Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 07:06 AM GMT

PDB ID	:	2ZK3
Title	:	Human peroxisome proliferator-activated receptor gamma ligand binding domain complexed with 8-oxo-eicosatetraenoic acid
Authors	:	Waku, T.; Shiraki, T.; Oyama, T.; Fujimoto, Y.; Morikawa, K.
Deposited on	:	2008-03-12
Resolution	:	2.58 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
http://wwpdb.org/validation/2016/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:

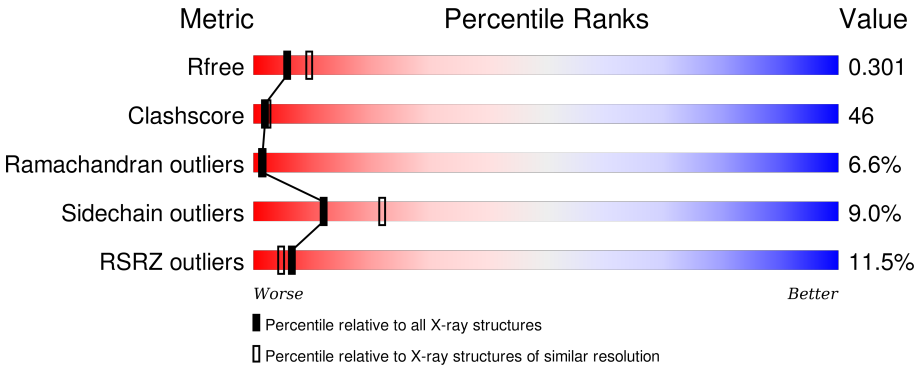
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.58 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}	91344	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (2.60-2.56)

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. 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	286	7%, 44%, 44%, 7% • •
1	B	286	15%, 36%, 44%, 10% • 8%

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	OCX	A	1	-	-	-	X
2	OCX	B	2	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4409 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.

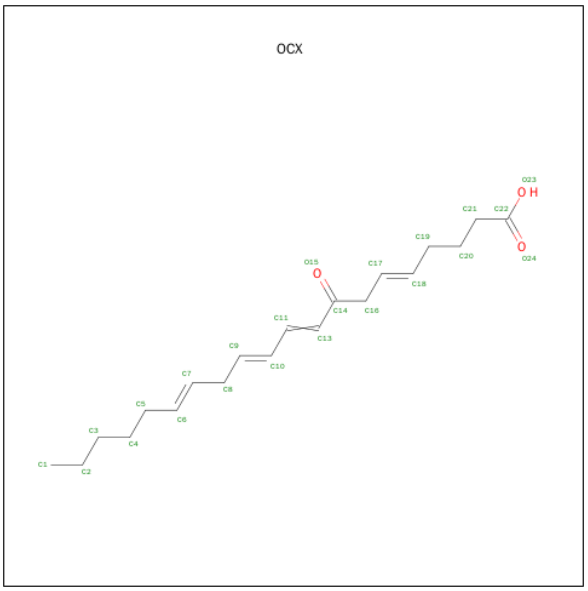
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2186	1409	358	409	10			
1	B	263	Total	C	N	O	S	0	0	0
			2110	1363	346	392	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	191	GLY	-	EXPRESSION TAG	UNP P37231
A	192	SER	-	EXPRESSION TAG	UNP P37231
A	193	HIS	-	EXPRESSION TAG	UNP P37231
A	194	MET	-	EXPRESSION TAG	UNP P37231
B	191	GLY	-	EXPRESSION TAG	UNP P37231
B	192	SER	-	EXPRESSION TAG	UNP P37231
B	193	HIS	-	EXPRESSION TAG	UNP P37231
B	194	MET	-	EXPRESSION TAG	UNP P37231

- Molecule 2 is (5E,11E,14E)-8-OXOICOSA-5,9,11,14-TETRAENOIC ACID (three-letter code: OCX) (formula: $C_{20}H_{30}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 23 20 3	0	0
2	B	1	Total C O 23 20 3	0	0

- Molecule 3 is water.

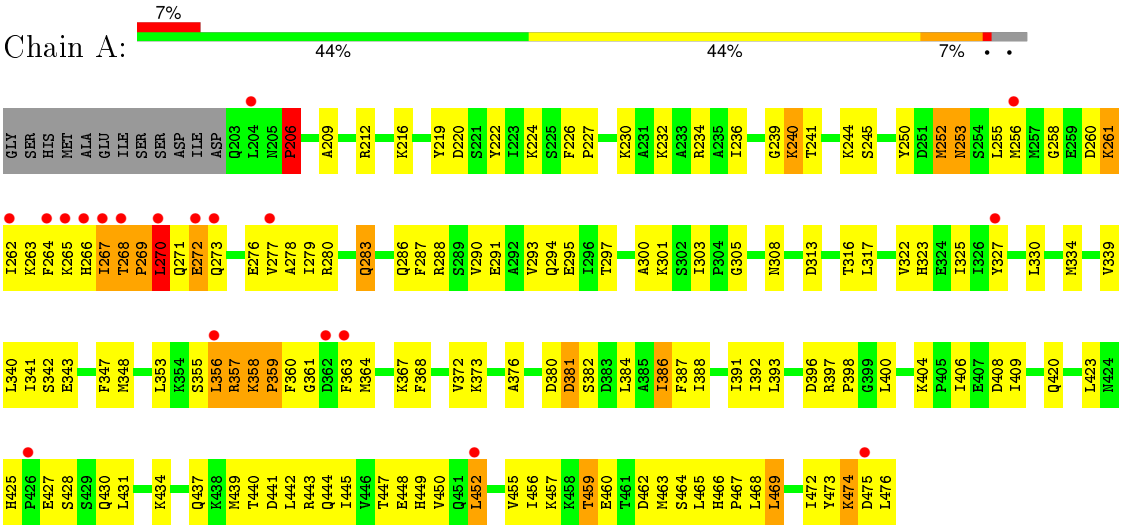
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	37	Total O 37 37	0	0
3	B	30	Total O 30 30	0	0

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 errors 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.

