Full wwPDB X-ray Structure Validation Report (i)

May 29, 2020 – 03:59 am BST

PDB ID	:	1G5Y
Title	:	THE 2.0 ANGSTROM RESOLUTION CRYSTAL STRUCTURE OF THE RXRALPHA LIGAND BINDING DOMAIN TETRAMER IN THE PRESENCE OF A NON-ACTIVATING RETINOIC ACID ISOMER.
Authors	:	Gampe Jr., R.T.; Montana, V.G.; Lambert, M.H.; Wisely, G.B.; Milburn, M.V.; Xu, H.E.
Deposited on	:	2000-11-02
Resolution	:	2.00 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 (1)) were used in the production of this report:

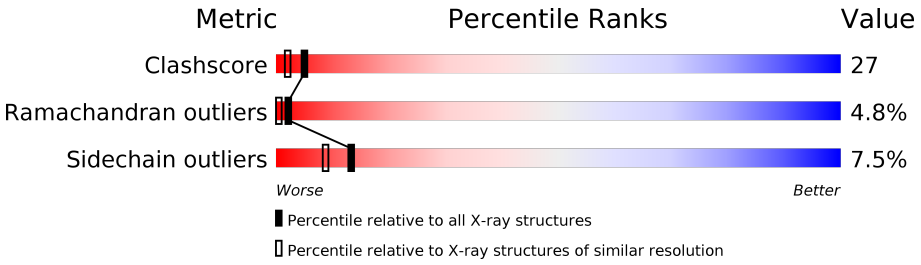
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	238	61% 26% 8%
1	B	238	63% 26% 7%
1	C	238	53% 37% 5%
1	D	238	57% 30% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	REA	B	501	-	-	X	-

2 Entry composition

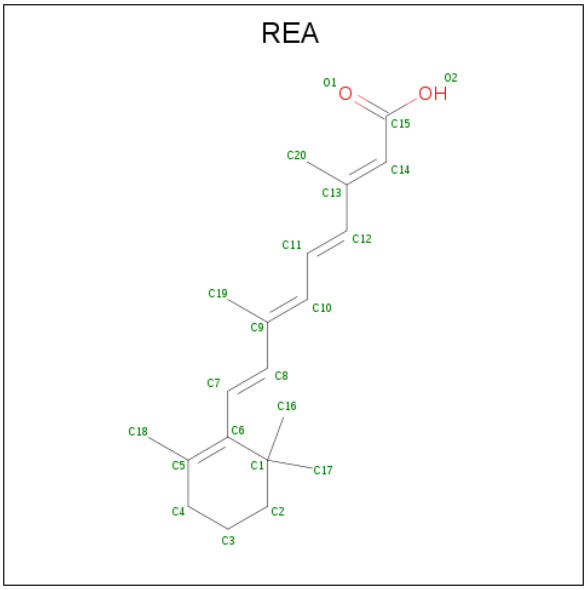
There are 3 unique types of molecules in this entry. The entry contains 7438 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RXR-ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1724	1104	301	310	9			
1	B	229	Total	C	N	O	S	0	0	0
			1739	1115	303	312	9			
1	C	226	Total	C	N	O	S	0	0	0
			1704	1093	293	309	9			
1	D	229	Total	C	N	O	S	0	0	0
			1731	1110	301	311	9			

- 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	C	1	Total	C	O	0	0
			22	20	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	138	Total O 138 138	0	0
3	B	145	Total O 145 145	0	0
3	C	99	Total O 99 99	0	0
3	D	114	Total O 114 114	0	0

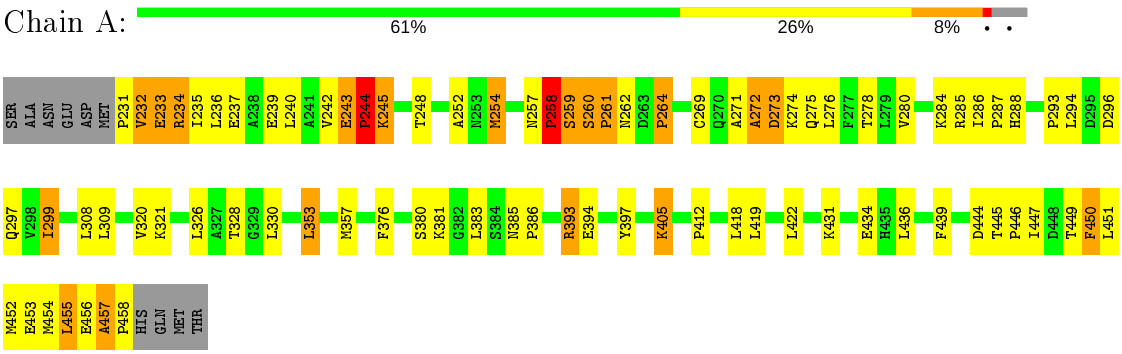
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

Note EDS was not executed.

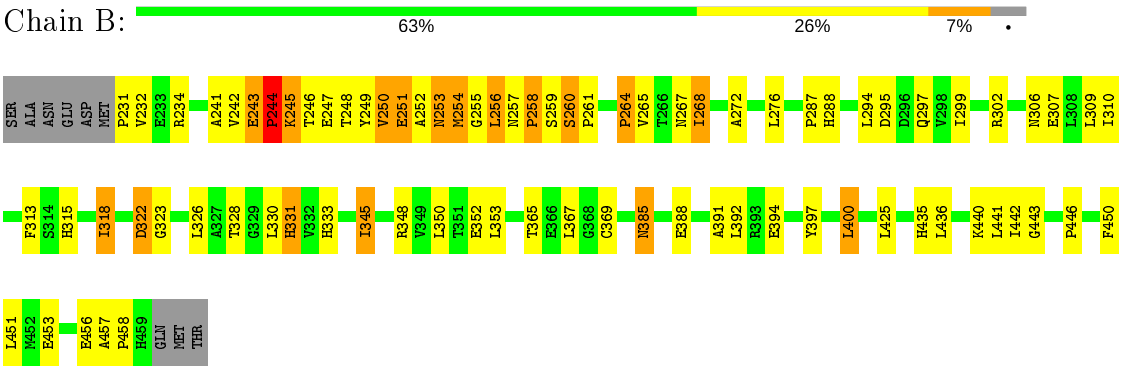
- Molecule 1: RETINOIC ACID RECEPTOR RXR-ALPHA

Chain A:



