.96
1:D:443:SER:O	1:D:447:LEU:HD13	1.65	0.96
1:C:310:LEU:HD22	1:C:314:GLU:OE1	1.66	0.94
1:D:326:GLU:HG3	1:D:331:TYR:CZ	2.03	0.94
1:B:311:THR:HG22	1:B:313:ASP:H	1.33	0.93
1:A:310:LEU:HD13	1:A:492:ARG:HH22	0.79	0.93
1:B:443:SER:O	1:B:447:LEU:HD12	1.67	0.92
1:B:333:THR:HA	1:B:336:ASP:HA	1.52	0.92
1:D:326:GLU:OE2	1:D:331:TYR:CE2	2.21	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:LEU:HD13	1:D:437:ILE:HD11	1.49	0.91
1:D:364:ILE:HG12	1:D:393:CYS:SG	2.10	0.91
1:D:383:ASN:HA	1:D:386:ILE:CD1	1.99	0.90
1:D:329:PHE:CZ	1:D:404:ARG:NH1	2.39	0.90
1:C:375:PRO:O	1:C:376:VAL:CG2	2.19	0.89
1:D:333:THR:HA	1:D:336:ASP:CA	1.98	0.89
1:D:310:LEU:HD12	1:D:314:GLU:CB	2.02	0.89
1:D:356:VAL:O	1:D:360:SER:OG	1.90	0.88
1:D:443:SER:O	1:D:447:LEU:HD12	1.71	0.88
1:B:453:GLU:OE1	1:B:495:ARG:NH2	2.05	0.88
1:A:310:LEU:HB3	1:A:314:GLU:OE1	1.74	0.87
1:A:418:LEU:HD11	1:A:420:LEU:CD2	2.04	0.87
1:C:359:LEU:HD11	1:C:416:ASN:ND2	1.89	0.87
1:D:444:LEU:HD23	1:D:454:TYR:CZ	2.10	0.87
1:D:326:GLU:CD	1:D:331:TYR:CZ	2.48	0.86
1:D:357:SER:O	1:D:361:THR:OG1	1.93	0.86
1:D:353:TRP:CH2	1:D:527:ARG:HD3	2.10	0.86
1:B:507:LEU:HD21	1:C:506:LEU:HD13	1.58	0.85
1:A:464:SER:OG	1:A:466:ASP:OD1	1.95	0.84
1:D:444:LEU:HD21	1:D:454:TYR:HE1	1.42	0.84
1:A:337:LYS:CB	1:A:419:THR:OG1	2.25	0.84
1:C:375:PRO:CA	1:C:378:THR:OG1	2.24	0.83
1:A:530:MET:HE2	1:A:533:GLU:HA	1.60	0.83
1:D:326:GLU:CG	1:D:331:TYR:OH	2.26	0.83
1:D:421:THR:HG1	1:D:424:GLN:HG3	1.44	0.83
1:B:443:SER:O	1:B:447:LEU:HD13	1.77	0.82
1:B:540:GLU:OE1	1:B:540:GLU:N	2.11	0.82
1:A:527:ARG:O	1:A:530:MET:CB	2.27	0.82
1:D:329:PHE:CE1	1:D:404:ARG:NH1	2.48	0.82
1:C:330:PRO:O	1:C:404:ARG:NH2	2.12	0.81
1:D:444:LEU:HD21	1:D:454:TYR:CE1	2.15	0.81
1:A:530:MET:CE	1:A:533:GLU:HA	2.09	0.81
1:D:383:ASN:CA	1:D:386:ILE:CD1	2.57	0.81
1:A:535:PRO:CB	1:A:536:PRO:HD3	2.10	0.81
1:D:444:LEU:CD2	1:D:454:TYR:CE1	2.63	0.81
1:B:453:GLU:CD	1:B:495:ARG:HH22	1.84	0.80
1:D:376:VAL:O	1:D:379:GLN:HB3	1.82	0.80
1:D:430:PHE:HB2	1:D:434:THR:OG1	1.81	0.80
1:A:467:ARG:HH12	1:A:513:ARG:NE	1.78	0.80
1:D:330:PRO:O	1:D:404:ARG:NH2	2.13	0.80
1:D:326:GLU:HG3	1:D:331:TYR:CE2	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:GLN:NE2	1:B:342:GLN:HA	1.97	0.79
1:A:359:LEU:HD11	1:A:416:ASN:ND2	1.96	0.79
1:D:422:GLN:O	1:D:426:GLU:CG	2.16	0.78
1:A:510:THR:HG1	1:D:510:THR:HG1	1.24	0.78
1:A:421:THR:OG1	1:A:424:GLN:CG	2.31	0.78
1:A:398:ILE:HG21	1:A:515:LEU:HD23	1.66	0.78
1:D:539:LEU:H	1:D:539:LEU:HD23	1.49	0.78
1:A:333:THR:HG23	1:A:334:ASP:OD2	1.84	0.77
1:B:443:SER:OG	1:B:508:LYS:NZ	2.18	0.77
1:D:326:GLU:CD	1:D:331:TYR:CE2	2.57	0.77
1:C:364:ILE:HG23	1:C:393:CYS:SG	2.25	0.77
1:A:453:GLU:CD	1:A:495:ARG:HH12	1.88	0.77
1:D:422:GLN:O	1:D:426:GLU:HG3	1.84	0.76
1:A:528:MET:HG3	1:A:529:GLU:OE1	1.84	0.76
1:D:326:GLU:HG3	1:D:331:TYR:OH	1.85	0.76
1:A:527:ARG:O	1:A:530:MET:HB3	1.86	0.75
1:D:333:THR:C	1:D:336:ASP:CA	2.49	0.75
1:A:408:LYS:O	1:B:375:PRO:HA	1.87	0.75
1:D:311:THR:HB	1:D:314:GLU:CG	2.15	0.75
1:A:398:ILE:HG21	1:A:515:LEU:CD2	2.17	0.74
1:D:416:ASN:OD1	1:D:418:LEU:N	2.13	0.74
1:B:421:THR:OG1	1:B:424:GLN:HG3	1.88	0.73
1:B:342:GLN:HE21	1:B:342:GLN:HA	1.51	0.73
1:D:444:LEU:CD2	1:D:454:TYR:HE1	2.01	0.73
1:A:395:GLU:OE1	1:A:467:ARG:NH2	2.19	0.73
1:B:374:VAL:CG1	1:B:375:PRO:HD2	2.18	0.73
1:D:333:THR:C	1:D:336:ASP:HA	2.08	0.72
1:B:338:TYR:CE1	1:B:418:LEU:HD12	2.25	0.72
1:A:317:MET:O	1:A:321:ILE:HG12	1.90	0.72
1:A:416:ASN:OD1	1:A:417:GLY:N	2.22	0.72
1:D:374:VAL:HG13	1:D:375:PRO:HD2	1.71	0.71
1:A:527:ARG:O	1:A:530:MET:HB2	1.88	0.71
1:D:430:PHE:CB	1:D:434:THR:OG1	2.38	0.71
1:D:422:GLN:OE1	1:D:438:PHE:CD2	2.44	0.71
1:D:386:ILE:N	1:D:386:ILE:HD12	2.04	0.71
1:D:377:PHE:HZ	1:D:389:LEU:HD11	1.54	0.71
1:A:376:VAL:HA	1:A:379:GLN:HG3	1.71	0.71
1:A:514:SER:OG	1:D:513:ARG:HD2	1.91	0.71
1:A:453:GLU:OE1	1:A:494:ARG:NH1	2.25	0.70
1:A:535:PRO:HB3	1:A:536:PRO:HD3	1.73	0.70
1:A:535:PRO:HB2	1:A:536:PRO:CD	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:PRO:CB	1:A:536:PRO:CD	2.70	0.70
1:D:422:GLN:HB2	1:D:438:PHE:CZ	2.27	0.70
1:D:421:THR:OG1	1:D:424:GLN:CG	2.35	0.69
1:A:309:GLU:O	1:A:314:GLU:OE1	2.11	0.69
1:A:342:GLN:HA	1:A:342:GLN:NE2	2.03	0.69
1:A:467:ARG:NH1	1:A:513:ARG:CZ	2.55	0.69
1:B:374:VAL:HG13	1:B:375:PRO:HD2	1.72	0.69
1:D:311:THR:CB	1:D:314:GLU:HG3	2.19	0.68
1:D:392:ALA:O	1:D:396:ILE:HD12	1.94	0.68
1:A:529:GLU:N	1:A:529:GLU:OE1	2.28	0.67
1:A:423:GLN:HA	1:A:426:GLU:HG3	1.76	0.67
1:D:326:GLU:OE2	1:D:331:TYR:OH	2.10	0.67
1:B:337:LYS:HB3	1:B:419:THR:OG1	1.94	0.67