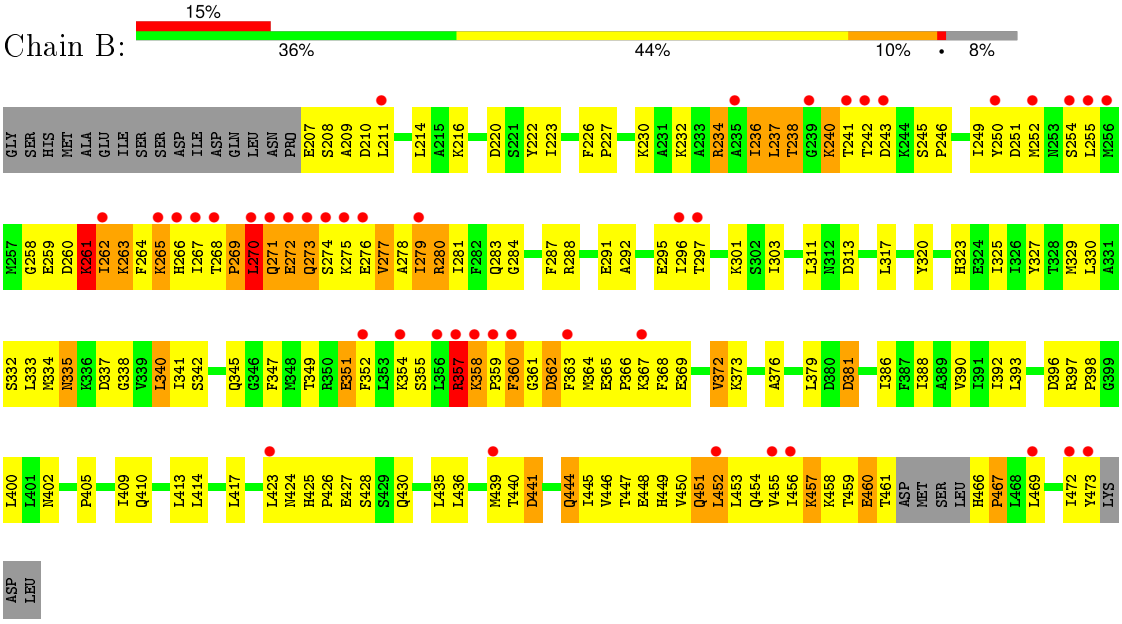
- Molecule 1: Peroxisome proliferator-activated receptor gamma

Chain A:



- Molecule 1: Peroxisome proliferator-activated receptor gamma

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	93.30Å 60.99Å 118.39Å 90.00° 103.00° 90.00°	Depositor
Resolution (Å)	32.66 – 2.58 48.68 – 2.58	Depositor EDS
% Data completeness (in resolution range)	93.4 (32.66-2.58) 93.4 (48.68-2.58)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.02 (at 2.58Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.299 0.246 , 0.301	Depositor DCC
R_{free} test set	937 reflections (4.85%)	DCC
Wilson B-factor (Å^2)	48.5	Xtriage
Anisotropy	0.574	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 55.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 20113 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4409	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.46	0/2223	0.69	1/2995 (0.0%)
1	B	0.47	0/2146	0.70	0/2891
All	All	0.47	0/4369	0.69	1/5886 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	206	PRO	N-CA-CB	5.15	109.48	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2186	0	2238	179	0
1	B	2110	0	2173	238	0
2	A	23	0	29	7	0
2	B	23	0	29	4	0
3	A	37	0	0	3	0
3	B	30	0	0	4	0
All	All	4409	0	4469	409	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 46.