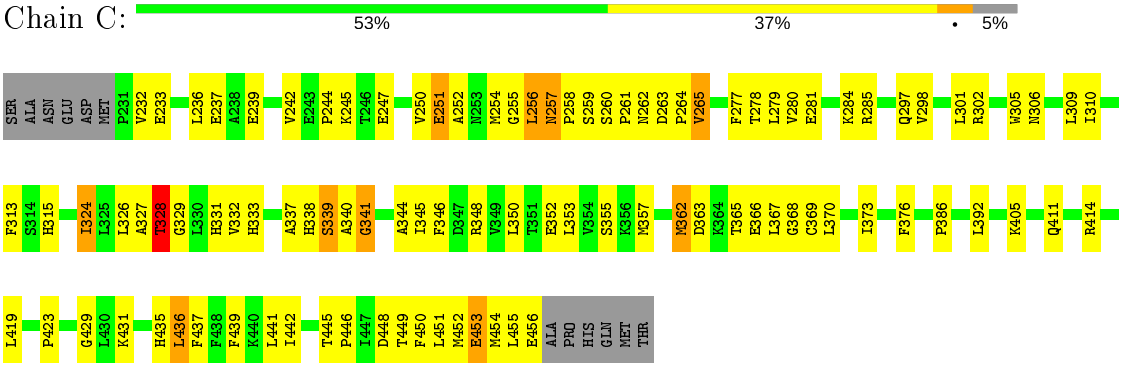
- Molecule 1: RETINOIC ACID RECEPTOR RXR-ALPHA

Chain B:



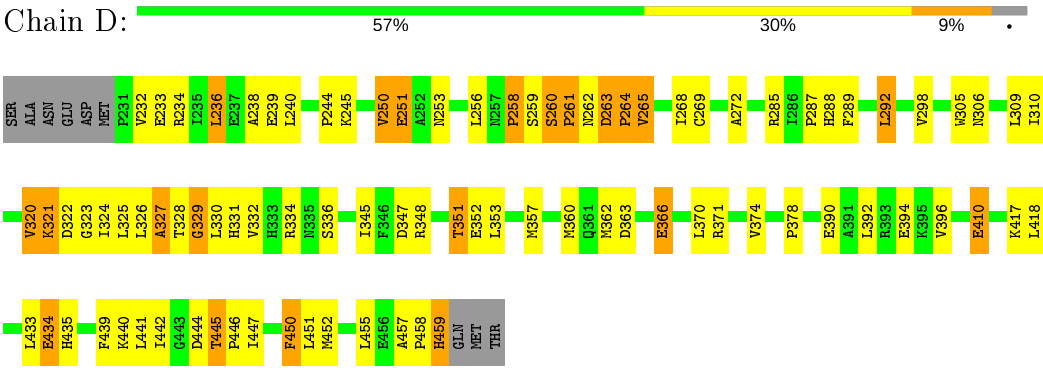
- Molecule 1: RETINOIC ACID RECEPTOR RXR-ALPHA

Chain C:



• Molecule 1: RETINOIC ACID RECEPTOR RXR-ALPHA

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.05Å 99.70Å 96.28Å 90.00° 96.70° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	99.5 (20.00-2.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS, CNX 2000	Depositor
R, R_{free}	0.231 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7438	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.44	1/1756 (0.1%)	0.72	6/2378 (0.3%)
1	B	0.40	0/1773	0.65	3/2403 (0.1%)
1	C	0.36	0/1736	0.62	3/2356 (0.1%)
1	D	0.40	0/1765	0.70	5/2394 (0.2%)
All	All	0.40	1/7030 (0.0%)	0.67	17/9531 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	233	GLU	CG-CD	5.56	1.60	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	459	HIS	N-CA-C	-10.31	83.15	111.00
1	A	234	ARG	N-CA-C	-7.46	90.87	111.00
1	B	244	PRO	N-CA-CB	6.41	110.99	103.30
1	D	265	VAL	N-CA-C	-5.79	95.38	111.00
1	D	258	PRO	N-CA-CB	5.78	110.23	103.30
1	A	458	PRO	N-CA-CB	5.76	110.22	103.30
1	B	261	PRO	N-CA-CB	5.72	110.17	103.30
1	A	258	PRO	N-CA-CB	5.65	110.08	103.30
1	A	244	PRO	N-CA-CB	5.64	110.07	103.30
1	D	244	PRO	N-CA-CB	5.63	110.06	103.30
1	B	258	PRO	N-CA-CB	5.63	110.06	103.30
1	C	258	PRO	N-CA-CB	5.63	110.05	103.30
1	C	261	PRO	N-CA-CB	5.62	110.05	103.30
1	A	264	PRO	N-CA-CB	5.61	110.04	103.30
1	C	244	PRO	N-CA-CB	5.58	109.99	103.30
1	D	261	PRO	N-CA-CB	5.51	109.91	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	261	PRO	N-CA-CB	5.40	109.78	103.30

There are no chirality outliers.

There are no planarity outliers.

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	1724	0	1692	105	0
1	B	1739	0	1719	78	0
1	C	1704	0	1672	106	0
1	D	1731	0	1702	99	0
2	B	22	0	27	14	0
2	C	22	0	27	5	0
3	A	138	0	0	8	0
3	B	145	0	0	2	1
3	C	99	0	0	8	0
3	D	114	0	0	7	1
All	All	7438	0	6839	373	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 27.