1:B:380:LEU:O	1:B:385:GLN:NE2	2.28	0.67
1:D:539:LEU:N	1:D:539:LEU:HD23	2.10	0.66
1:D:392:ALA:O	1:D:396:ILE:CD1	2.44	0.66
1:A:418:LEU:CD1	1:A:420:LEU:HD21	2.20	0.66
1:A:499:PRO:HG2	1:D:485:GLU:OE2	1.96	0.66
1:B:527:ARG:HG3	1:B:527:ARG:HH11	1.61	0.66
1:D:429:GLY:O	1:D:522:ARG:NE	2.27	0.65
1:D:459:LEU:HD13	1:D:483:ILE:HD13	1.77	0.65
1:C:311:THR:HG22	1:C:313:ASP:H	1.62	0.65
1:B:389:LEU:O	1:B:393:CYS:HB2	1.97	0.65
1:D:394:LEU:O	1:D:398:ILE:HG13	1.95	0.65
1:C:453:GLU:O	1:C:457:LEU:HB2	1.96	0.65
1:D:353:TRP:O	1:D:357:SER:OG	2.13	0.65
1:A:419:THR:O	1:A:420:LEU:HD23	1.97	0.65
1:D:311:THR:HG22	1:D:313:ASP:H	1.62	0.64
1:A:418:LEU:CD1	1:A:420:LEU:CD2	2.75	0.64
1:D:421:THR:OG1	1:D:424:GLN:N	2.23	0.64
1:B:447:LEU:HD12	1:B:447:LEU:N	2.13	0.64
1:A:364:ILE:HD11	1:A:542:LEU:HD21	1.80	0.64
1:A:463:ILE:O	1:A:480:GLN:CG	2.42	0.63
1:D:444:LEU:HD23	1:D:454:TYR:CE1	2.31	0.63
1:D:354:GLU:O	1:D:358:GLU:HB2	1.98	0.63
1:A:467:ARG:NH1	1:A:513:ARG:NE	2.45	0.62
1:C:359:LEU:CD1	1:C:416:ASN:HD22	2.08	0.62
1:C:496:PRO:HD2	1:C:497:ASP:OD1	1.99	0.62
1:D:453:GLU:O	1:D:457:LEU:HD22	1.98	0.62
1:D:332:LEU:O	1:D:333:THR:HG22	2.00	0.62
1:D:456:MET:O	1:D:460:ILE:HG13	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:SER:O	1:B:361:THR:HB	2.00	0.62
1:A:418:LEU:HD12	1:A:419:THR:N	2.14	0.62
1:D:311:THR:HG22	1:D:313:ASP:N	2.14	0.62
1:B:513:ARG:HG3	1:C:510:THR:HG23	1.81	0.62
1:D:362:LYS:O	1:D:366:ASN:ND2	2.32	0.62
1:A:310:LEU:CB	1:A:314:GLU:OE1	2.48	0.62
1:D:314:GLU:CD	1:D:489:HIS:HD1	1.94	0.61
1:C:464:SER:OG	1:C:466:ASP:OD1	2.19	0.60
1:A:535:PRO:HB2	1:A:536:PRO:HD3	1.83	0.60
1:B:451:THR:O	1:B:454:TYR:HB2	2.01	0.60
1:B:507:LEU:O	1:B:510:THR:HB	2.01	0.60
1:B:485:GLU:OE1	1:B:488:LYS:HE2	2.02	0.60
1:D:386:ILE:H	1:D:386:ILE:CD1	2.09	0.60
1:D:370:PHE:O	1:D:374:VAL:HG23	2.01	0.60
1:A:361:THR:HA	1:A:538:ILE:HG13	1.83	0.60
1:B:370:PHE:O	1:B:374:VAL:HG23	2.01	0.59
1:D:426:GLU:H	1:D:426:GLU:CD	2.05	0.59
1:C:374:VAL:HG11	1:C:459:LEU:HD11	1.84	0.59
1:B:514:SER:OG	1:C:513:ARG:HD2	2.02	0.59
1:D:453:GLU:OE1	1:D:494:ARG:NH1	2.35	0.59
1:B:540:GLU:C	1:B:542:LEU:H	2.06	0.59
1:B:433:LEU:HD12	1:B:437:ILE:CD1	2.32	0.59
1:D:399:LEU:O	1:D:402:ALA:HB3	2.03	0.59
1:B:330:PRO:O	1:B:404:ARG:NH2	2.36	0.59
1:D:542:LEU:O	1:D:543:ASP:HB2	2.02	0.59
1:D:328:THR:HG22	1:D:369:ASP:HB3	1.85	0.58
1:D:392:ALA:HB1	1:D:396:ILE:CD1	2.33	0.58
1:D:353:TRP:CD1	1:D:530:MET:HE1	2.38	0.58
1:B:433:LEU:HD21	1:B:518:LYS:HB3	1.86	0.58
1:C:400:ARG:O	1:C:403:SER:HB3	2.04	0.58
1:C:447:LEU:HD23	1:C:505:LEU:HD23	1.86	0.58
1:D:444:LEU:HD23	1:D:454:TYR:HH	1.67	0.58
1:A:353:TRP:CH2	1:A:526:LEU:HB3	2.38	0.57
1:B:376:VAL:HG13	1:B:479:LYS:HG3	1.85	0.57
1:C:447:LEU:O	1:C:495:ARG:NH2	2.26	0.57
1:D:314:GLU:O	1:D:318:VAL:HG23	2.03	0.57
1:D:392:ALA:HB1	1:D:396:ILE:HD11	1.86	0.57
1:A:342:GLN:HE21	1:A:342:GLN:CA	2.09	0.57
1:A:439:LYS:CB	1:A:439:LYS:CD	2.76	0.57
1:B:311:THR:HG22	1:B:312:GLU:N	2.19	0.57
1:A:400:ARG:O	1:A:403:SER:OG	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:THR:CG2	1:D:369:ASP:HB3	2.34	0.57
1:B:409:GLU:HB3	1:B:411:THR:HG23	1.87	0.57
1:B:447:LEU:HD12	1:B:447:LEU:H	1.69	0.57
1:A:309:GLU:O	1:A:314:GLU:HB2	2.05	0.56
1:D:539:LEU:H	1:D:539:LEU:CD2	2.12	0.56
1:D:310:LEU:CD1	1:D:314:GLU:HB2	2.26	0.56
1:A:333:THR:CG2	1:A:334:ASP:OD2	2.52	0.56
1:B:375:PRO:HB2	1:B:376:VAL:HG23	1.88	0.56
1:B:311:THR:HG22	1:B:313:ASP:N	2.13	0.56
1:C:407:ASP:HB2	3:C:609:HOH:O	2.07	0.55
1:A:319:GLU:O	1:A:323:LYS:HB2	2.06	0.55
1:D:524:LEU:HD11	1:D:541:MET:CE	2.35	0.55
1:A:412:MET:HE1	1:A:437:ILE:HG22	1.88	0.55
1:D:375:PRO:O	1:D:377:PHE:N	2.29	0.55
1:A:395:GLU:CD	1:A:467:ARG:HH22	2.10	0.55
1:D:447:LEU:HD12	1:D:447:LEU:N	2.21	0.55
1:C:449:VAL:HG22	1:C:505:LEU:HD21	1.88	0.55
1:C:377:PHE:CZ	1:C:385:GLN:HB3	2.42	0.55
1:C:440:PHE:O	1:C:443:SER:OG	2.13	0.55
1:C:359:LEU:CD1	1:C:416:ASN:ND2	2.66	0.55
1:D:325:HIS:O	1:D:329:PHE:N	2.40	0.55
1:A:353:TRP:O	1:A:357:SER:OG	2.23	0.54
1:A:325:HIS:O	1:A:329:PHE:N	2.40	0.54
1:A:513:ARG:O	1:A:517:VAL:HG23	2.06	0.54
1:D:400:ARG:O	1:D:403:SER:OG	2.24	0.54
1:C:432:THR:O	1:C:435:PRO:HD2	2.07	0.54
1:B:311:THR:HG21	1:B:313:ASP:HB2	1.89	0.54
1:D:396:ILE:HD12	1:D:396:ILE:H	1.71	0.54
1:B:320:LYS:HG2	1:B:375:PRO:HG3	1.90	0.53
1:C:453:GLU:OE1	1:C:495:ARG:NH1	2.33	0.53
1:D:395:GLU:OE1	1:D:461:CYS:SG	2.66	0.53
1:D:396:ILE:N	1:D:396:ILE:HD12	2.24	0.53
1:A:359:LEU:HD11	1:A:416:ASN:HD22	1.71	0.53
1:B:317:MET:O	1:B:321:ILE:HG13	2.08	0.53
1:D:497:ASP:O	1:D:499:PRO:HD3	2.09	0.53