All (409) 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:358:LYS:HB2	1:A:359:PRO:HD3	1.26	1.11
1:A:268:THR:HB	1:A:280:ARG:HH11	1.11	1.08
1:B:459:THR:HG22	1:B:460:GLU:H	1.24	1.02
1:A:241:THR:HG21	1:A:244:LYS:HD2	1.44	0.99
1:B:362:ASP:O	1:B:366:PRO:HD3	1.69	0.93
1:A:268:THR:HG23	1:A:283:GLN:HB2	1.50	0.93
1:B:280:ARG:HA	1:B:283:GLN:NE2	1.86	0.91
1:A:264:PHE:HD2	1:A:266:HIS:HB3	1.33	0.91
1:B:451:GLN:HE21	1:B:451:GLN:HA	1.35	0.91
1:A:469:LEU:HG	2:A:1:OCX:H20A	1.52	0.90
1:B:363:PHE:O	1:B:366:PRO:HD2	1.72	0.90
1:A:271:GLN:O	1:A:273:GLN:N	2.06	0.89
1:A:268:THR:HB	1:A:280:ARG:NH1	1.87	0.89
1:A:325:ILE:HG23	1:A:388:ILE:HD12	1.54	0.88
1:B:358:LYS:CB	1:B:359:PRO:HD3	2.03	0.88
1:A:293:VAL:HG22	1:A:322:VAL:HG11	1.54	0.87
1:A:358:LYS:HB2	1:A:359:PRO:CD	2.05	0.87
1:A:268:THR:CG2	1:A:283:GLN:HB2	2.05	0.87
1:A:363:PHE:HD2	1:A:452:LEU:HD13	1.40	0.86
1:B:360:PHE:CE1	1:B:456:ILE:HD11	2.11	0.86
1:B:255:LEU:HD23	1:B:277:VAL:HG12	1.57	0.85
1:B:263:LYS:C	1:B:265:LYS:H	1.78	0.84
1:B:358:LYS:HB2	1:B:359:PRO:HD3	1.59	0.84
1:A:273:GLN:HA	1:A:280:ARG:NH2	1.95	0.81
1:B:446:VAL:O	1:B:450:VAL:HG23	1.81	0.81
1:B:216:LYS:HE3	1:B:220:ASP:OD1	1.82	0.79
1:B:262:ILE:O	1:B:264:PHE:N	2.16	0.79
1:A:439:MET:HA	1:A:442:LEU:HD12	1.64	0.79
1:B:255:LEU:HD21	1:B:281:ILE:HD11	1.65	0.79
1:A:268:THR:HG21	1:A:280:ARG:HD3	1.64	0.78
1:A:265:LYS:HB3	1:A:342:SER:HA	1.65	0.78
1:A:273:GLN:HA	1:A:280:ARG:CZ	2.14	0.77
1:B:273:GLN:HE22	1:B:469:LEU:CD2	1.96	0.77
1:B:363:PHE:CZ	1:B:452:LEU:HB2	2.20	0.77
1:B:311:LEU:H	1:B:311:LEU:HD22	1.50	0.77
1:A:291:GLU:HA	1:A:294:GLN:OE1	1.85	0.77
1:B:269:PRO:O	1:B:270:LEU:HD12	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ARG:NH1	1:B:358:LYS:HE2	2.00	0.76
1:A:441:ASP:O	1:A:445:ILE:HG12	1.86	0.76
1:B:270:LEU:HB2	1:B:273:GLN:OE1	1.86	0.75
1:A:363:PHE:CD2	1:A:452:LEU:HD13	2.22	0.74
1:A:327:TYR:CE2	1:A:367:LYS:HE3	2.22	0.74
1:B:288:ARG:HH21	2:B:2:OCX:H3	1.50	0.74
1:A:268:THR:CB	1:A:280:ARG:HH11	1.96	0.74
1:B:273:GLN:HE22	1:B:469:LEU:HD22	1.52	0.74
1:B:270:LEU:HD22	1:B:273:GLN:NE2	2.03	0.74
1:B:460:GLU:O	1:B:460:GLU:HG3	1.89	0.73
1:B:250:TYR:HA	1:B:349:THR:CG2	2.18	0.72
1:A:241:THR:HG21	1:A:244:LYS:CD	2.20	0.72
1:B:265:LYS:HA	1:B:268:THR:OG1	1.90	0.72
1:B:402:ASN:O	1:B:405:PRO:HD2	1.90	0.72
1:A:264:PHE:C	1:A:266:HIS:H	1.90	0.72
1:A:327:TYR:CZ	1:A:367:LYS:HE3	2.25	0.71
1:A:469:LEU:O	1:A:473:TYR:HD2	1.73	0.71
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.73	0.71
1:A:456:ILE:HA	1:A:459:THR:CG2	2.20	0.71
1:A:260:ASP:O	1:A:261:LYS:HG2	1.91	0.71
1:A:276:GLU:HB3	1:A:279:ILE:HB	1.73	0.71
1:B:368:PHE:O	1:B:372:VAL:HG23	1.91	0.71
1:B:250:TYR:HA	1:B:349:THR:HG22	1.72	0.70
1:B:359:PRO:HA	1:B:362:ASP:OD2	1.89	0.70
1:B:335:ASN:ND2	1:B:338:GLY:H	1.88	0.70
1:B:330:LEU:HG	1:B:334:MET:HE3	1.73	0.70
1:B:207:GLU:C	1:B:209:ALA:H	1.94	0.70
1:A:437:GLN:HG2	1:B:439:MET:HE3	1.74	0.69
1:A:267:ILE:O	1:A:269:PRO:HD3	1.93	0.69
1:A:437:GLN:HG2	1:B:439:MET:CE	2.23	0.69
1:A:293:VAL:HG22	1:A:322:VAL:CG1	2.23	0.68
1:B:292:ALA:O	1:B:296:ILE:HG12	1.93	0.68
1:B:459:THR:HG22	1:B:460:GLU:N	2.05	0.68
1:B:335:ASN:HD22	1:B:337:ASP:H	1.40	0.68
1:B:388:ILE:O	1:B:392:ILE:HG13	1.92	0.68
1:B:472:ILE:HG22	1:B:472:ILE:O	1.94	0.68
1:A:241:THR:CG2	1:A:244:LYS:HD2	2.23	0.68
1:B:358:LYS:CB	1:B:359:PRO:CD	2.70	0.67
1:A:252:MET:HE2	1:A:255:LEU:HD12	1.77	0.67
1:B:358:LYS:HB3	1:B:359:PRO:HD3	1.73	0.67
1:B:277:VAL:O	1:B:281:ILE:HG12	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ASN:ND2	1:B:337:ASP:H	1.93	0.67
1:B:449:HIS:NE2	2:B:2:OCX:H19	2.11	0.66
1:A:276:GLU:OE1	1:A:276:GLU:HA	1.95	0.66