All (373) 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:232:VAL:HG23	1:A:235:ILE:HD12	1.25	1.09
1:A:233:GLU:HA	1:A:236:LEU:HB3	1.38	1.05
1:A:232:VAL:HG13	3:A:501:HOH:O	1.56	1.04
1:D:327:ALA:N	1:D:331:HIS:NE2	2.10	0.98
1:D:253:ASN:HA	1:D:329:GLY:H	1.26	0.98
1:C:411:GLN:NE2	1:C:414:ARG:HD2	1.78	0.96
1:A:232:VAL:CG2	1:A:235:ILE:HD12	1.96	0.96
1:A:232:VAL:O	1:A:236:LEU:N	2.01	0.94
1:D:253:ASN:CA	1:D:329:GLY:H	1.80	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:THR:HG23	1:A:450:PHE:H	1.33	0.93
1:D:253:ASN:HA	1:D:329:GLY:N	1.84	0.91
1:D:263:ASP:O	1:D:265:VAL:N	2.08	0.87
1:C:252:ALA:CB	1:C:328:THR:O	2.24	0.86
1:A:449:THR:HG23	1:A:450:PHE:N	1.91	0.84
1:D:328:THR:O	1:D:330:LEU:O	1.96	0.84
1:A:248:THR:HA	3:A:565:HOH:O	1.78	0.83
1:B:442:ILE:HD11	2:B:501:REA:H171	1.61	0.83
1:D:253:ASN:CB	1:D:329:GLY:H	1.92	0.83
1:A:233:GLU:O	1:A:237:GLU:HB2	1.77	0.82
1:A:232:VAL:CG1	3:A:501:HOH:O	2.16	0.82
1:D:328:THR:N	1:D:331:HIS:NE2	2.28	0.82
1:B:245:LYS:O	1:B:247:GLU:N	2.13	0.80
1:C:252:ALA:HB3	1:C:328:THR:O	1.81	0.80
1:D:310:ILE:HA	1:D:313:PHE:CE2	2.17	0.78
1:A:233:GLU:O	1:A:237:GLU:CB	2.32	0.77
1:A:299:ILE:HD11	1:A:380:SER:HB3	1.65	0.77
1:D:234:ARG:HE	1:D:287:PRO:HG3	1.49	0.77
1:A:273:ASP:OD2	1:C:265:VAL:HG22	1.85	0.77
1:B:251:GLU:HA	1:B:256:LEU:O	1.85	0.76
1:D:268:ILE:H	1:D:268:ILE:HD12	1.50	0.76
1:C:348:ARG:HH21	1:C:431:LYS:HD3	1.51	0.75
1:D:327:ALA:H	1:D:331:HIS:CD2	2.05	0.75
1:D:458:PRO:O	1:D:459:HIS:C	2.20	0.75
1:A:232:VAL:O	1:A:232:VAL:HG13	1.86	0.75
1:C:233:GLU:O	1:C:237:GLU:HG3	1.87	0.74
1:D:326:LEU:H	1:D:331:HIS:CD2	2.05	0.74
1:B:310:ILE:HG23	1:B:425:LEU:HD11	1.68	0.74
1:A:271:ALA:C	1:A:273:ASP:H	1.92	0.73
1:C:333:HIS:O	1:C:337:ALA:HB2	1.88	0.72
1:C:324:ILE:HD11	1:C:441:LEU:HD21	1.71	0.72
1:D:239:GLU:HB2	3:D:529:HOH:O	1.91	0.71
1:C:411:GLN:HE22	1:C:414:ARG:HD2	1.55	0.71
1:C:262:ASN:CB	3:C:575:HOH:O	2.38	0.71
1:A:299:ILE:CD1	1:A:380:SER:HB3	2.21	0.70
1:C:411:GLN:HE21	1:C:414:ARG:HD2	1.55	0.70
1:D:328:THR:H	1:D:331:HIS:CE1	2.09	0.70
1:D:435:HIS:O	1:D:440:LYS:HE2	1.92	0.70
1:A:376:PHE:O	1:A:393:ARG:HD3	1.91	0.70
1:B:252:ALA:HB3	1:B:328:THR:HB	1.73	0.70
1:A:252:ALA:HB3	1:A:328:THR:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:ASP:N	1:D:264:PRO:HD2	2.08	0.69
1:C:348:ARG:HD2	1:C:352:GLU:OE2	1.93	0.69
1:A:446:PRO:C	1:A:449:THR:HG22	2.14	0.68
1:A:449:THR:CG2	1:A:450:PHE:H	2.04	0.68
1:A:237:GLU:HA	3:A:515:HOH:O	1.94	0.68
1:C:251:GLU:HA	1:C:256:LEU:CB	2.23	0.67
1:D:378:PRO:HG3	1:D:390:GLU:OE1	1.93	0.67
1:C:280:VAL:O	1:C:284:LYS:HG3	1.94	0.67
1:B:276:LEU:HD11	2:B:501:REA:H182	1.77	0.67
1:C:405:LYS:HE3	3:C:562:HOH:O	1.95	0.67
1:A:232:VAL:C	1:A:235:ILE:H	1.98	0.67
1:A:447:ILE:O	1:A:451:LEU:HB2	1.94	0.67
1:B:255:GLY:O	1:B:257:ASN:N	2.28	0.66
1:B:322:ASP:OD2	1:B:333:HIS:HD2	1.79	0.66
1:A:260:SER:O	1:A:262:ASN:N	2.25	0.66
1:C:252:ALA:HA	1:C:255:GLY:HA2	1.78	0.66
1:D:360:MET:CE	1:D:418:LEU:HD23	2.26	0.66
1:B:231:PRO:N	1:B:234:ARG:HD3	2.11	0.65
1:C:353:LEU:O	1:C:357:MET:HG3	1.96	0.65
1:C:324:ILE:HD11	1:C:326:LEU:HD21	1.78	0.65
1:A:274:LYS:O	1:A:278:THR:HG23	1.96	0.65
1:B:315:HIS:O	1:B:318:ILE:HD12	1.95	0.65
1:C:348:ARG:NH2	1:C:431:LYS:HD3	2.10	0.65
1:B:252:ALA:O	1:B:330:LEU:HB2	1.95	0.65
1:B:326:LEU:HD22	2:B:501:REA:H201	1.77	0.65
1:B:243:GLU:O	1:B:244:PRO:CB	2.44	0.64
1:C:252:ALA:C	1:C:255:GLY:H	2.00	0.64
1:D:234:ARG:NE	1:D:287:PRO:HG3	2.11	0.64
1:B:252:ALA:HB3	1:B:328:THR:CB	2.26	0.64
1:D:330:LEU:N	1:D:330:LEU:HD12	2.13	0.64
1:A:450:PHE:O	1:A:454:MET:HG3	1.97	0.63
1:A:280:VAL:HG11	1:C:454:MET:HB3	1.79	0.63
1:C:350:LEU:O	1:C:355:SER:HB2	1.99	0.63
1:B:245:LYS:C	1:B:247:GLU:H	2.02	0.63
1:C:435:HIS:C	1:C:436:LEU:HD12	2.19	0.63
1:A:231:PRO:HG2	1:A:234:ARG:NH2	2.14	0.63
1:A:383:LEU:HD11	1:A:386:PRO:HA	1.81	0.63
1:C:451:LEU:O	1:C:455:LEU:HD23	1.99	0.63
1:A:271:ALA:O	1:A:273:ASP:N	2.31	0.62
1:C:338:HIS:O	1:C:340:ALA:N	2.31	0.62
1:D:262:ASN:C	1:D:264:PRO:HD2	2.19	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:ASP:O	1:D:265:VAL:HG23	1.99	0.62
1:B:345:ILE:O	1:B:345:ILE:HD13	1.99	0.62
1:A:235:ILE:HG12	1:A:286:ILE:HD13	1.82	0.62
1:B:385:ASN:O	1:B:388:GLU:HG2	2.00	0.62
1:C:327:ALA:C	1:C:329:GLY:H	2.03	0.62
1:A:233:GLU:HA	1:A:236:LEU:CB	2.23	0.62
1:B:232:VAL:HG13	1:B:365:THR:CG2	2.30	0.62
1:D:239:GLU:OE2	1:D:371:ARG:HD3	2.00	0.62
1:C:326:LEU:HD22	2:C:502:REA:H201	1.81	0.61
1:A:449:THR:CG2	1:A:450:PHE:N	2.62	0.61
1:A:383:LEU:HD11	1:A:386:PRO:CA	2.30	0.61
1:B:249:TYR:HA	1:B:328:THR:C	2.21	0.61
1:B:242:VAL:O	1:B:243:GLU:CB	2.49	0.60
1:D:360:MET:HE1	1:D:418:LEU:HD23	1.83	0.60
1:B:435:HIS:O	1:B:440:LYS:HE2	2.02	0.60
1:A:260:SER:C	1:A:262:ASN:H	2.05	0.60
1:B:323:GLY:H	1:B:331:HIS:HE1	1.46	0.60
1:A:243:GLU:O	1:A:244:PRO:C	2.40	0.60
1:B:315:HIS:CG	1:B:367:LEU:HD22	2.37	0.60
1:A:326:LEU:HD22	1:A:330:LEU:HD23	1.82	0.60
1:C:445:THR:HB	1:C:446:PRO:HD3	1.84	0.59
1:A:446:PRO:O	1:A:449:THR:HG22	2.03	0.59
1:C:344:ALA:HB3	3:C:551:HOH:O	2.03	0.59
1:A:436:LEU:N	1:A:436:LEU:HD22	2.18	0.59
1:C:324:ILE:CD1	1:C:441:LEU:HD21	2.32	0.59
1:D:238:ALA:HA	1:D:285:ARG:HE	1.67	0.59
1:A:244:PRO:O	1:A:245:LYS:O	2.21	0.58
1:A:405:LYS:NZ	3:A:560:HOH:O	2.36	0.58
1:D:421:ARG:CD	3:D:570:HOH:O	2.50	0.58
1:D:232:VAL:HG12	1:D:233:GLU:OE2	2.04	0.58
1:B:294:LEU:HD23	1:D:452:MET:SD	2.44	0.58
1:B:244:PRO:O	1:B:248:THR:CB	2.51	0.58
1:D:236:LEU:C	1:D:236:LEU:HD13	2.24	0.58
