



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 10, 2014 – 01:23 PM EDT

PDB ID : 3WCG
Title : The complex structure of TcSQS with ligand, BPH1344
Authors : Shang, N.; Li, Q.; Ko, T.P.; Chan, H.C.; Huang, C.H.; Ren, F.; Zheng, Y.;
Zhu, Z.; Chen, C.C.; Guo, R.T.
Deposited on : 2013-05-27
Resolution : 2.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

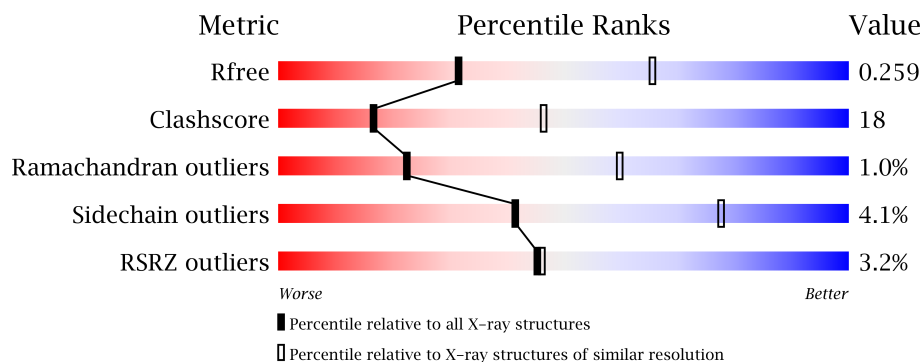
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23161
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23161

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	365	
1	B	365	
1	C	365	
1	D	365	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11294 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

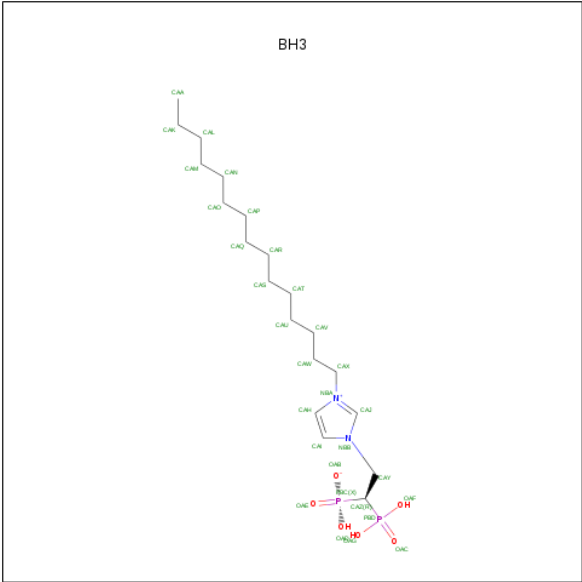
- Molecule 1 is a protein called Farnesyltransferase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2751	1745	473	511	22			
1	B	341	Total	C	N	O	S	0	0	0
			2751	1745	473	511	22			
1	C	341	Total	C	N	O	S	0	0	0
			2751	1745	473	511	22			
1	D	341	Total	C	N	O	S	0	0	0
			2752	1745	473	512	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	GLU	ASP	ENGINEERED MUTATION	UNP Q4CWB4
B	82	GLU	ASP	ENGINEERED MUTATION	UNP Q4CWB4
C	82	GLU	ASP	ENGINEERED MUTATION	UNP Q4CWB4
D	82	GLU	ASP	ENGINEERED MUTATION	UNP Q4CWB4

- Molecule 2 is HYDROGEN [(1R)-2-(3-PENTADECYL-1H-IMIDAZOL-3-IUM-1-YL)-1-PHOSPHONOETHYL]PHOSPHONATE (three-letter code: BH3) (formula: C₂₀H₄₀N₂O₆P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			30	20	2	6	2		
2	B	1	Total	C	N	O	P	0	0
			30	20	2	6	2		
2	C	1	Total	C	N	O	P	0	0
			30	20	2	6	2		
2	D	1	Total	C	N	O	P	0	0
			30	20	2	6	2		

- Molecule 3 is water.