1:B:351:GLU:OE1	1:B:354:LYS:HE3	1.96	0.66
1:A:288:ARG:HH11	1:A:291:GLU:HB3	1.62	0.65
1:B:365:GLU:OE1	1:B:365:GLU:HA	1.97	0.65
1:B:269:PRO:O	1:B:270:LEU:C	2.35	0.65
1:B:341:ILE:HD12	1:B:342:SER:OG	1.97	0.65
1:A:363:PHE:CE2	1:A:452:LEU:HD22	2.31	0.65
1:A:240:LYS:O	1:A:241:THR:HG23	1.97	0.64
1:B:255:LEU:CD2	1:B:277:VAL:HG12	2.27	0.64
1:B:358:LYS:HB2	1:B:359:PRO:CD	2.27	0.64
1:A:252:MET:HA	1:A:255:LEU:HB3	1.80	0.64
1:A:323:HIS:CE1	1:A:472:ILE:HG21	2.33	0.64
1:B:335:ASN:HD22	1:B:335:ASN:C	2.01	0.63
1:B:238:THR:OG1	1:B:240:LYS:HG3	1.99	0.62
1:A:262:ILE:HG13	1:A:262:ILE:O	1.98	0.62
1:A:455:VAL:O	1:A:459:THR:HG22	2.00	0.62
1:B:207:GLU:O	1:B:209:ALA:N	2.33	0.62
1:B:263:LYS:NZ	1:B:265:LYS:HD2	2.14	0.62
1:B:270:LEU:HD13	1:B:273:GLN:CG	2.29	0.62
1:B:277:VAL:HG23	1:B:278:ALA:H	1.64	0.62
1:B:270:LEU:O	1:B:273:GLN:HG2	2.00	0.62
1:A:276:GLU:CB	1:A:279:ILE:HD12	2.30	0.61
1:A:469:LEU:CG	2:A:1:OCX:H20A	2.28	0.61
1:B:263:LYS:HZ2	1:B:265:LYS:CD	2.14	0.61
1:A:473:TYR:HA	1:A:476:LEU:HB2	1.81	0.61
1:A:277:VAL:HG13	1:A:278:ALA:H	1.64	0.61
1:B:452:LEU:HA	1:B:455:VAL:HB	1.81	0.61
1:A:276:GLU:HB3	1:A:279:ILE:HD12	1.83	0.61
1:B:453:LEU:O	1:B:456:ILE:HG22	2.02	0.60
1:A:393:LEU:HG	1:A:409:ILE:HG21	1.83	0.60
1:A:290:VAL:O	1:A:294:GLN:HG3	2.00	0.60
1:B:258:GLY:O	1:B:262:ILE:HG13	2.01	0.60
1:B:466:HIS:HB3	1:B:467:PRO:HD3	1.84	0.60
1:A:393:LEU:HG	1:A:409:ILE:CG2	2.32	0.60
1:B:351:GLU:HA	1:B:351:GLU:OE1	2.01	0.60
1:B:452:LEU:H	1:B:452:LEU:HD12	1.67	0.59
1:B:466:HIS:O	1:B:469:LEU:N	2.35	0.59
1:A:428:SER:OG	1:A:431:LEU:HB2	2.01	0.59
1:A:468:LEU:C	1:A:468:LEU:HD13	2.22	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:LEU:O	1:A:473:TYR:CD2	2.55	0.59
1:B:207:GLU:C	1:B:209:ALA:N	2.55	0.59
1:B:263:LYS:C	1:B:265:LYS:N	2.51	0.59
1:B:272:GLU:O	1:B:272:GLU:HG3	2.03	0.59
1:B:255:LEU:CD2	1:B:281:ILE:HD11	2.30	0.59
1:A:317:LEU:HD21	1:A:406:ILE:HD13	1.83	0.59
1:B:262:ILE:O	1:B:263:LYS:C	2.41	0.59
1:B:379:LEU:HD11	1:B:435:LEU:HD13	1.83	0.59
1:A:265:LYS:HG2	1:A:343:GLU:CG	2.33	0.59
1:B:357:ARG:HH12	1:B:358:LYS:HE2	1.65	0.59
1:A:450:VAL:HG22	1:A:473:TYR:CE1	2.37	0.59
1:B:269:PRO:O	1:B:271:GLN:N	2.36	0.59
1:B:288:ARG:NH2	2:B:2:OCX:H3	2.18	0.58
1:A:297:THR:O	1:A:301:LYS:HG3	2.03	0.58
1:A:340:LEU:HD23	1:A:347:PHE:HD1	1.69	0.58
1:B:363:PHE:CE1	1:B:452:LEU:HD13	2.39	0.58
1:B:267:ILE:HG22	1:B:287:PHE:CG	2.39	0.58
1:B:338:GLY:HA3	1:B:347:PHE:CZ	2.39	0.58
1:B:214:LEU:HD12	1:B:214:LEU:O	2.03	0.58
1:B:325:ILE:HD11	1:B:392:ILE:HG12	1.84	0.58
1:B:397:ARG:O	1:B:400:LEU:HG	2.04	0.58
1:A:355:SER:O	1:A:357:ARG:N	2.37	0.58
1:A:267:ILE:HG22	1:A:269:PRO:HG3	1.85	0.57
1:B:274:SER:C	1:B:280:ARG:HE	2.07	0.57
1:A:239:GLY:O	1:A:241:THR:N	2.33	0.57
1:A:240:LYS:HB3	1:A:240:LYS:NZ	2.19	0.57
1:A:323:HIS:HB2	3:A:1060:HOH:O	2.04	0.57
1:A:404:LYS:O	1:A:404:LYS:HD3	2.05	0.57
1:B:291:GLU:O	1:B:295:GLU:HG3	2.05	0.57
1:A:384:LEU:O	1:A:388:ILE:HG12	2.05	0.57
1:B:272:GLU:O	1:B:273:GLN:HB3	2.04	0.57
1:B:320:TYR:HB3	1:B:397:ARG:HD2	1.86	0.57
1:A:464:SER:C	1:A:465:LEU:HD23	2.24	0.57
1:A:265:LYS:HG2	1:A:343:GLU:HG2	1.86	0.56
1:B:311:LEU:H	1:B:311:LEU:CD2	2.18	0.56
1:A:363:PHE:HE2	1:A:452:LEU:HB3	1.69	0.56
1:B:264:PHE:O	1:B:268:THR:HG23	2.05	0.56
1:B:249:ILE:O	1:B:349:THR:HG22	2.06	0.56
1:A:241:THR:CB	1:A:244:LYS:HB2	2.36	0.56
1:A:325:ILE:HD11	1:A:392:ILE:CG1	2.35	0.56
1:B:452:LEU:HA	1:B:455:VAL:CG2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:LYS:HE3	1:A:408:ASP:OD1	2.06	0.56
1:B:448:GLU:HA	1:B:451:GLN:HG2	1.88	0.56
1:A:288:ARG:HA	1:A:288:ARG:NH1	2.21	0.55
1:A:288:ARG:HA	1:A:288:ARG:CZ	2.36	0.55