1:D:310:LEU:CD1	1:D:314:GLU:CB	2.84	0.53
1:B:314:GLU:O	1:B:318:VAL:HG23	2.09	0.53
1:B:333:THR:O	1:B:333:THR:HG23	2.08	0.53
1:D:353:TRP:CH2	1:D:527:ARG:CD	2.89	0.53
1:D:482:PRO:O	1:D:486:THR:OG1	2.24	0.53
1:A:524:LEU:O	1:A:528:MET:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:LYS:HB2	1:C:419:THR:OG1	2.09	0.52
1:C:541:MET:C	1:C:542:LEU:HD12	2.29	0.52
1:D:374:VAL:HG12	1:D:375:PRO:O	2.08	0.52
1:C:327:GLU:OE2	1:C:373:GLN:NE2	2.41	0.52
1:B:338:TYR:HE1	1:B:418:LEU:HD12	1.70	0.52
1:B:453:GLU:O	1:B:457:LEU:HD22	2.10	0.52
1:A:310:LEU:HD22	1:A:489:HIS:CE1	2.44	0.52
1:A:337:LYS:CB	1:A:417:GLY:O	2.58	0.52
1:D:429:GLY:H	2:D:601:REA:H14	1.74	0.52
1:A:377:PHE:O	1:A:380:LEU:HD12	2.09	0.52
1:A:519:GLY:O	1:A:523:VAL:HG23	2.09	0.52
1:B:485:GLU:OE1	1:B:488:LYS:CE	2.58	0.52
1:B:510:THR:HG23	1:C:513:ARG:HG3	1.91	0.51
1:B:369:ASP:O	1:B:372:LYS:HB2	2.11	0.51
1:C:333:THR:HA	1:C:336:ASP:HA	1.93	0.51
1:C:497:ASP:OD1	1:C:497:ASP:N	2.44	0.51
1:A:423:GLN:H	1:A:423:GLN:NE2	2.09	0.51
1:D:317:MET:O	1:D:321:ILE:HG13	2.10	0.51
1:D:373:GLN:OE1	1:D:373:GLN:N	2.41	0.51
1:A:421:THR:OG1	1:A:424:GLN:CD	2.48	0.50
1:A:481:GLU:HG2	1:D:504:LYS:NZ	2.26	0.50
1:B:421:THR:H	1:B:424:GLN:HE21	1.57	0.50
1:C:360:SER:O	1:C:364:ILE:HG13	2.10	0.50
1:B:374:VAL:HG12	1:B:375:PRO:HD2	1.90	0.50
1:B:513:ARG:HG3	1:C:510:THR:CG2	2.42	0.50
1:C:311:THR:HG22	1:C:313:ASP:N	2.25	0.50
1:D:531:PRO:O	1:D:534:LEU:HB2	2.11	0.50
1:A:322:LEU:O	1:A:326:GLU:HG3	2.12	0.50
1:D:423:GLN:O	1:D:427:VAL:HG23	2.11	0.50
1:A:341:THR:O	1:A:342:GLN:NE2	2.44	0.50
1:C:418:LEU:HD11	1:C:420:LEU:HD21	1.92	0.50
1:D:524:LEU:HD11	1:D:541:MET:HE1	1.94	0.50
1:B:429:GLY:H	2:B:601:REA:H14	1.77	0.50
1:C:381:SER:O	1:C:385:GLN:HG3	2.12	0.50
1:A:408:LYS:HB3	1:B:375:PRO:HG3	1.93	0.49
1:B:374:VAL:HG12	1:B:375:PRO:O	2.12	0.49
1:C:391:ALA:CB	1:C:467:ARG:HG3	2.42	0.49
1:B:327:GLU:OE2	1:B:373:GLN:NE2	2.45	0.49
1:C:341:THR:O	1:C:342:GLN:NE2	2.45	0.49
1:C:329:PHE:CZ	1:C:400:ARG:HB3	2.47	0.49
1:A:311:THR:O	1:A:315:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:MET:HE3	1:B:437:ILE:HG22	1.95	0.49
1:C:333:THR:OG1	1:C:336:ASP:OD1	2.20	0.48
1:B:340:LEU:HG	1:B:341:THR:N	2.28	0.48
1:D:375:PRO:HB2	1:D:376:VAL:HG22	1.95	0.48
1:C:322:LEU:HD22	1:C:326:GLU:OE1	2.13	0.48
1:C:513:ARG:HH11	1:C:513:ARG:CG	2.27	0.48
1:D:394:LEU:HD13	1:D:516:SER:HB2	1.94	0.48
1:A:433:LEU:HD21	1:A:518:LYS:HB3	1.96	0.48
1:B:506:LEU:O	1:B:509:LEU:HB2	2.13	0.48
1:C:322:LEU:CD2	1:C:326:GLU:OE1	2.61	0.48
1:D:374:VAL:CG1	1:D:375:PRO:HD2	2.41	0.48
1:D:383:ASN:C	1:D:386:ILE:HD13	2.33	0.48
1:A:353:TRP:CZ3	1:A:526:LEU:HD13	2.49	0.48
1:A:375:PRO:O	1:A:376:VAL:CG2	2.62	0.48
1:D:416:ASN:OD1	1:D:417:GLY:N	2.46	0.47
1:B:439:LYS:HZ2	1:C:466:ASP:HA	1.79	0.47
1:B:311:THR:CG2	1:B:313:ASP:H	2.14	0.47
1:A:506:LEU:O	1:A:509:LEU:HB2	2.14	0.47
1:C:332:LEU:O	1:C:333:THR:HG22	2.14	0.47
1:D:333:THR:OG1	1:D:336:ASP:OD1	2.25	0.47
1:D:465:GLY:HA3	1:D:477:GLU:HG3	1.97	0.47
1:C:463:ILE:O	1:C:480:GLN:HG3	2.14	0.47
1:A:332:LEU:O	1:A:333:THR:HG22	2.15	0.47
1:C:395:GLU:OE2	1:C:513:ARG:HG2	2.15	0.47
1:D:339:ARG:NH1	1:D:409:GLU:CD	2.66	0.47
1:B:333:THR:CA	1:B:336:ASP:HA	2.37	0.47
1:B:433:LEU:HD21	1:B:518:LYS:CB	2.44	0.47
1:B:538:ILE:HG23	1:B:539:LEU:N	2.30	0.47
1:D:333:THR:HG23	1:D:336:ASP:OD1	2.13	0.47
1:A:452:ALA:O	1:A:456:MET:HG3	2.15	0.47
1:A:337:LYS:HA	1:A:417:GLY:O	2.15	0.46
1:D:311:THR:CG2	1:D:313:ASP:H	2.26	0.46
1:A:525:GLN:O	1:A:529:GLU:HB2	2.15	0.46
1:B:313:ASP:HB3	3:B:710:HOH:O	2.15	0.46
1:A:500:HIS:CD2	1:A:500:HIS:C	2.89	0.46
1:A:352:LEU:O	1:A:355:ARG:HB2	2.15	0.46
1:D:377:PHE:CZ	1:D:389:LEU:HD11	2.42	0.46
1:B:539:LEU:HB2	1:B:540:GLU:OE1	2.16	0.46
1:D:444:LEU:CD2	1:D:454:TYR:CZ	2.86	0.46
1:B:310:LEU:HD12	1:B:493:LYS:HD3	1.97	0.46
1:D:430:PHE:HB3	1:D:434:THR:OG1	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:LEU:HD23	1:C:322:LEU:O	2.16	0.46
1:D:524:LEU:HD11	1:D:541:MET:HE3	1.98	0.46
1:A:375:PRO:O	1:A:376:VAL:HG23	2.17	0.45
1:D:376:VAL:O	1:D:379:GLN:CB	2.58	0.45
1:D:380:LEU:O	1:D:385:GLN:NE2	2.34	0.45
1:D:433:LEU:CD1	1:D:437:ILE:HD11	2.33	0.45
1:A:457:LEU:HD11	1:A:505:LEU:HD22	1.98	0.45
1:D:352:LEU:O	1:D:355:ARG:N	2.44	0.45
1:D:512:LEU:O	1:D:516:SER:N	2.47	0.45
1:A:530:MET:HE3	1:A:533:GLU:HA	1.96	0.45
1:C:389:LEU:O	1:C:393:CYS:HB2	2.17	0.45
1:D:376:VAL:HA	1:D:379:GLN:HB2	1.99	0.45
1:A:433:LEU:C	1:A:435:PRO:HD2	2.37	0.44
1:D:392:ALA:O	1:D:396:ILE:HD13	2.16	0.44
1:B:374:VAL:CG1	1:B:375:PRO:CD	2.93	0.44
1:D:317:MET:HG2	1:D:321:ILE:HD11	1.99	0.44