1:B:443:GLY:O	1:B:446:PRO:HD2	2.03	0.57
1:C:309:LEU:HD13	2:C:502:REA:C19	2.34	0.57
1:C:333:HIS:O	1:C:337:ALA:CB	2.53	0.57
1:A:434:GLU:HG3	3:A:553:HOH:O	2.05	0.56
1:C:250:VAL:O	1:C:252:ALA:N	2.39	0.56
1:C:242:VAL:HG21	1:C:278:THR:O	2.06	0.56
1:C:257:ASN:C	1:C:259:SER:H	2.09	0.56
1:D:390:GLU:O	1:D:394:GLU:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:325:LEU:HD12	1:D:331:HIS:HD2	1.69	0.56
1:C:309:LEU:HD13	2:C:502:REA:H193	1.87	0.56
1:C:338:HIS:O	1:C:341:GLY:N	2.32	0.56
1:A:232:VAL:HA	1:A:235:ILE:HG13	1.88	0.56
1:D:363:ASP:OD1	1:D:366:GLU:HG2	2.05	0.56
1:A:232:VAL:HA	1:A:235:ILE:CG1	2.36	0.56
1:C:306:ASN:HB3	3:C:589:HOH:O	2.05	0.55
1:D:236:LEU:HD22	1:D:236:LEU:O	2.06	0.55
1:D:348:ARG:HD3	1:D:352:GLU:OE2	2.06	0.55
1:C:357:MET:HA	1:C:362:MET:SD	2.46	0.55
1:D:326:LEU:HB2	1:D:331:HIS:CE1	2.41	0.55
1:D:421:ARG:HD2	3:D:570:HOH:O	2.06	0.55
1:B:268:ILE:HD11	2:B:501:REA:H172	1.89	0.55
1:A:236:LEU:O	1:A:236:LEU:HD13	2.07	0.55
1:B:264:PRO:HG3	1:B:450:PHE:CG	2.41	0.55
1:C:411:GLN:NE2	1:C:414:ARG:HH11	2.04	0.55
1:C:346:PHE:O	1:C:350:LEU:HD22	2.06	0.54
1:D:439:PHE:HE1	1:D:447:ILE:HD11	1.72	0.54
1:D:263:ASP:N	1:D:264:PRO:CD	2.70	0.54
1:C:411:GLN:HE22	1:C:414:ARG:HH11	1.54	0.54
1:A:296:ASP:HA	1:A:299:ILE:CG2	2.38	0.54
1:B:265:VAL:HG11	1:D:272:ALA:HB3	1.89	0.54
1:C:452:MET:O	1:C:456:GLU:HA	2.06	0.54
1:A:446:PRO:HA	1:A:449:THR:CG2	2.37	0.54
1:C:455:LEU:O	1:C:456:GLU:HG3	2.07	0.54
1:D:334:ARG:HG2	3:D:474:HOH:O	2.07	0.54
1:A:271:ALA:C	1:A:273:ASP:N	2.60	0.54
1:C:411:GLN:HB3	1:C:414:ARG:HB2	1.90	0.54
1:A:259:SER:O	1:A:260:SER:C	2.46	0.54
1:B:297:GLN:NE2	1:D:455:LEU:HD22	2.23	0.53
1:C:332:VAL:HG22	1:C:337:ALA:HB2	1.91	0.53
1:A:276:LEU:O	1:A:280:VAL:HG23	2.08	0.53
1:B:245:LYS:C	1:B:247:GLU:N	2.60	0.53
1:B:255:GLY:O	1:B:256:LEU:C	2.47	0.53
1:B:333:HIS:HE1	3:B:554:HOH:O	1.91	0.53
1:D:234:ARG:HE	1:D:287:PRO:CG	2.21	0.53
1:D:457:ALA:O	1:D:458:PRO:C	2.44	0.53
1:C:232:VAL:HG23	1:C:369:CYS:SG	2.48	0.52
1:A:381:LYS:HE3	3:C:558:HOH:O	2.09	0.52
1:B:302:ARG:HH12	1:D:444:ASP:HB2	1.74	0.52
1:A:452:MET:O	1:A:456:GLU:CB	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:LEU:HD12	1:A:439:PHE:HD2	1.75	0.52
1:B:232:VAL:HG13	1:B:365:THR:HG23	1.91	0.52
1:D:445:THR:N	1:D:446:PRO:CD	2.73	0.52
1:B:253:ASN:O	1:B:254:MET:CB	2.56	0.52
1:C:386:PRO:HD2	3:C:588:HOH:O	2.09	0.52
1:D:353:LEU:O	1:D:357:MET:HG3	2.10	0.52
1:D:360:MET:HE3	1:D:418:LEU:HD23	1.91	0.52
1:D:317:SER:OG	1:D:324:ILE:HA	2.11	0.51
1:A:452:MET:O	1:A:456:GLU:HB2	2.10	0.51
1:B:248:THR:C	1:B:250:VAL:H	2.12	0.51
1:A:242:VAL:O	1:A:244:PRO:N	2.44	0.51
1:D:421:ARG:HD3	3:D:570:HOH:O	2.10	0.51
1:B:244:PRO:O	1:B:245:LYS:O	2.28	0.51
1:B:369:CYS:CB	1:B:400:LEU:HG	2.40	0.51
1:D:351:THR:HG22	1:D:352:GLU:HG3	1.92	0.51
1:A:259:SER:O	1:A:260:SER:O	2.28	0.51
1:A:450:PHE:HA	1:A:453:GLU:HB3	1.92	0.51
1:D:253:ASN:CB	1:D:329:GLY:N	2.69	0.51
1:D:289:PHE:O	1:D:292:LEU:HB2	2.11	0.51
1:A:296:ASP:HA	1:A:299:ILE:HG22	1.93	0.51
1:D:268:ILE:N	1:D:268:ILE:HD12	2.21	0.51
1:C:411:GLN:HE22	1:C:414:ARG:NH1	2.08	0.51
1:C:338:HIS:O	1:C:339:SER:C	2.49	0.50
1:C:437:PHE:O	1:C:441:LEU:HB2	2.11	0.50
1:A:276:LEU:HG	1:C:450:PHE:HE2	1.76	0.50
1:D:434:GLU:HG2	1:D:435:HIS:CD2	2.46	0.50
1:C:306:ASN:HD21	1:C:429:GLY:C	2.14	0.50
1:B:442:ILE:HD11	2:B:501:REA:C17	2.38	0.50
1:D:324:ILE:O	1:D:331:HIS:HB2	2.11	0.50
1:A:287:PRO:O	1:A:288:HIS:HB2	2.12	0.50
1:C:328:THR:OG1	1:C:328:THR:O	2.26	0.50
1:D:360:MET:HE3	1:D:418:LEU:CD2	2.42	0.50
1:B:309:LEU:CD1	2:B:501:REA:H193	2.42	0.50
1:C:332:VAL:CG2	1:C:337:ALA:HB2	2.42	0.50
1:C:345:ILE:HD11	1:C:437:PHE:CD2	2.47	0.50
1:D:439:PHE:CE1	1:D:447:ILE:HD11	2.47	0.50
1:B:457:ALA:HB1	1:B:458:PRO:HD2	1.94	0.49
1:A:232:VAL:HG22	1:A:235:ILE:HB	1.94	0.49
1:B:245:LYS:O	1:B:248:THR:N	2.40	0.49
1:A:233:GLU:O	1:A:237:GLU:HB3	2.11	0.49
1:A:232:VAL:O	1:A:235:ILE:HB	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:LEU:HD22	3:B:520:HOH:O	2.11	0.49
1:D:236:LEU:HD11	1:D:240:LEU:HD12	1.93	0.49
1:C:326:LEU:HD22	2:C:502:REA:C20	2.43	0.49
1:B:443:GLY:C	1:B:446:PRO:HD2	2.33	0.49
1:C:298:VAL:O	1:C:302:ARG:HG3	2.13	0.49
1:D:317:SER:HB3	1:D:323:GLY:O	2.13	0.49
1:B:249:TYR:O	1:B:328:THR:O	2.30	0.49
1:B:306:ASN:O	1:B:310:ILE:HG22	2.13	0.48
1:C:448:ASP:O	1:C:452:MET:HG2	2.13	0.48
1:D:305:TRP:O	1:D:309:LEU:HD23	2.13	0.48
1:B:451:LEU:HD23	1:D:298:VAL:HG13	1.94	0.48
1:C:245:LYS:C	1:C:247:GLU:H	2.16	0.48
1:B:272:ALA:HB2	2:B:501:REA:C17	2.44	0.48
1:C:232:VAL:HG22	1:C:365:THR:HG23	1.96	0.48
1:C:313:PHE:CD1	1:C:324:ILE:HD12	2.48	0.48
1:D:250:VAL:O	1:D:253:ASN:N	2.45	0.48
1:A:257:ASN:O	1:A:258:PRO:O	2.30	0.48
1:C:232:VAL:CG2	1:C:365:THR:HG23	2.44	0.48
1:C:315:HIS:CG	1:C:367:LEU:HD22	2.49	0.48
1:C:449:THR:O	1:C:453:GLU:HG2	2.13	0.48
1:A:232:VAL:CG2	1:A:235:ILE:CD1	2.82	0.47
1:C:369:CYS:O	1:C:373:ILE:HG13	2.14	0.47
1:A:451:LEU:HD23	1:C:298:VAL:HG13	1.96	0.47
2:B:501:REA:H181	2:B:501:REA:H7	1.49	0.47
1:A:276:LEU:HG	1:C:450:PHE:CE2	2.50	0.47
1:D:317:SER:O	1:D:320:VAL:HG13	2.14	0.47
1:D:362:MET:HA	1:D:366:GLU:OE2	2.15	0.47
1:B:348:ARG:HD3	1:B:352:GLU:OE2	2.15	0.47
1:B:391:ALA:O	1:B:394:GLU:HG3	2.14	0.47
1:B:231:PRO:CD	1:B:234:ARG:HH11	2.27	0.47
1:B:259:SER:O	1:B:260:SER:O	2.33	0.47
1:A:273:ASP:OD1	1:C:265:VAL:HG13	2.14	0.47
1:D:332:VAL:HG11	1:D:441:LEU:HD22	1.97	0.47
1:C:252:ALA:C	1:C:254:MET:N	2.65	0.47
1:C:255:GLY:O	1:C:256:LEU:CB	2.62	0.47