1:B:333:LEU:HD12	1:B:333:LEU:N	2.21	0.55
1:B:423:LEU:O	1:B:426:PRO:HD3	2.06	0.55
1:A:425:HIS:HB3	1:A:428:SER:HB2	1.87	0.55
1:A:397:ARG:O	1:A:400:LEU:HG	2.05	0.55
1:B:266:HIS:O	1:B:269:PRO:HD2	2.06	0.55
1:B:267:ILE:HG21	1:B:284:GLY:HA2	1.87	0.55
1:B:250:TYR:HA	1:B:349:THR:HG21	1.89	0.55
1:B:234:ARG:O	1:B:238:THR:HG23	2.07	0.55
1:B:445:ILE:HG22	1:B:446:VAL:N	2.21	0.55
1:B:266:HIS:C	1:B:269:PRO:HD2	2.27	0.55
1:B:273:GLN:HE22	1:B:469:LEU:HD21	1.72	0.55
1:B:349:THR:HG23	1:B:352:PHE:CB	2.37	0.55
1:B:456:ILE:C	1:B:458:LYS:H	2.09	0.55
1:A:457:LYS:HG2	1:A:457:LYS:O	2.07	0.54
1:A:273:GLN:CA	1:A:280:ARG:NH2	2.70	0.54
1:A:440:THR:HG22	1:B:440:THR:HA	1.88	0.54
1:B:265:LYS:HG2	1:B:269:PRO:HG3	1.88	0.54
1:B:436:LEU:O	1:B:439:MET:HG3	2.07	0.54
1:A:255:LEU:O	1:A:255:LEU:HD22	2.08	0.54
1:B:267:ILE:HG22	1:B:287:PHE:CB	2.38	0.54
1:A:269:PRO:O	1:A:271:GLN:N	2.41	0.54
1:B:280:ARG:HA	1:B:283:GLN:HE21	1.69	0.54
1:A:271:GLN:O	1:A:271:GLN:HG2	2.07	0.54
1:A:287:PHE:HE2	1:A:288:ARG:HH22	1.54	0.54
1:B:357:ARG:HH11	1:B:357:ARG:CG	2.20	0.54
1:A:264:PHE:CD2	1:A:266:HIS:HB3	2.26	0.54
1:B:237:LEU:HD21	1:B:340:LEU:HD13	1.90	0.54
1:B:357:ARG:HH11	1:B:357:ARG:HG3	1.72	0.53
1:B:451:GLN:NE2	1:B:451:GLN:HA	2.16	0.53
1:B:271:GLN:O	1:B:272:GLU:HG2	2.09	0.53
1:B:260:ASP:O	1:B:260:ASP:OD1	2.27	0.53
1:A:241:THR:HG21	1:A:244:LYS:HB2	1.90	0.53
1:B:365:GLU:N	1:B:366:PRO:CD	2.71	0.53
1:B:259:GLU:HA	1:B:264:PHE:CE1	2.43	0.53
1:B:274:SER:CA	1:B:280:ARG:HE	2.22	0.53
1:B:279:ILE:HD11	1:B:459:THR:HG21	1.91	0.53
1:B:357:ARG:NH1	1:B:357:ARG:HG3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ARG:NH1	1:A:291:GLU:HB3	2.23	0.53
1:B:472:ILE:HB	1:B:473:TYR:CE2	2.43	0.53
1:B:265:LYS:C	1:B:269:PRO:HD3	2.29	0.52
1:B:330:LEU:HG	1:B:334:MET:CE	2.40	0.52
1:B:249:ILE:HA	1:B:254:SER:HB3	1.91	0.52
1:A:443:ARG:HG3	1:B:440:THR:CG2	2.40	0.52
1:A:252:MET:HE1	1:A:277:VAL:HG21	1.91	0.52
1:B:323:HIS:O	1:B:327:TYR:HD2	1.93	0.52
1:B:320:TYR:CB	1:B:397:ARG:HD2	2.38	0.52
1:B:393:LEU:HG	1:B:409:ILE:HG22	1.92	0.52
1:A:440:THR:HA	1:B:440:THR:HG23	1.91	0.52
1:A:373:LYS:O	1:A:376:ALA:HB3	2.10	0.52
1:A:277:VAL:O	1:A:280:ARG:HB3	2.09	0.52
1:A:239:GLY:C	1:A:241:THR:H	2.12	0.52
1:A:212:ARG:HD3	1:A:423:LEU:CD1	2.39	0.52
1:B:390:VAL:O	1:B:410:GLN:NE2	2.40	0.51
1:B:251:ASP:HA	1:B:352:PHE:CD1	2.45	0.51
1:A:288:ARG:NH1	1:A:291:GLU:CB	2.74	0.51
1:B:258:GLY:O	1:B:262:ILE:CG1	2.59	0.51
1:B:269:PRO:C	1:B:270:LEU:HD12	2.31	0.51
1:B:349:THR:HG23	1:B:352:PHE:HB2	1.93	0.51
1:A:404:LYS:C	1:A:404:LYS:HD3	2.31	0.51
1:A:466:HIS:ND1	1:A:467:PRO:HD2	2.25	0.51
1:B:327:TYR:CE1	1:B:367:LYS:HE2	2.47	0.50
1:B:386:ILE:HB	1:B:417:LEU:HD13	1.93	0.50
1:A:268:THR:HG22	1:A:283:GLN:HB2	1.89	0.50
1:A:449:HIS:CD2	2:A:1:OCX:O23	2.64	0.50
1:A:240:LYS:O	1:A:241:THR:CG2	2.59	0.50
1:A:450:VAL:HG22	1:A:473:TYR:CD1	2.47	0.50
1:A:348:MET:SD	1:A:353:LEU:HD21	2.51	0.50
1:A:380:ASP:HB2	3:A:1044:HOH:O	2.12	0.50
1:B:363:PHE:CE1	1:B:452:LEU:HB2	2.46	0.50
1:B:267:ILE:HG13	1:B:268:THR:N	2.27	0.50
1:B:335:ASN:ND2	1:B:338:GLY:N	2.57	0.49
1:B:261:LYS:HA	1:B:261:LYS:HE3	1.94	0.49
1:B:357:ARG:HH12	1:B:358:LYS:CE	2.24	0.49
1:B:330:LEU:HD21	1:B:334:MET:HE1	1.94	0.49
1:B:263:LYS:HZ3	1:B:265:LYS:HD2	1.78	0.49
1:B:335:ASN:HD22	1:B:337:ASP:N	2.07	0.49
1:A:474:LYS:HG3	1:A:475:ASP:OD1	2.13	0.49
1:B:226:PHE:HE1	1:B:296:ILE:HD13	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ARG:NH2	1:A:460:GLU:OE1	2.45	0.49
1:A:232:LYS:O	1:A:236:ILE:HG13	2.12	0.49
1:A:240:LYS:C	1:A:241:THR:HG23	2.32	0.49
1:B:273:GLN:HG3	1:B:273:GLN:O	2.12	0.49