1:D:449:VAL:HG22	1:D:505:LEU:HD21	2.00	0.44
1:A:497:ASP:OD1	1:A:497:ASP:N	2.43	0.44
1:B:397:ILE:O	1:B:401:LEU:HB2	2.18	0.44
1:A:538:ILE:CD1	1:A:538:ILE:N	2.80	0.44
1:B:527:ARG:HG3	1:B:527:ARG:NH1	2.29	0.44
1:C:474:GLU:HG2	1:C:475:LYS:N	2.31	0.44
1:D:352:LEU:O	1:D:355:ARG:HG3	2.18	0.44
1:A:433:LEU:HD21	1:A:518:LYS:CB	2.48	0.44
1:B:507:LEU:CD2	1:C:506:LEU:HD13	2.38	0.44
1:D:463:ILE:O	1:D:480:GLN:HG3	2.17	0.44
1:A:310:LEU:HB3	1:A:311:THR:H	1.68	0.44
1:B:409:GLU:CB	1:B:411:THR:HG23	2.47	0.44
1:C:535:PRO:O	1:C:539:LEU:HB2	2.18	0.44
1:A:506:LEU:HD12	1:D:506:LEU:HD12	2.00	0.44
1:D:440:PHE:CZ	1:D:512:LEU:HD13	2.53	0.44
1:A:380:LEU:O	1:A:385:GLN:NE2	2.46	0.43
1:B:453:GLU:CD	1:B:495:ARG:NH2	2.64	0.43
1:D:383:ASN:ND2	1:D:471:GLU:OE1	2.50	0.43
1:A:513:ARG:HG3	1:D:514:SER:OG	2.17	0.43
1:D:374:VAL:HG11	1:D:459:LEU:HD21	2.00	0.43
1:D:524:LEU:O	1:D:527:ARG:N	2.51	0.43
1:A:443:SER:HB2	1:A:508:LYS:NZ	2.32	0.43
1:D:422:GLN:O	1:D:426:GLU:N	2.51	0.43
1:D:443:SER:HB2	1:D:508:LYS:NZ	2.32	0.43
1:B:311:THR:HB	1:B:314:GLU:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:PHE:O	1:C:374:VAL:HG23	2.19	0.43
1:A:374:VAL:HG12	1:A:375:PRO:HD2	2.00	0.43
1:A:513:ARG:HA	1:A:513:ARG:HD3	1.67	0.43
1:A:381:SER:O	1:A:385:GLN:HG3	2.19	0.43
1:D:423:GLN:H	1:D:423:GLN:CD	2.21	0.43
1:C:506:LEU:O	1:C:509:LEU:HB2	2.18	0.43
1:B:360:SER:O	1:B:364:ILE:HG13	2.18	0.43
1:B:399:LEU:HD13	1:B:512:LEU:HD21	2.00	0.43
1:D:442:ARG:O	1:D:445:VAL:CG2	2.66	0.43
1:B:374:VAL:HG12	1:B:375:PRO:CD	2.49	0.43
1:B:412:MET:CE	1:B:437:ILE:HG22	2.49	0.43
1:C:542:LEU:N	1:C:542:LEU:HD12	2.34	0.43
1:A:513:ARG:HH11	1:A:513:ARG:HG2	1.84	0.42
1:C:396:ILE:O	1:C:400:ARG:HG3	2.19	0.42
1:D:413:SER:OG	1:D:419:THR:HG23	2.19	0.42
1:A:490:TYR:CE1	1:A:494:ARG:HD3	2.54	0.42
1:B:356:VAL:HA	2:B:601:REA:H192	2.01	0.42
1:B:364:ILE:HG23	1:B:393:CYS:SG	2.58	0.42
1:D:527:ARG:HA	1:D:527:ARG:HD2	1.68	0.42
1:B:376:VAL:CG1	1:B:479:LYS:CG	2.97	0.42
1:B:540:GLU:C	1:B:542:LEU:N	2.70	0.42
1:A:467:ARG:NH1	1:A:513:ARG:NH2	2.66	0.42
1:C:359:LEU:HD13	1:C:414:PHE:HB3	2.02	0.42
1:D:442:ARG:O	1:D:445:VAL:HG23	2.19	0.42
1:B:355:ARG:HD3	2:B:601:REA:H202	2.02	0.42
1:C:386:ILE:O	1:C:390:LYS:HB2	2.20	0.42
1:C:423:GLN:N	1:C:423:GLN:OE1	2.39	0.42
1:B:447:LEU:CD1	1:B:447:LEU:N	2.83	0.42
1:D:449:VAL:HA	1:D:453:GLU:OE2	2.20	0.42
1:D:459:LEU:HA	1:D:459:LEU:HD23	1.96	0.42
1:B:443:SER:O	1:B:447:LEU:HD11	2.05	0.42
1:C:496:PRO:CD	1:C:497:ASP:OD1	2.67	0.42
1:D:517:VAL:O	1:D:521:GLU:HG3	2.20	0.42
1:D:535:PRO:O	1:D:539:LEU:HD21	2.20	0.42
1:A:513:ARG:HG2	1:A:513:ARG:NH1	2.35	0.41
1:C:340:LEU:HG	1:C:341:THR:N	2.34	0.41
1:C:513:ARG:HH11	1:C:513:ARG:HG2	1.85	0.41
1:D:331:TYR:N	1:D:331:TYR:CD2	2.88	0.41
1:B:505:LEU:HD23	1:B:505:LEU:HA	1.87	0.41
1:C:423:GLN:H	1:C:423:GLN:CD	2.22	0.41
1:C:421:THR:OG1	1:C:424:GLN:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:421:THR:OG1	1:D:424:GLN:CB	2.68	0.41
1:B:491:VAL:HA	1:B:495:ARG:NH1	2.36	0.41
1:D:388:LEU:CD2	1:D:470:LEU:HD21	2.51	0.41
1:C:322:LEU:HD23	1:C:322:LEU:C	2.40	0.41
1:D:310:LEU:HD12	1:D:314:GLU:HB3	1.93	0.41
1:A:375:PRO:C	1:A:376:VAL:HG22	2.41	0.41
1:A:418:LEU:CD1	1:A:420:LEU:HD23	2.50	0.41
1:A:530:MET:CE	1:A:532:GLY:O	2.68	0.41
1:C:364:ILE:HG12	1:C:397:ILE:HD11	2.02	0.41
1:D:447:LEU:HD12	1:D:447:LEU:H	1.84	0.41
1:A:534:LEU:N	1:A:534:LEU:HD23	2.36	0.41
1:B:428:GLY:HA3	2:B:601:REA:O1	2.21	0.41
1:C:507:LEU:HD23	1:C:507:LEU:HA	1.87	0.41
1:D:384:ASP:O	1:D:388:LEU:HG	2.21	0.41
1:D:389:LEU:O	1:D:393:CYS:HB2	2.20	0.41
1:A:375:PRO:C	1:A:376:VAL:CG2	2.89	0.41
1:A:314:GLU:CD	1:A:489:HIS:HD1	2.24	0.41
1:A:524:LEU:O	1:A:528:MET:CG	2.68	0.41
1:A:527:ARG:C	1:A:530:MET:HB2	2.40	0.40
1:C:522:ARG:HG2	1:C:522:ARG:H	1.51	0.40
1:A:449:VAL:HA	1:A:453:GLU:OE2	2.21	0.40
1:B:356:VAL:HA	2:B:601:REA:C19	2.51	0.40
1:C:376:VAL:H	1:C:379:GLN:HG3	1.86	0.40
1:B:421:THR:OG1	1:B:424:GLN:CG	2.64	0.40
1:B:527:ARG:CG	1:B:527:ARG:HH11	2.32	0.40
1:C:322:LEU:CD2	1:C:326:GLU:CD	2.90	0.40
1:D:328:THR:HG21	1:D:370:PHE:N	2.37	0.40
1:A:527:ARG:HA	1:A:530:MET:SD	2.62	0.40
1:B:371:GLY:O	1:B:377:PHE:HD2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	223/241 (92%)	211 (95%)	10 (4%)	2 (1%)	17	40
1	B	223/241 (92%)	215 (96%)	8 (4%)	0	100	100
1	C	211/241 (88%)	200 (95%)	9 (4%)	2 (1%)	17	40
1	D	223/241 (92%)	216 (97%)	6 (3%)	1 (0%)	34	60
All	All	880/964 (91%)	842 (96%)	33 (4%)	5 (1%)	25	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	535	PRO
1	C	376	VAL
1	C	536	PRO
1	D	376	VAL
1	A	376	VAL