1:A:235:ILE:O	1:A:239:GLU:HG3	2.15	0.47
1:B:248:THR:C	1:B:250:VAL:N	2.68	0.47
1:C:250:VAL:C	1:C:252:ALA:H	2.18	0.47
1:A:232:VAL:CA	1:A:235:ILE:HB	2.44	0.46
1:B:307:GLU:HA	1:B:310:ILE:HG22	1.98	0.46
1:C:310:ILE:HA	1:C:313:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:ILE:H	1:D:268:ILE:CD1	2.23	0.46
1:A:252:ALA:C	1:A:254:MET:H	2.19	0.46
1:A:269:CYS:O	1:A:271:ALA:O	2.33	0.46
1:C:327:ALA:C	1:C:329:GLY:N	2.68	0.46
1:C:313:PHE:CE1	1:C:324:ILE:HD12	2.49	0.46
1:C:324:ILE:HG23	1:C:346:PHE:CZ	2.50	0.46
1:A:232:VAL:HA	1:A:235:ILE:HB	1.97	0.46
1:D:450:PHE:CD1	1:D:451:LEU:N	2.83	0.46
1:B:276:LEU:HD21	2:B:501:REA:H181	1.98	0.46
1:C:285:ARG:NH1	3:C:570:HOH:O	2.49	0.46
1:C:337:ALA:C	1:C:339:SER:N	2.69	0.46
1:D:321:LYS:NZ	1:D:322:ASP:OD2	2.49	0.45
1:B:309:LEU:CD1	2:B:501:REA:C19	2.94	0.45
1:D:236:LEU:HD11	1:D:240:LEU:CD1	2.46	0.45
1:D:265:VAL:O	1:D:269:CYS:SG	2.75	0.45
1:A:353:LEU:O	1:A:357:MET:HG3	2.17	0.45
1:A:436:LEU:HD12	1:A:439:PHE:CD2	2.51	0.45
1:C:236:LEU:HD13	1:C:236:LEU:C	2.37	0.45
1:B:287:PRO:O	1:B:288:HIS:HB2	2.17	0.45
1:B:330:LEU:HD13	1:B:331:HIS:N	2.31	0.45
1:D:329:GLY:C	1:D:330:LEU:HD12	2.37	0.45
1:B:436:LEU:N	1:B:436:LEU:HD12	2.32	0.45
1:D:417:LYS:NZ	3:D:490:HOH:O	2.42	0.45
1:B:323:GLY:H	1:B:331:HIS:CE1	2.31	0.44
1:C:363:ASP:OD1	1:C:366:GLU:HG3	2.17	0.44
1:B:295:ASP:O	1:B:299:ILE:HG12	2.17	0.44
1:D:259:SER:O	1:D:260:SER:C	2.55	0.44
1:A:234:ARG:HG3	3:A:541:HOH:O	2.18	0.44
1:C:324:ILE:HG12	1:C:332:VAL:CG1	2.48	0.44
1:C:252:ALA:C	1:C:254:MET:H	2.21	0.44
1:A:258:PRO:C	1:A:260:SER:H	2.21	0.44
1:C:239:GLU:OE1	1:C:368:GLY:HA2	2.17	0.44
1:C:439:PHE:CD1	1:C:439:PHE:C	2.91	0.44
1:A:394:GLU:HA	1:A:397:TYR:CE2	2.53	0.44
1:B:309:LEU:HD13	2:B:501:REA:H193	1.99	0.44
1:B:394:GLU:HA	1:B:397:TYR:CE2	2.52	0.44
1:D:236:LEU:HD22	1:D:240:LEU:HG	2.00	0.44
1:D:260:SER:O	1:D:262:ASN:N	2.50	0.44
1:C:346:PHE:O	1:C:350:LEU:CD2	2.66	0.44
1:A:260:SER:C	1:A:262:ASN:N	2.71	0.44
1:A:258:PRO:O	1:A:260:SER:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:ILE:HD11	1:B:353:LEU:CD1	2.48	0.44
1:C:252:ALA:CA	1:C:255:GLY:H	2.31	0.44
1:D:330:LEU:O	1:D:331:HIS:CD2	2.71	0.44
1:D:347:ASP:O	1:D:351:THR:HB	2.18	0.43
1:A:252:ALA:CB	1:A:328:THR:O	2.65	0.43
1:C:277:PHE:CE2	1:C:281:GLU:OE2	2.71	0.43
1:C:279:LEU:HD21	1:C:305:TRP:HA	1.98	0.43
1:D:250:VAL:O	1:D:251:GLU:C	2.56	0.43
1:D:445:THR:N	1:D:446:PRO:HD3	2.33	0.43
1:B:268:ILE:HD13	1:B:268:ILE:C	2.39	0.43
1:B:307:GLU:HA	1:B:310:ILE:CG2	2.47	0.43
1:C:251:GLU:HA	1:C:255:GLY:O	2.19	0.43
1:A:231:PRO:HD2	1:A:287:PRO:HG2	2.00	0.43
1:B:309:LEU:HD13	2:B:501:REA:C19	2.49	0.43
1:B:436:LEU:N	1:B:436:LEU:CD1	2.80	0.43
1:D:328:THR:O	1:D:329:GLY:C	2.57	0.43
1:A:455:LEU:HD22	1:C:297:GLN:HE21	1.84	0.43
1:D:263:ASP:O	1:D:264:PRO:C	2.56	0.43
1:D:313:PHE:C	1:D:313:PHE:CD1	2.92	0.43
1:A:232:VAL:HG11	3:A:501:HOH:O	2.04	0.43
1:A:236:LEU:HD13	1:A:240:LEU:HD12	2.01	0.43
1:D:239:GLU:OE1	1:D:239:GLU:HA	2.18	0.43
1:A:444:ASP:HB2	1:C:302:ARG:HH12	1.84	0.42
1:C:236:LEU:HD23	1:C:365:THR:HA	2.01	0.42
1:D:332:VAL:HG13	1:D:336:SER:HB2	2.00	0.42
1:D:370:LEU:O	1:D:374:VAL:HG23	2.19	0.42
1:B:315:HIS:CB	1:B:367:LEU:HD22	2.49	0.42
1:A:451:LEU:HD12	1:A:451:LEU:HA	1.89	0.42
1:A:456:GLU:O	1:A:457:ALA:O	2.36	0.42
1:A:297:GLN:OE1	1:C:455:LEU:HD12	2.20	0.42
1:D:321:LYS:CE	1:D:322:ASP:OD2	2.67	0.42
1:A:436:LEU:CD2	1:A:436:LEU:N	2.82	0.42
1:D:327:ALA:CA	1:D:331:HIS:NE2	2.80	0.42
1:A:280:VAL:O	1:A:284:LYS:HG3	2.19	0.42
1:B:264:PRO:HG3	1:B:450:PHE:CD2	2.55	0.42
1:C:331:HIS:C	1:C:331:HIS:CD2	2.92	0.42
1:A:285:ARG:HH11	1:A:285:ARG:HG3	1.85	0.42
1:A:383:LEU:HD11	1:A:386:PRO:N	2.35	0.42
1:B:253:ASN:HA	1:B:330:LEU:HD23	2.02	0.42
1:D:392:LEU:O	1:D:396:VAL:HG23	2.20	0.42
1:C:423:PRO:HD2	3:C:597:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:GLN:HE21	1:D:455:LEU:HD22	1.83	0.41
1:C:327:ALA:O	1:C:329:GLY:N	2.49	0.41
1:C:337:ALA:O	1:C:339:SER:N	2.53	0.41
1:B:313:PHE:C	1:B:313:PHE:CD1	2.94	0.41
1:C:250:VAL:C	1:C:252:ALA:N	2.74	0.41
1:A:272:ALA:H	1:A:275:GLN:HG2	1.85	0.41
1:C:452:MET:O	1:C:456:GLU:N	2.54	0.41
1:A:296:ASP:CA	1:A:299:ILE:HG22	2.50	0.41
1:A:455:LEU:HD22	1:C:297:GLN:NE2	2.35	0.41
1:C:245:LYS:C	1:C:247:GLU:N	2.73	0.41
1:D:259:SER:O	1:D:260:SER:O	2.37	0.41
1:A:293:PRO:HD2	1:A:296:ASP:HB2	2.03	0.41
1:A:320:VAL:HG12	1:A:321:LYS:N	2.35	0.41
1:A:405:LYS:NZ	1:A:412:PRO:HA	2.36	0.41
1:C:376:PHE:CE1	1:C:392:LEU:HD23	2.56	0.41
1:D:236:LEU:CD2	1:D:240:LEU:HG	2.50	0.41
1:A:444:ASP:O	1:A:447:ILE:HB	2.21	0.41
1:B:369:CYS:HB3	1:B:400:LEU:HG	2.03	0.41
1:C:331:HIS:HD2	1:C:332:VAL:N	2.19	0.41
2:C:502:REA:H12	2:C:502:REA:H191	2.03	0.41
1:D:363:ASP:CG	1:D:366:GLU:HG2	2.42	0.41
1:A:280:VAL:HG11	1:C:454:MET:CB	2.49	0.41
1:A:232:VAL:HA	1:A:235:ILE:CB	2.50	0.41
1:B:441:LEU:HD23	2:B:501:REA:H202	2.03	0.41
1:D:251:GLU:O	1:D:256:LEU:N	2.42	0.41
1:D:287:PRO:O	1:D:288:HIS:HB2	2.20	0.41
1:C:357:MET:HG2	1:C:362:MET:SD	2.60	0.40
1:D:442:ILE:HD11	3:D:550:HOH:O	2.20	0.40
1:A:320:VAL:CG1	1:A:321:LYS:N	2.84	0.40
1:A:431:LYS:HA	1:A:431:LYS:HD3	1.82	0.40
1:B:251:GLU:O	1:B:257:ASN:CB	2.69	0.40
1:B:272:ALA:HB2	2:B:501:REA:H173	2.04	0.40
1:A:296:ASP:C	1:A:299:ILE:HG22	2.42	0.40
1:D:410:GLU:HG3	1:D:410:GLU:H	1.55	0.40
1:C:436:LEU:N	1:C:436:LEU:HD12	2.36	0.40
1:D:329:GLY:C	1:D:330:LEU:O	2.55	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)
3:B:554:HOH:O	3:D:492:HOH:O[1_455]	1.79	0.41