1:B:226:PHE:CE1	1:B:296:ILE:HD13	2.48	0.49
1:B:236:ILE:O	1:B:237:LEU:C	2.51	0.49
1:B:320:TYR:CZ	1:B:398:PRO:HG2	2.48	0.49
1:A:270:LEU:O	1:A:271:GLN:HB3	2.13	0.49
1:B:267:ILE:HD12	1:B:267:ILE:C	2.33	0.49
1:B:352:PHE:O	1:B:355:SER:HB3	2.13	0.49
1:B:327:TYR:CE1	1:B:367:LYS:CE	2.95	0.48
1:B:472:ILE:O	1:B:472:ILE:CG2	2.61	0.48
1:A:465:LEU:N	1:A:465:LEU:HD23	2.28	0.48
1:B:236:ILE:O	1:B:238:THR:N	2.46	0.48
1:A:447:THR:O	1:A:449:HIS:N	2.46	0.48
1:A:252:MET:HE3	1:A:252:MET:HA	1.95	0.48
1:B:327:TYR:OH	1:B:449:HIS:CG	2.67	0.48
1:A:206:PRO:O	1:A:209:ALA:HB3	2.14	0.48
1:A:239:GLY:C	1:A:241:THR:N	2.67	0.48
1:B:466:HIS:O	1:B:467:PRO:C	2.52	0.48
1:B:335:ASN:HD21	1:B:338:GLY:N	2.12	0.48
1:B:279:ILE:O	1:B:283:GLN:HG3	2.13	0.48
1:B:466:HIS:HA	1:B:469:LEU:HB2	1.96	0.48
1:B:393:LEU:HG	1:B:409:ILE:CG2	2.43	0.48
1:B:313:ASP:O	1:B:317:LEU:HG	2.13	0.48
1:A:277:VAL:HG13	1:A:278:ALA:N	2.29	0.48
1:A:443:ARG:HG3	1:B:440:THR:HG21	1.96	0.48
1:B:452:LEU:HA	1:B:455:VAL:CB	2.44	0.47
1:B:270:LEU:HD13	1:B:273:GLN:HG3	1.95	0.47
1:B:373:LYS:O	1:B:376:ALA:HB3	2.14	0.47
1:B:451:GLN:CA	1:B:451:GLN:HE21	2.13	0.47
1:B:279:ILE:HG13	1:B:360:PHE:CZ	2.49	0.47
1:A:474:LYS:HE3	1:A:475:ASP:OD1	2.14	0.47
1:B:223:ILE:HD13	1:B:223:ILE:HA	1.70	0.47
1:B:230:LYS:HB3	1:B:381:ASP:OD2	2.14	0.47
1:A:252:MET:O	1:A:253:ASN:C	2.53	0.47
1:B:325:ILE:HD11	1:B:392:ILE:CG1	2.44	0.47
1:B:264:PHE:C	1:B:266:HIS:H	2.18	0.47
1:B:329:MET:O	1:B:332:SER:HB2	2.15	0.47
1:B:243:ASP:O	1:B:243:ASP:OD1	2.33	0.47
1:B:448:GLU:O	1:B:451:GLN:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:PHE:HZ	1:A:456:ILE:HG13	1.80	0.46
1:B:262:ILE:HG22	1:B:345:GLN:CB	2.44	0.46
1:B:311:LEU:N	1:B:311:LEU:HD22	2.25	0.46
1:B:268:THR:OG1	1:B:269:PRO:HD3	2.15	0.46
1:A:240:LYS:HB3	1:A:240:LYS:HZ3	1.80	0.46
1:B:355:SER:OG	1:B:355:SER:O	2.30	0.46
1:A:462:ASP:N	1:A:462:ASP:OD1	2.36	0.46
1:A:263:LYS:HG3	1:A:263:LYS:O	2.15	0.46
1:B:268:THR:N	1:B:269:PRO:CD	2.78	0.46
1:A:359:PRO:O	1:A:361:GLY:N	2.49	0.46
1:A:473:TYR:HA	1:A:476:LEU:HD12	1.97	0.46
1:B:425:HIS:HB3	1:B:428:SER:OG	2.15	0.46
1:B:447:THR:O	1:B:451:GLN:HG2	2.16	0.45
1:B:364:MET:O	1:B:368:PHE:HD2	1.99	0.45
1:A:268:THR:CG2	1:A:280:ARG:HD3	2.39	0.45
1:B:270:LEU:HD22	1:B:273:GLN:CD	2.37	0.45
1:A:212:ARG:NH1	1:A:420:GLN:OE1	2.49	0.45
1:A:353:LEU:HD12	1:A:368:PHE:CE2	2.51	0.45
1:A:273:GLN:C	1:A:280:ARG:NH2	2.70	0.45
1:B:279:ILE:HD11	1:B:459:THR:CG2	2.46	0.45
1:B:222:TYR:CE1	1:B:381:ASP:HB3	2.52	0.45
1:B:278:ALA:HB3	1:B:357:ARG:HD3	1.98	0.45
1:A:287:PHE:CE2	1:A:288:ARG:NH2	2.84	0.45
1:B:236:ILE:HG22	1:B:237:LEU:N	2.31	0.45
1:A:268:THR:CB	1:A:280:ARG:NH1	2.67	0.45
1:B:459:THR:CG2	1:B:460:GLU:N	2.74	0.45
1:B:441:ASP:O	1:B:445:ILE:HB	2.17	0.45
1:A:288:ARG:HG2	2:A:1:OCX:H5	1.99	0.45
1:A:323:HIS:CE1	1:A:473:TYR:HH	2.33	0.45
1:A:252:MET:HA	1:A:252:MET:CE	2.46	0.45
1:A:265:LYS:HG2	1:A:343:GLU:HG3	1.99	0.45
1:A:264:PHE:C	1:A:266:HIS:N	2.63	0.45
1:B:245:SER:HA	1:B:246:PRO:HD3	1.74	0.44
1:B:230:LYS:HB3	1:B:381:ASP:CG	2.38	0.44
1:B:427:GLU:HG3	1:B:428:SER:N	2.33	0.44
1:A:437:GLN:HG2	1:B:439:MET:HE1	1.98	0.44
1:B:303:ILE:HD11	1:B:392:ILE:HD12	2.00	0.44
1:A:387:PHE:CE2	1:A:391:ILE:HD11	2.53	0.44
1:A:252:MET:HE2	1:A:255:LEU:CD1	2.45	0.44
1:A:456:ILE:HG21	1:A:463:MET:HE1	2.00	0.44
1:A:430:GLN:NE2	1:B:414:LEU:HB3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ALA:O	1:A:303:ILE:HG13	2.17	0.44
1:B:402:ASN:HB3	3:B:1011:HOH:O	2.18	0.44
1:A:230:LYS:O	1:A:234:ARG:HG2	2.18	0.43
1:B:327:TYR:CD1	1:B:445:ILE:HG21	2.53	0.43
1:B:267:ILE:CG1	1:B:268:THR:N	2.81	0.43
1:B:335:ASN:ND2	1:B:337:ASP:N	2.64	0.43