5.3.2　Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	197/219 (90%)	159 (81%)	38 (19%)	1	3
1	B	199/219 (91%)	168 (84%)	31 (16%)	2	7
1	C	190/219 (87%)	155 (82%)	35 (18%)	1	4
1	D	201/219 (92%)	160 (80%)	41 (20%)	1	3
All	All	787/876 (90%)	642 (82%)	145 (18%)	1	4

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	321	ILE
1	A	322	LEU
1	A	323	LYS
1	A	331	TYR
1	A	332	LEU
1	A	333	THR

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Mol	Chain	Res	Type
1	A	334	ASP
1	A	335	ASP
1	A	339	ARG
1	A	340	LEU
1	A	341	THR
1	A	342	GLN
1	A	353	TRP
1	A	357	SER
1	A	376	VAL
1	A	380	LEU
1	A	381	SER
1	A	390	LYS
1	A	401	LEU
1	A	403	SER
1	A	412	MET
1	A	415	SER
1	A	418	LEU
1	A	432	THR
1	A	434	THR
1	A	436	THR
1	A	444	LEU
1	A	450	ASP
1	A	474	GLU
1	A	477	GLU
1	A	495	ARG
1	A	511	ASP
1	A	513	ARG
1	A	515	LEU
1	A	522	ARG
1	A	534	LEU
1	A	538	ILE
1	A	543	ASP
1	B	313	ASP
1	B	320	LYS
1	B	322	LEU
1	B	332	LEU
1	B	336	ASP
1	B	337	LYS
1	B	340	LEU
1	B	341	THR
1	B	342	GLN
1	B	351	ILE