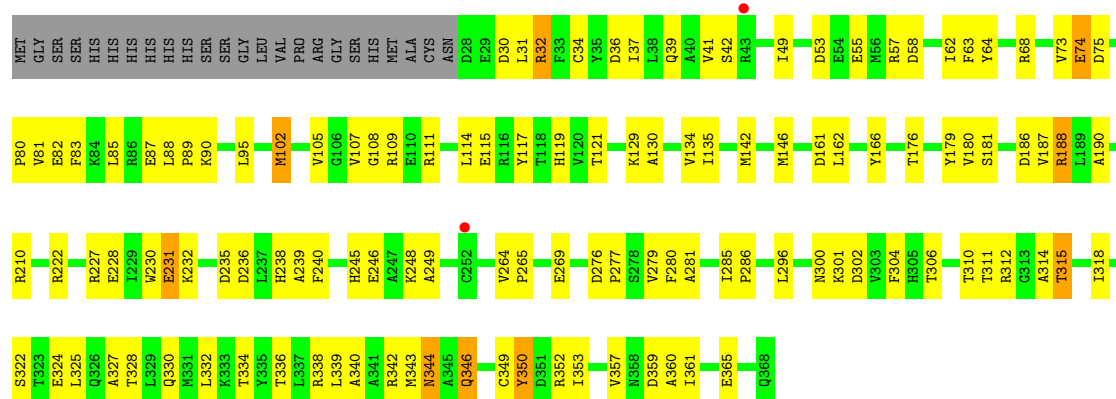
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	54	Total	O	0	0
			54	54		
3	B	35	Total	O	0	0
			35	35		
3	C	41	Total	O	0	0
			41	41		
3	D	39	Total	O	0	0
			39	39		

3 Residue-property plots

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.

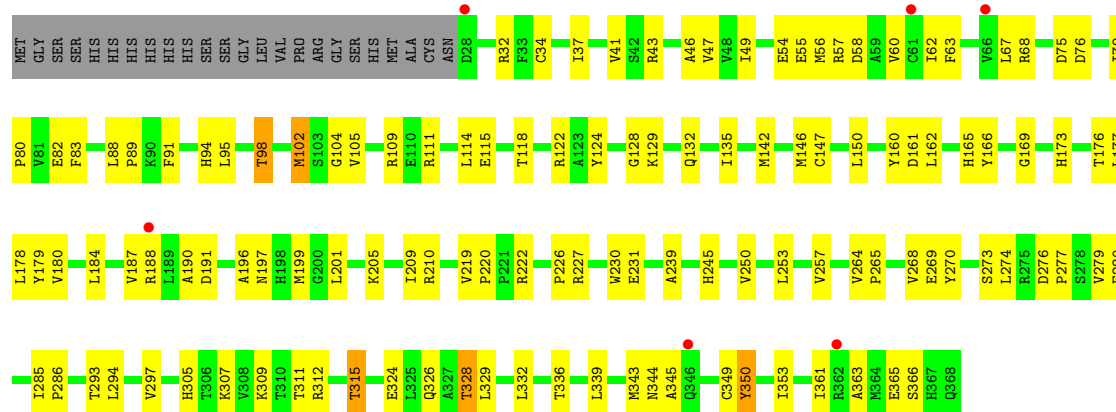
- Molecule 1: Farnesyltransferase, putative

Chain A: 



- Molecule 1: Farnesyltransferase, putative

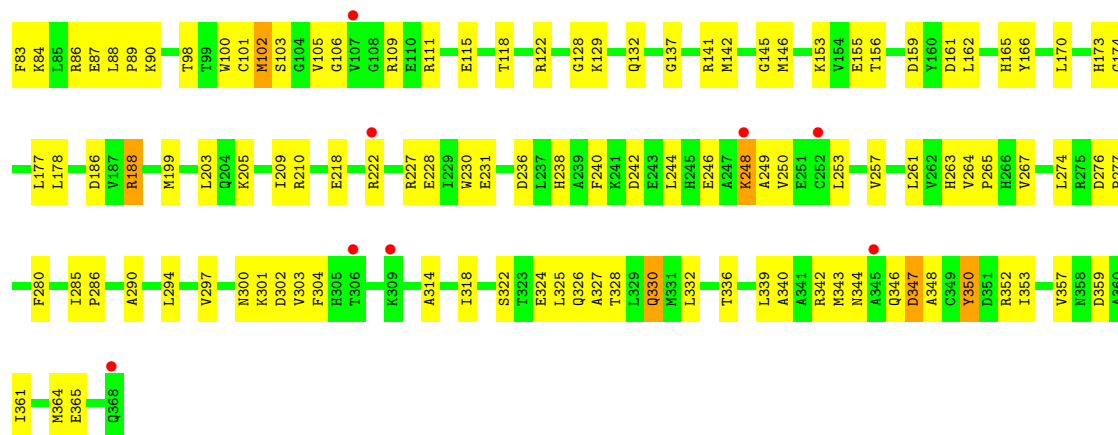
Chain B: 