1:B:327:TYR:CE1	1:B:445:ILE:HG23	2.53	0.43
1:B:263:LYS:NZ	1:B:265:LYS:CD	2.76	0.43
1:B:267:ILE:HG22	1:B:287:PHE:HB3	1.99	0.43
1:B:251:ASP:O	1:B:254:SER:HB2	2.19	0.43
1:A:434:LYS:HA	1:A:437:GLN:NE2	2.34	0.43
1:A:334:MET:HG2	1:A:339:VAL:HB	2.00	0.43
1:A:226:PHE:HA	1:A:227:PRO:HD3	1.87	0.43
1:A:368:PHE:O	1:A:372:VAL:HG23	2.19	0.43
1:A:220:ASP:O	1:A:224:LYS:HG3	2.18	0.43
1:A:386:ILE:H	1:A:386:ILE:HG12	1.69	0.43
1:A:452:LEU:O	1:A:456:ILE:HG12	2.19	0.43
1:B:270:LEU:HB2	1:B:273:GLN:CD	2.38	0.43
1:B:262:ILE:HG22	1:B:345:GLN:HB2	2.00	0.43
1:A:250:TYR:CD2	1:A:250:TYR:N	2.87	0.43
1:A:241:THR:CG2	1:A:244:LYS:HB2	2.49	0.43
1:B:276:GLU:O	1:B:277:VAL:C	2.57	0.43
1:A:440:THR:HG23	3:B:1049:HOH:O	2.18	0.43
1:B:366:PRO:O	1:B:369:GLU:HB2	2.19	0.42
1:B:366:PRO:O	1:B:369:GLU:N	2.52	0.42
1:A:291:GLU:O	1:A:294:GLN:HB2	2.19	0.42
1:B:296:ILE:HD12	1:B:325:ILE:HG21	2.01	0.42
1:B:360:PHE:CZ	1:B:456:ILE:HD11	2.52	0.42
1:B:330:LEU:CD2	1:B:334:MET:HE1	2.49	0.42
1:A:323:HIS:CD2	2:A:1:OCX:H18	2.54	0.42
1:A:325:ILE:HD13	1:A:388:ILE:HG23	2.01	0.42
1:B:430:GLN:HA	3:B:1019:HOH:O	2.19	0.42
2:A:1:OCX:H8	2:A:1:OCX:H11	1.90	0.42
1:A:341:ILE:O	1:A:342:SER:C	2.57	0.42
1:B:333:LEU:HB3	1:B:340:LEU:HB2	2.01	0.42
1:A:222:TYR:CE2	1:A:381:ASP:HB3	2.54	0.42
1:B:451:GLN:HA	1:B:454:GLN:OE1	2.19	0.42
1:A:469:LEU:HD12	1:A:469:LEU:HA	1.80	0.42
1:B:262:ILE:C	1:B:264:PHE:N	2.73	0.42
1:A:356:LEU:HD23	1:A:356:LEU:HA	1.85	0.42
1:A:339:VAL:HG22	1:A:340:LEU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:TYR:CD1	1:A:382:SER:HA	2.55	0.42
1:B:327:TYR:HE1	1:B:367:LYS:HE2	1.83	0.42
1:B:410:GLN:O	1:B:413:LEU:HB2	2.20	0.42
1:B:230:LYS:N	1:B:381:ASP:OD2	2.44	0.42
1:B:288:ARG:HD2	1:B:288:ARG:O	2.20	0.42
1:A:363:PHE:CE2	1:A:452:LEU:HB3	2.54	0.41
1:B:402:ASN:OD1	1:B:405:PRO:HD3	2.20	0.41
1:A:256:MET:C	1:A:258:GLY:N	2.73	0.41
1:B:457:LYS:HD3	1:B:457:LYS:HA	1.88	0.41
1:B:263:LYS:O	1:B:265:LYS:N	2.54	0.41
1:B:271:GLN:HE21	1:B:271:GLN:HB2	1.62	0.41
1:A:313:ASP:O	1:A:317:LEU:HG	2.20	0.41
1:A:330:LEU:O	1:A:334:MET:HG3	2.20	0.41
1:B:335:ASN:C	1:B:335:ASN:ND2	2.71	0.41
1:A:305:GLY:HA2	1:A:308:ASN:HD22	1.85	0.41
1:A:308:ASN:HB2	3:A:1023:HOH:O	2.21	0.41
1:B:449:HIS:HA	1:B:452:LEU:CD1	2.51	0.41
1:A:450:VAL:HG22	1:A:473:TYR:HE1	1.83	0.41
1:A:443:ARG:HG3	1:B:444:GLN:HE22	1.86	0.41
1:A:271:GLN:HG2	1:A:273:GLN:O	2.21	0.41
1:B:330:LEU:HD13	2:B:2:OCX:H8	2.03	0.41
1:B:357:ARG:NH1	1:B:357:ARG:CG	2.82	0.41
1:A:341:ILE:HA	2:A:1:OCX:H4A	2.02	0.41
1:B:275:LYS:HA	1:B:280:ARG:HH21	1.86	0.41
1:B:327:TYR:CD1	1:B:445:ILE:CG2	3.04	0.41
1:A:291:GLU:O	1:A:295:GLU:HG3	2.21	0.41
1:B:251:ASP:OD1	1:B:251:ASP:C	2.59	0.41
1:A:466:HIS:HB3	1:A:469:LEU:HB2	2.02	0.41
1:A:404:LYS:C	1:A:404:LYS:CD	2.89	0.41
1:B:297:THR:HG22	1:B:301:LYS:HE3	2.02	0.41
1:B:274:SER:HA	1:B:280:ARG:HE	1.86	0.40
1:A:447:THR:C	1:A:449:HIS:N	2.75	0.40
1:B:270:LEU:HD13	1:B:273:GLN:HG2	2.03	0.40
1:B:349:THR:CG2	1:B:352:PHE:HB2	2.51	0.40
1:A:271:GLN:O	1:A:272:GLU:C	2.57	0.40
1:B:268:THR:O	1:B:269:PRO:O	2.39	0.40
1:A:212:ARG:HA	1:A:212:ARG:HD2	1.73	0.40
1:B:430:GLN:NE2	3:B:1019:HOH:O	2.54	0.40
1:B:448:GLU:CA	1:B:451:GLN:HG2	2.52	0.40
1:B:246:PRO:HB3	1:B:345:GLN:O	2.21	0.40
1:B:252:MET:SD	1:B:277:VAL:HG11	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:PRO:C	1:B:361:GLY:H	2.24	0.40
1:A:364:MET:HA	1:A:367:LYS:HG3	2.03	0.40
1:A:283:GLN:HE21	1:A:283:GLN:HB3	1.68	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	272/286 (95%)	230 (85%)	27 (10%)	15 (6%)	2	2
1	B	259/286 (91%)	211 (82%)	28 (11%)	20 (8%)	1	1
All	All	531/572 (93%)	441 (83%)	55 (10%)	35 (7%)	1	1