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Mol	Chain	Res	Type
1	B	352	LEU
1	B	361	THR
1	B	378	THR
1	B	394	LEU
1	B	433	LEU
1	B	436	THR
1	B	457	LEU
1	B	458	SER
1	B	461	CYS
1	B	464	SER
1	B	479	LYS
1	B	493	LYS
1	B	504	LYS
1	B	511	ASP
1	B	512	LEU
1	B	524	LEU
1	B	527	ARG
1	B	528	MET
1	B	533	GLU
1	B	537	LEU
1	B	542	LEU
1	C	310	LEU
1	C	312	GLU
1	C	315	GLU
1	C	316	GLU
1	C	332	LEU
1	C	336	ASP
1	C	337	LYS
1	C	339	ARG
1	C	340	LEU
1	C	341	THR
1	C	342	GLN
1	C	351	ILE
1	C	353	TRP
1	C	373	GLN
1	C	390	LYS
1	C	394	LEU
1	C	401	LEU
1	C	403	SER
1	C	433	LEU
1	C	436	THR
1	C	459	LEU

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Mol	Chain	Res	Type
1	C	461	CYS
1	C	467	ARG
1	C	479	LYS
1	C	493	LYS
1	C	498	SER
1	C	505	LEU
1	C	506	LEU
1	C	511	ASP
1	C	513	ARG
1	C	522	ARG
1	C	523	VAL
1	C	537	LEU
1	C	539	LEU
1	C	540	GLU
1	D	310	LEU
1	D	311	THR
1	D	312	GLU
1	D	322	LEU
1	D	323	LYS
1	D	332	LEU
1	D	333	THR
1	D	336	ASP
1	D	340	LEU
1	D	351	ILE
1	D	357	SER
1	D	358	GLU
1	D	360	SER
1	D	361	THR
1	D	369	ASP
1	D	376	VAL
1	D	382	THR
1	D	389	LEU
1	D	390	LYS
1	D	394	LEU
1	D	433	LEU
1	D	436	THR
1	D	437	ILE
1	D	443	SER
1	D	444	LEU
1	D	446	GLU
1	D	450	ASP
1	D	457	LEU