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	226/238 (95%)	201 (89%)	14 (6%)	11 (5%)	2	0
1	B	227/238 (95%)	202 (89%)	11 (5%)	14 (6%)	1	0
1	C	224/238 (94%)	196 (88%)	20 (9%)	8 (4%)	3	1
1	D	227/238 (95%)	206 (91%)	11 (5%)	10 (4%)	2	0
All	All	904/952 (95%)	805 (89%)	56 (6%)	43 (5%)	2	0

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	PRO
1	A	245	LYS
1	A	258	PRO
1	A	264	PRO
1	A	457	ALA
1	B	243	GLU
1	B	244	PRO
1	B	246	THR
1	B	251	GLU
1	B	253	ASN
1	B	254	MET
1	B	256	LEU
1	B	260	SER
1	B	264	PRO
1	C	256	LEU
1	C	339	SER
1	D	245	LYS

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Mol	Chain	Res	Type
1	D	264	PRO
1	A	259	SER
1	B	241	ALA
1	C	251	GLU
1	C	264	PRO
1	D	250	VAL
1	D	329	GLY
1	A	243	GLU
1	A	254	MET
1	A	261	PRO
1	B	245	LYS
1	B	258	PRO
1	C	260	SER
1	D	258	PRO
1	D	260	SER
1	D	327	ALA
1	A	260	SER
1	C	257	ASN
1	C	328	THR
1	C	341	GLY
1	D	251	GLU
1	A	272	ALA
1	D	261	PRO
1	B	322	ASP
1	D	263	ASP
1	B	250	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	172/205 (84%)	156 (91%)	16 (9%)	9 5
1	B	176/205 (86%)	165 (94%)	11 (6%)	18 13
1	C	172/205 (84%)	161 (94%)	11 (6%)	17 13
1	D	174/205 (85%)	160 (92%)	14 (8%)	12 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	694/820 (85%)	642 (92%)	52 (8%)	13 9