- Molecule 1: Farnesyltransferase, putative

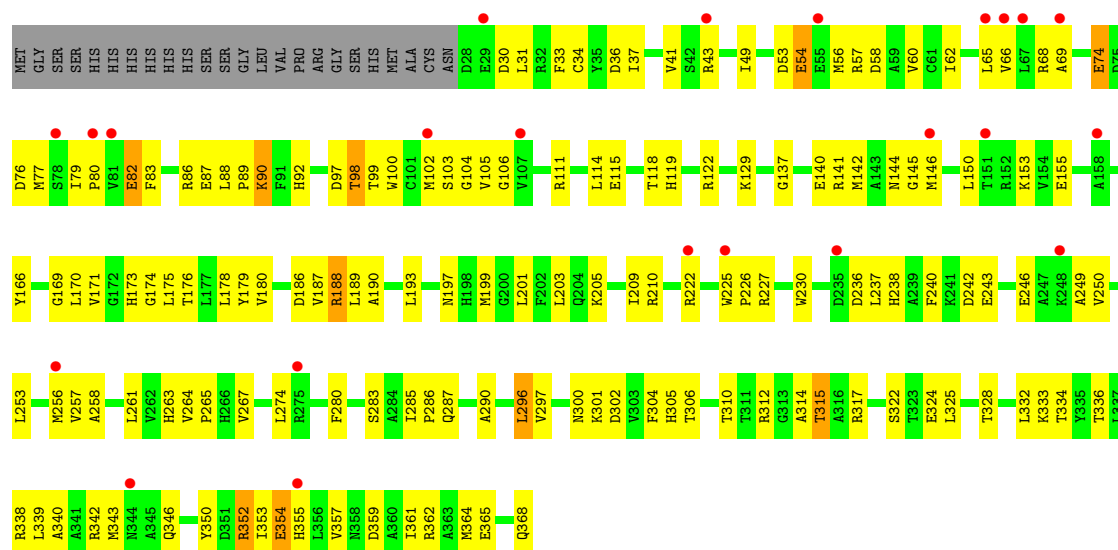
Chain C: 





- Molecule 1: Farnesyltransferase, putative

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.09Å 128.97Å 144.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.80 23.62 – 2.78	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.80) 92.5 (23.62-2.78)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.20 (at 2.75Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.221 , 0.271 0.238 , 0.259	Depositor DCC
R_{free} test set	1816 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	64.4	Xtriage
Anisotropy	0.671	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 30.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 36990 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11294	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BH3

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	0.31	0/2809	0.49	0/3806
1	B	0.25	0/2809	0.46	0/3806
1	C	0.28	0/2809	0.46	0/3806
1	D	0.25	0/2810	0.46	0/3806
All	All	0.27	0/11237	0.47	0/15224

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2751	0	2698	95	0
1	B	2751	0	2698	89	0
1	C	2751	0	2698	105	0
1	D	2752	0	2698	116	0
2	A	30	0	0	0	0
2	B	30	0	0	0	0
2	C	30	0	0	0	0
2	D	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	54	0	0	0	0
3	B	35	0	0	0	0
3	C	41	0	0	0	0
3	D	39	0	0	0	0
All	All	11294	0	10792	393	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