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Mol	Chain	Res	Type
1	D	458	SER
1	D	459	LEU
1	D	464	SER
1	D	486	THR
1	D	493	LYS
1	D	498	SER
1	D	501	SER
1	D	511	ASP
1	D	513	ARG
1	D	522	ARG
1	D	524	LEU
1	D	537	LEU
1	D	539	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	342	GLN
1	A	423	GLN
1	A	500	HIS
1	B	342	GLN
1	B	424	GLN
1	C	424	GLN
1	D	366	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands 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	#$|Z| > 2$
2	REA	B	601	-	19,22,22	1.60	3 (15%)	26,30,30	2.55	9 (34%)
2	REA	D	601	-	19,22,22	1.21	1 (5%)	26,30,30	1.57	6 (23%)

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
2	REA	B	601	-	-	1/13/32/32	0/1/1/1
2	REA	D	601	-	-	0/13/32/32	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	REA	C14-C13	3.55	1.39	1.35
2	B	601	REA	C1-C6	3.48	1.58	1.53
2	B	601	REA	C14-C13	3.28	1.38	1.35
2	B	601	REA	C5-C6	2.87	1.39	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	REA	C10-C11-C12	-7.86	98.68	123.22
2	B	601	REA	C11-C10-C9	4.69	134.00	127.31
2	D	601	REA	C10-C11-C12	-4.23	110.03	123.22
2	B	601	REA	C7-C8-C9	-4.08	120.07	126.23
2	B	601	REA	C18-C5-C6	-3.59	120.50	124.53
2	B	601	REA	C11-C12-C13	3.57	136.43	126.42
2	D	601	REA	C11-C10-C9	3.17	131.84	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	REA	C12-C13-C14	-2.73	111.82	119.11
2	B	601	REA	C18-C5-C4	2.52	118.46	113.62
2	D	601	REA	C19-C9-C8	2.46	121.95	118.08
2	B	601	REA	C20-C13-C14	2.40	129.66	124.64
2	B	601	REA	C17-C1-C16	-2.26	101.58	108.53
2	D	601	REA	C8-C9-C10	-2.23	115.52	118.94
2	D	601	REA	C11-C12-C13	2.16	132.47	126.42
2	D	601	REA	C4-C5-C6	-2.05	119.76	122.73

There are no chirality outliers.
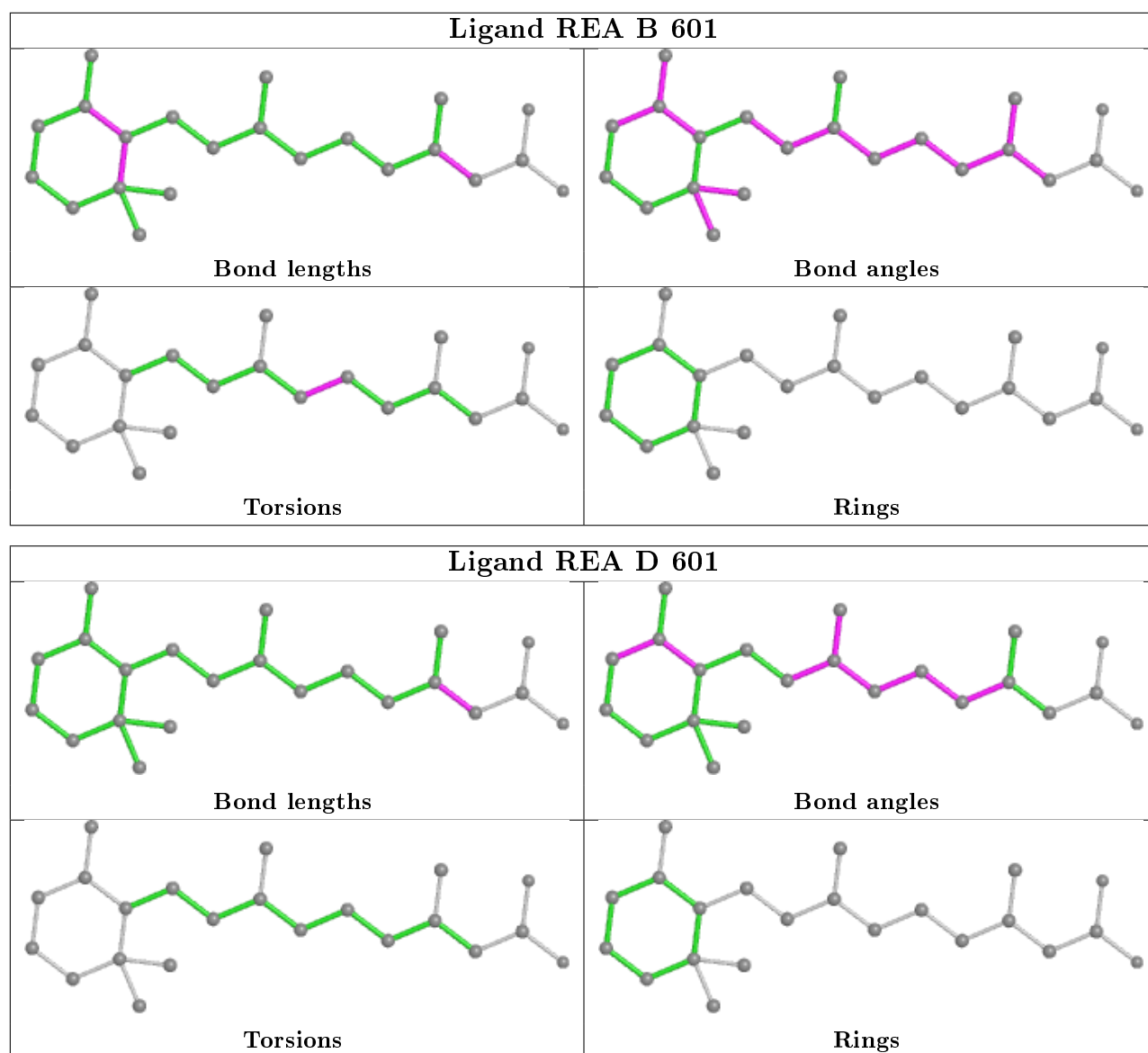
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	REA	C9-C10-C11-C12