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	232	VAL
1	A	273	ASP
1	A	294	LEU
1	A	299	ILE
1	A	308	LEU
1	A	309	LEU
1	A	353	LEU
1	A	385	ASN
1	A	393	ARG
1	A	405	LYS
1	A	418	LEU
1	A	419	LEU
1	A	422	LEU
1	A	445	THR
1	A	450	PHE
1	A	455	LEU
1	B	267	ASN
1	B	268	ILE
1	B	318	ILE
1	B	331	HIS
1	B	345	ILE
1	B	350	LEU
1	B	385	ASN
1	B	392	LEU
1	B	400	LEU
1	B	453	GLU
1	B	456	GLU
1	C	263	ASP
1	C	265	VAL
1	C	301	LEU
1	C	324	ILE
1	C	328	THR
1	C	362	MET
1	C	370	LEU
1	C	419	LEU
1	C	436	LEU
1	C	442	ILE

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Mol	Chain	Res	Type
1	C	453	GLU
1	D	236	LEU
1	D	292	LEU
1	D	306	ASN
1	D	320	VAL
1	D	321	LYS
1	D	345	ILE
1	D	351	THR
1	D	366	GLU
1	D	410	GLU
1	D	425	LEU
1	D	433	LEU
1	D	434	GLU
1	D	445	THR
1	D	450	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	A	275	GLN
1	A	335	ASN
1	A	338	HIS
1	B	267	ASN
1	B	270	GLN
1	B	288	HIS
1	B	297	GLN
1	B	331	HIS
1	B	333	HIS
1	B	385	ASN
1	C	270	GLN
1	C	288	HIS
1	C	297	GLN
1	C	306	ASN
1	C	411	GLN
1	D	267	ASN
1	D	435	HIS

5.3.3 RNA

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 carbohydrates 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	501	-	19,22,22	3.10	8 (42%)	26,30,30	3.85	18 (69%)
2	REA	C	502	-	19,22,22	3.15	9 (47%)	26,30,30	3.46	17 (65%)

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	501	-	-	5/13/32/32	0/1/1/1
2	REA	C	502	-	-	1/13/32/32	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	REA	C1-C6	8.80	1.65	1.53
2	C	502	REA	C1-C6	8.08	1.64	1.53
2	B	501	REA	C12-C13	-5.52	1.34	1.45
2	C	502	REA	C12-C13	-5.21	1.34	1.45
2	C	502	REA	C5-C6	4.84	1.42	1.34
2	C	502	REA	C8-C9	-4.24	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	REA	C8-C9	-3.92	1.37	1.45
2	C	502	REA	C18-C5	3.87	1.57	1.50
2	B	501	REA	C18-C5	3.54	1.56	1.50
2	B	501	REA	C14-C13	3.46	1.39	1.35
2	C	502	REA	C14-C13	3.44	1.39	1.35
2	B	501	REA	C5-C6	3.23	1.40	1.34
2	B	501	REA	C11-C10	-2.98	1.34	1.43
2	C	502	REA	C4-C5	2.82	1.56	1.51
2	C	502	REA	C11-C10	-2.69	1.35	1.43
2	C	502	REA	C17-C1	2.38	1.58	1.53
2	B	501	REA	C4-C5	2.32	1.55	1.51