All (393) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:108:GLY:HA2	1:B:366:SER:HA	1.48	0.96
1:D:103:SER:HA	1:D:115:GLU:HG2	1.55	0.88
1:A:73:VAL:HG22	1:A:102:MET:HE1	1.54	0.88
1:D:41:VAL:HG11	1:D:68:ARG:HG2	1.58	0.85
1:D:43:ARG:HB2	1:D:43:ARG:NH2	1.93	0.84
1:D:80:PRO:HG2	1:D:83:PHE:HB2	1.59	0.83
1:A:322:SER:HA	1:A:328:THR:HG22	1.58	0.82
1:C:88:LEU:HB2	1:C:89:PRO:HD3	1.61	0.82
1:A:32:ARG:HH12	1:C:301:LYS:NZ	1.81	0.79
1:D:352:ARG:O	1:D:352:ARG:HD3	1.84	0.76
1:B:227:ARG:HA	1:B:230:TRP:NE1	2.00	0.75
1:C:246:GLU:OE2	1:C:301:LYS:HD2	1.87	0.74
1:B:118:THR:O	1:B:122:ARG:HG2	1.87	0.74
1:C:264:VAL:HB	1:C:265:PRO:HD3	1.71	0.73
1:D:300:ASN:HD21	1:D:302:ASP:HB2	1.53	0.72
1:C:80:PRO:HB2	1:C:82:GLU:OE2	1.91	0.71
1:C:248:LYS:HA	1:C:248:LYS:HE3	1.73	0.71
1:C:188:ARG:HA	1:C:188:ARG:HE	1.54	0.71
1:C:285:ILE:HB	1:C:286:PRO:HD3	1.73	0.71
1:C:76:ASP:HB3	1:C:79:ILE:HD11	1.71	0.70
1:B:180:VAL:HG13	1:B:187:VAL:HA	1.72	0.70
1:A:30:ASP:HA	1:A:119:HIS:HD2	1.57	0.70
1:D:188:ARG:HE	1:D:188:ARG:HA	1.54	0.70
1:C:257:VAL:HG13	1:C:294:LEU:HD11	1.72	0.69
1:D:352:ARG:HD3	1:D:352:ARG:C	2.13	0.69
1:D:322:SER:HA	1:D:328:THR:HG22	1.73	0.69
1:D:334:THR:O	1:D:338:ARG:HG2	1.92	0.68
1:D:97:ASP:OD2	1:D:100:TRP:HB2	1.94	0.68
1:A:32:ARG:HH12	1:C:301:LYS:HZ1	1.41	0.68
1:B:55:GLU:HB2	1:D:338:ARG:HH22	1.57	0.68
1:B:41:VAL:HG12	1:B:68:ARG:NH1	2.09	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:32:ARG:NH1	1:C:301:LYS:NZ	2.42	0.67
1:A:227:ARG:O	1:A:231:GLU:HB3	1.94	0.67
1:D:180:VAL:HG13	1:D:187:VAL:HA	1.76	0.67
1:A:285:ILE:HB	1:A:286:PRO:HD3	1.75	0.67
1:D:227:ARG:HA	1:D:230:TRP:NE1	2.10	0.67
1:D:340:ALA:HB2	1:D:357:VAL:HG21	1.77	0.67
1:A:264:VAL:HB	1:A:265:PRO:HD3	1.76	0.67
1:D:80:PRO:HB2	1:D:82:GLU:OE1	1.94	0.67
1:D:86:ARG:NH1	1:D:86:ARG:HB3	2.10	0.67
1:A:142:MET:HG3	1:A:166:TYR:O	1.96	0.66
1:B:37:ILE:O	1:B:41:VAL:HG23	1.96	0.66
1:D:76:ASP:HB3	1:D:79:ILE:HD12	1.77	0.66
1:D:361:ILE:O	1:D:365:GLU:HG3	1.96	0.65
1:A:81:VAL:HG12	1:A:85:LEU:HD11	1.78	0.65
1:B:102:MET:CE	1:B:105:VAL:HG21	2.27	0.65
1:B:80:PRO:HB2	1:B:82:GLU:OE1	1.96	0.64
1:A:227:ARG:HA	1:A:230:TRP:NE1	2.12	0.64
1:D:285:ILE:HB	1:D:286:PRO:HD3	1.80	0.64
1:C:142:MET:HG3	1:C:166:TYR:O	1.98	0.64
1:D:350:TYR:O	1:D:354:GLU:HB2	1.98	0.63
1:D:31:LEU:HD21	1:D:58:ASP:OD1	1.98	0.63
1:A:186:ASP:OD2	1:A:188:ARG:HB2	1.99	0.63
1:C:102:MET:HE3	1:C:105:VAL:HG21	1.80	0.63
1:C:103:SER:HA	1:C:115:GLU:HG2	1.80	0.63