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	REA	5	0
2	D	601	REA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand REA B 601

Bond lengths

Bond angles

Torsions

Rings

Ligand REA D 601

Bond lengths

Bond angles

Torsions

Rings

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	227/241 (94%)	0.48	13 (5%)	23	22	19, 45, 109, 183	0
1	B	227/241 (94%)	0.29	5 (2%)	62	63	23, 46, 72, 110	0
1	C	217/241 (90%)	0.23	7 (3%)	47	48	20, 48, 84, 121	0
1	D	227/241 (94%)	0.41	14 (6%)	20	19	31, 56, 90, 124	0
All	All	898/964 (93%)	0.35	39 (4%)	35	33	19, 50, 93, 183	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	531	PRO	6.1
1	A	430	PHE	6.1
1	C	334	ASP	4.0
1	D	352	LEU	3.9
1	C	429	GLY	3.9
1	A	541	MET	3.6
1	A	528	MET	3.5
1	B	335	ASP	3.2
1	A	530	MET	3.1
1	C	335	ASP	3.1
1	A	355	ARG	3.0
1	D	370	PHE	2.8
1	A	533	GLU	2.7
1	A	537	LEU	2.6
1	D	364	ILE	2.6
1	D	310	LEU	2.5
1	B	376	VAL	2.5
1	B	401	LEU	2.5
1	A	340	LEU	2.5
1	A	356	VAL	2.5
1	A	542	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	377	PHE	2.4
1	C	355	ARG	2.4
1	C	351	ILE	2.4
1	C	356	VAL	2.3
1	D	414	PHE	2.3
1	D	312	GLU	2.3
1	D	515	LEU	2.3
1	D	420	LEU	2.2
1	B	543	ASP	2.2
1	D	354	GLU	2.2
1	D	376	VAL	2.2
1	B	420	LEU	2.2
1	C	430	PHE	2.2
1	D	356	VAL	2.1
1	A	334	ASP	2.1
1	A	420	LEU	2.0
1	D	332	LEU	2.0
1	D	539	LEU	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)
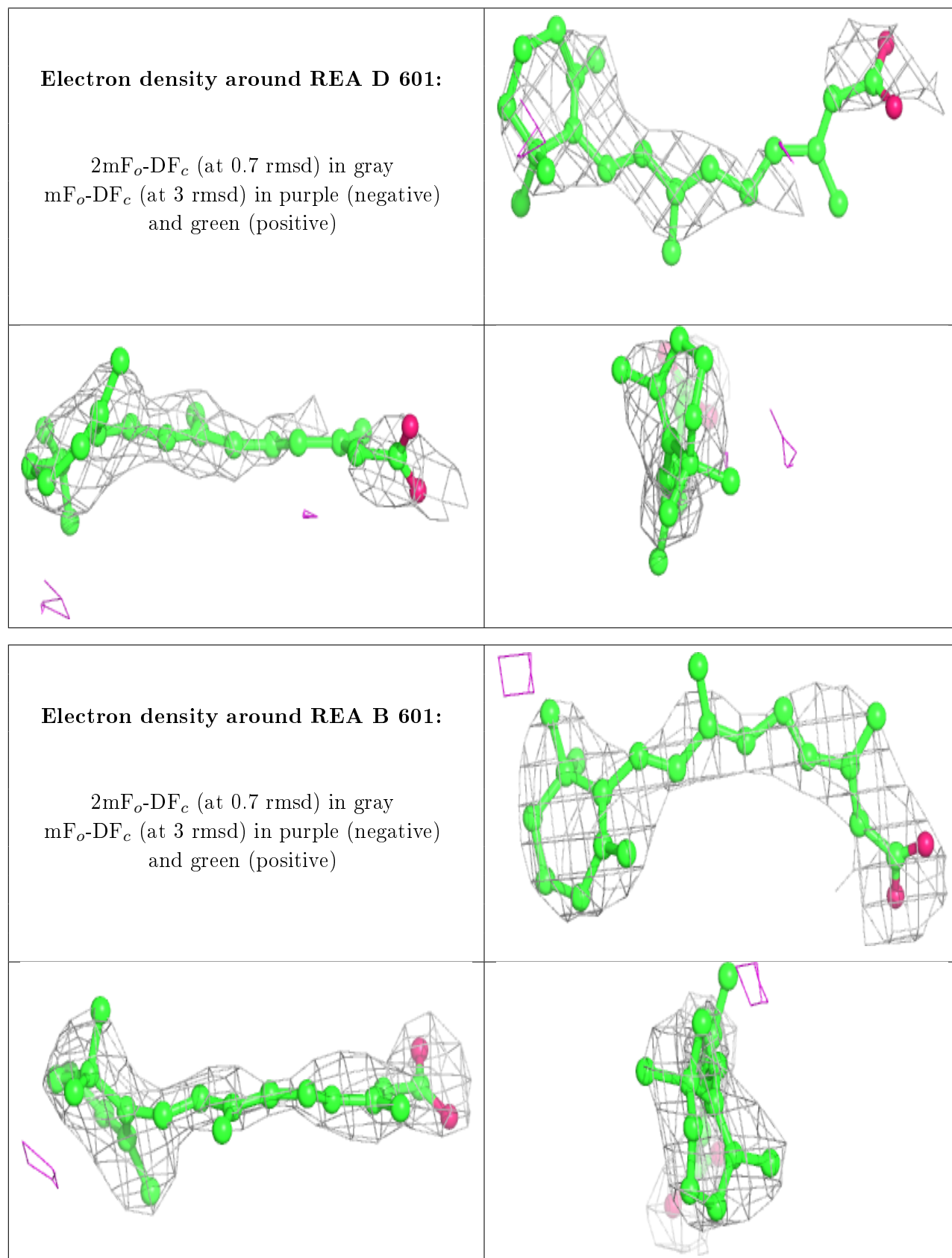
There are no monosaccharides in this entry.

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	REA	D	601	22/22	0.85	0.61	76,84,108,111	0
2	REA	B	601	22/22	0.88	0.54	35,49,71,73	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around REA D 601:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around REA B 601:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers (i)

There are no such residues in this entry.