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	REA	C11-C10-C9	11.23	143.34	127.31
2	C	502	REA	C11-C10-C9	8.66	139.67	127.31
2	B	501	REA	C17-C1-C6	6.67	121.11	110.30
2	C	502	REA	C17-C1-C6	5.94	119.94	110.30
2	C	502	REA	C18-C5-C6	5.68	130.91	124.53
2	C	502	REA	C1-C6-C5	-5.35	115.08	122.61
2	B	501	REA	C1-C6-C5	-5.29	115.17	122.61
2	B	501	REA	C1-C6-C7	5.01	129.96	115.78
2	C	502	REA	C1-C6-C7	4.40	128.24	115.78
2	B	501	REA	C8-C9-C10	-4.30	112.35	118.94
2	B	501	REA	C18-C5-C6	-4.19	119.82	124.53
2	B	501	REA	C10-C11-C12	4.04	135.82	123.22
2	B	501	REA	C7-C8-C9	3.93	132.18	126.23
2	B	501	REA	C2-C3-C4	-3.71	103.09	111.38
2	C	502	REA	C2-C3-C4	-3.68	103.15	111.38
2	C	502	REA	C18-C5-C4	-3.50	106.89	113.62
2	B	501	REA	C2-C1-C6	3.39	115.70	110.48
2	C	502	REA	C16-C1-C6	3.36	115.75	110.30
2	C	502	REA	C10-C11-C12	3.23	133.31	123.22
2	B	501	REA	C16-C1-C6	3.13	115.37	110.30
2	C	502	REA	C7-C8-C9	3.07	130.88	126.23
2	C	502	REA	C20-C13-C12	3.07	122.91	118.08
2	C	502	REA	C8-C9-C10	-3.00	114.33	118.94
2	C	502	REA	C2-C1-C6	3.00	115.10	110.48
2	B	501	REA	C20-C13-C12	2.72	122.36	118.08
2	B	501	REA	C7-C6-C5	-2.72	114.88	121.46
2	B	501	REA	C16-C1-C2	-2.68	98.19	108.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	REA	C18-C5-C4	2.64	118.70	113.62
2	C	502	REA	C16-C1-C2	-2.64	98.36	108.91
2	B	501	REA	C19-C9-C10	2.61	126.59	122.92
2	B	501	REA	C17-C1-C2	-2.18	100.19	108.91
2	C	502	REA	C8-C7-C6	2.16	133.28	127.20
2	B	501	REA	C8-C7-C6	2.09	133.09	127.20
2	C	502	REA	C19-C9-C10	2.05	125.79	122.92
2	C	502	REA	C17-C1-C2	-2.03	100.77	108.91

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	REA	C9-C10-C11-C12
2	B	501	REA	C11-C12-C13-C14
2	B	501	REA	C11-C12-C13-C20
2	C	502	REA	C9-C10-C11-C12
2	B	501	REA	C11-C10-C9-C8
2	B	501	REA	C11-C10-C9-C19

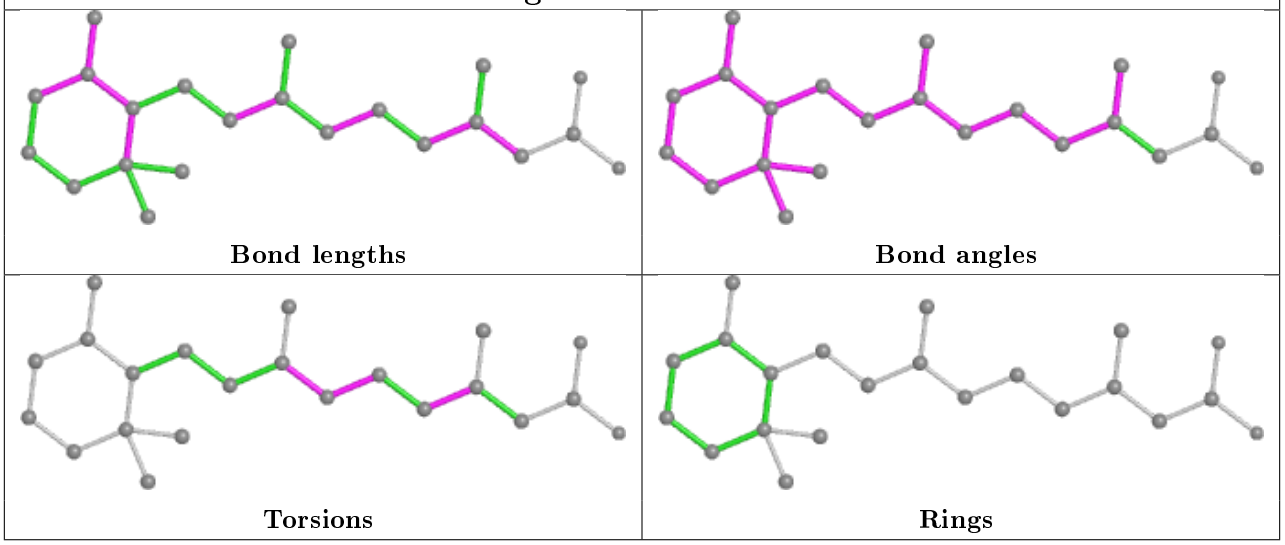
There are no ring outliers.

2 monomers are involved in 19 short contacts:

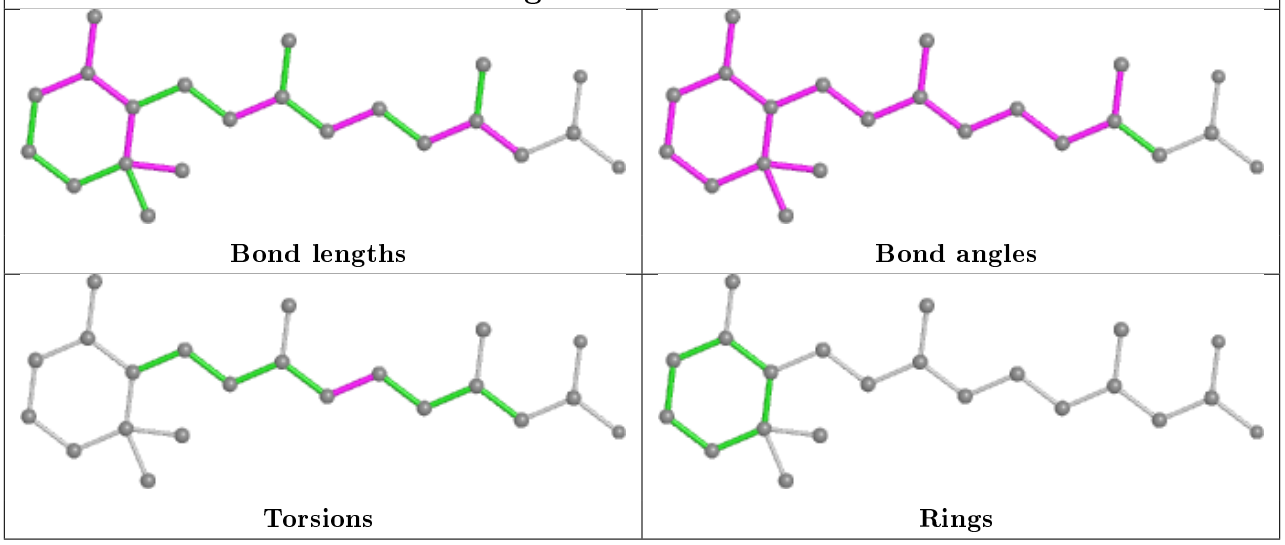
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	REA	14	0
2	C	502	REA	5	0

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 501



Ligand REA C 502



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.