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	PRO
1	A	270	LEU
1	A	272	GLU
1	A	356	LEU
1	A	360	PHE
1	B	236	ILE
1	B	263	LYS
1	B	269	PRO
1	B	273	GLN
1	B	277	VAL
1	B	357	ARG
1	B	358	LYS
1	A	261	LYS
1	A	267	ILE
1	B	208	SER

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Mol	Chain	Res	Type
1	B	237	LEU
1	B	240	LYS
1	B	261	LYS
1	B	270	LEU
1	B	272	GLU
1	B	360	PHE
1	A	357	ARG
1	A	381	ASP
1	A	448	GLU
1	B	241	THR
1	A	474	LYS
1	B	232	LYS
1	B	265	LYS
1	A	269	PRO
1	A	358	LYS
1	A	359	PRO
1	B	242	THR
1	B	457	LYS
1	A	398	PRO
1	B	227	PRO

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	243/257 (95%)	226 (93%)	17 (7%)	19 36
1	B	236/257 (92%)	210 (89%)	26 (11%)	8 13
All	All	479/514 (93%)	436 (91%)	43 (9%)	12 22

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	LYS
1	A	240	LYS
1	A	245	SER

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Mol	Chain	Res	Type
1	A	252	MET
1	A	253	ASN
1	A	268	THR
1	A	270	LEU
1	A	283	GLN
1	A	286	GLN
1	A	316	THR
1	A	386	ILE
1	A	396	ASP
1	A	427	GLU
1	A	444	GLN
1	A	452	LEU
1	A	459	THR
1	A	469	LEU
1	B	210	ASP
1	B	211	LEU
1	B	234	ARG
1	B	238	THR
1	B	261	LYS
1	B	262	ILE
1	B	270	LEU
1	B	271	GLN
1	B	279	ILE
1	B	280	ARG
1	B	335	ASN
1	B	340	LEU
1	B	351	GLU
1	B	357	ARG
1	B	362	ASP
1	B	372	VAL
1	B	381	ASP
1	B	396	ASP
1	B	424	ASN
1	B	441	ASP
1	B	444	GLN
1	B	451	GLN
1	B	452	LEU
1	B	460	GLU
1	B	461	THR
1	B	467	PRO

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

Mol	Chain	Res	Type
1	A	271	GLN
1	A	283	GLN
1	A	308	ASN
1	A	314	GLN
1	A	412	ASN
1	A	430	GLN
1	A	437	GLN
1	B	271	GLN
1	B	273	GLN
1	B	283	GLN
1	B	312	ASN
1	B	335	ASN
1	B	424	ASN
1	B	430	GLN
1	B	444	GLN
1	B	451	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	OCX	A	1	1	19,22,22	2.12	3 (15%)	16,23,23	1.26	1 (6%)
2	OCX	B	2	1	19,22,22	2.27	3 (15%)	16,23,23	1.49	1 (6%)

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	OCX	A	1	1	-	0/19/21/21	0/0/0/0
2	OCX	B	2	1	-	0/19/21/21	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	OCX	C13-C14	2.34	1.56	1.48
2	B	2	OCX	C13-C14	2.41	1.56	1.48
2	A	1	OCX	C11-C10	3.57	1.54	1.44
2	B	2	OCX	C11-C10	4.28	1.56	1.44
2	A	1	OCX	C11-C13	7.69	1.54	1.34
2	B	2	OCX	C11-C13	8.09	1.55	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	OCX	C10-C11-C13	-5.62	112.18	124.66
2	A	1	OCX	C10-C11-C13	-4.44	114.81	124.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	OCX	7	0
2	B	2	OCX	4	0

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

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, 95^{th} 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	274/286 (95%)	0.74	19 (6%) 20 16	27, 46, 72, 83	0
1	B	263/286 (91%)	0.95	43 (16%) 2 1	27, 46, 73, 84	0
All	All	537/572 (93%)	0.85	62 (11%) 6 5	27, 46, 73, 84	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	363	PHE	7.4
1	B	273	GLN	6.3
1	B	360	PHE	6.2
1	A	264	PHE	5.8
1	B	242	THR	5.6
1	B	241	THR	4.8
1	A	265	LYS	3.9
1	A	356	LEU	3.9
1	B	262	ILE	3.9
1	B	352	PHE	3.9
1	A	267	ILE	3.9
1	B	357	ARG	3.8
1	B	274	SER	3.8
1	B	452	LEU	3.5
1	B	255	LEU	3.5
1	A	268	THR	3.4
1	B	271	GLN	3.4
1	A	475	ASP	3.3
1	A	272	GLU	3.2
1	B	265	LYS	3.2
1	B	354	LYS	3.2
1	B	276	GLU	3.1
1	B	456	ILE	3.1
1	A	273	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	268	THR	3.0
1	B	243	ASP	3.0
1	B	252	MET	3.0
1	B	270	LEU	2.9
1	B	254	SER	2.9
1	B	235	ALA	2.9
1	B	211	LEU	2.8
1	A	262	ILE	2.8
1	B	256	MET	2.8
1	B	279	ILE	2.8
1	B	358	LYS	2.7
1	B	356	LEU	2.6
1	A	363	PHE	2.6
1	A	270	LEU	2.6
1	B	239	GLY	2.5
1	B	455	VAL	2.5
1	B	275	LYS	2.4
1	A	266	HIS	2.4
1	B	272	GLU	2.4
1	B	296	ILE	2.3
1	B	473	TYR	2.3
1	A	362	ASP	2.3
1	A	426	PRO	2.2
1	B	439	MET	2.2
1	A	452	LEU	2.2
1	A	277	VAL	2.2
1	B	472	ILE	2.2
1	B	469	LEU	2.1
1	B	250	TYR	2.1
1	A	204	LEU	2.1
1	B	266	HIS	2.1
1	A	327	TYR	2.1
1	A	256	MET	2.1
1	B	359	PRO	2.1
1	B	423	LEU	2.0
1	B	297	THR	2.0
1	B	267	ILE	2.0
1	B	367	LYS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	OCX	A	1	23/23	0.70	0.48	5.70	57,68,79,81	0
2	OCX	B	2	23/23	0.78	0.32	2.37	59,66,71,72	0

6.5 Other polymers (i)

There are no such residues in this entry.