1:D:274:LEU:HD13	1:D:280:PHE:HA	1.81	0.63
1:D:87:GLU:HA	1:D:90:LYS:HD2	1.81	0.63
1:D:34:CYS:O	1:D:37:ILE:HG22	1.98	0.63
1:A:180:VAL:HG13	1:A:187:VAL:HA	1.81	0.62
1:D:186:ASP:OD2	1:D:188:ARG:HB2	1.99	0.62
1:D:199:MET:SD	1:D:267:VAL:HG13	2.38	0.62
1:A:82:GLU:HA	1:A:85:LEU:HD12	1.81	0.62
1:C:326:GLN:O	1:C:330:GLN:HG2	2.00	0.62
1:A:332:LEU:O	1:A:336:THR:HG23	2.00	0.61
1:A:82:GLU:CD	1:A:82:GLU:H	2.03	0.61
1:B:264:VAL:HB	1:B:265:PRO:HD3	1.83	0.61
1:D:142:MET:O	1:D:146:MET:HG3	2.01	0.61
1:B:285:ILE:HB	1:B:286:PRO:HD3	1.83	0.60
1:B:49:ILE:HG12	1:B:57:ARG:HG3	1.82	0.60
1:C:41:VAL:HG13	1:C:68:ARG:CZ	2.32	0.60
1:A:343:MET:HE2	1:A:350:TYR:HA	1.83	0.60
1:B:332:LEU:O	1:B:336:THR:HG23	2.02	0.60
1:D:80:PRO:HG2	1:D:83:PHE:CB	2.32	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:340:ALA:HB2	1:C:357:VAL:HG21	1.84	0.59
1:D:364:MET:O	1:D:368:GLN:HG3	2.03	0.59
1:B:280:PHE:CZ	1:B:328:THR:HG21	2.37	0.59
1:C:343:MET:CE	1:C:350:TYR:HA	2.33	0.59
1:A:107:VAL:O	1:A:107:VAL:HG23	2.03	0.58
1:A:343:MET:CE	1:A:350:TYR:HA	2.33	0.58
1:B:361:ILE:O	1:B:365:GLU:HG3	2.03	0.58
1:A:300:ASN:OD1	1:A:302:ASP:HB2	2.03	0.58
1:B:176:THR:HA	1:B:179:TYR:CD2	2.37	0.58
1:D:222:ARG:HG3	1:D:222:ARG:HH11	1.68	0.58
1:D:258:ALA:HB2	1:D:353:ILE:HD11	1.86	0.58
1:D:264:VAL:HB	1:D:265:PRO:HD3	1.85	0.58
1:C:118:THR:O	1:C:122:ARG:HG2	2.03	0.58
1:D:142:MET:HG3	1:D:166:TYR:O	2.03	0.58
1:D:146:MET:O	1:D:150:LEU:HG	2.03	0.58
1:D:58:ASP:O	1:D:62:ILE:HG12	2.04	0.58
1:A:130:ALA:O	1:A:134:VAL:HG23	2.04	0.58
1:A:340:ALA:O	1:A:343:MET:HG2	2.04	0.58
1:B:98:THR:O	1:B:118:THR:HG23	2.04	0.58
1:C:199:MET:SD	1:C:267:VAL:HG13	2.43	0.57
1:D:332:LEU:O	1:D:336:THR:HG23	2.04	0.57
1:A:130:ALA:HB1	1:A:181:SER:OG	2.04	0.57
1:D:225:TRP:HA	1:D:256:MET:HE2	1.87	0.57
1:D:43:ARG:HH21	1:D:43:ARG:HB2	1.66	0.57
1:C:343:MET:HE1	1:C:350:TYR:HA	1.87	0.57
1:A:344:ASN:ND2	1:A:346:GLN:HG3	2.20	0.57
1:A:111:ARG:O	1:A:115:GLU:HG3	2.05	0.57
1:A:31:LEU:HD21	1:A:58:ASP:OD1	2.05	0.56
1:A:246:GLU:OE2	1:A:301:LYS:HD2	2.05	0.56
1:D:62:ILE:O	1:D:66:VAL:HG23	2.05	0.56
1:B:173:HIS:O	1:B:177:LEU:HG	2.05	0.56
1:B:205:LYS:O	1:B:209:ILE:HG13	2.05	0.56
1:D:257:VAL:O	1:D:261:LEU:HG	2.06	0.56
1:D:333:LYS:HE2	1:D:361:ILE:HG23	1.87	0.56
1:A:58:ASP:O	1:A:62:ILE:HG12	2.06	0.55
1:C:222:ARG:HH11	1:C:222:ARG:HG3	1.70	0.55
1:C:344:ASN:O	1:C:347:ASP:HB2	2.06	0.55
1:C:153:LYS:HB2	1:C:155:GLU:OE2	2.06	0.55
1:A:102:MET:HE3	1:A:105:VAL:HG21	1.89	0.55
1:D:343:MET:CE	1:D:350:TYR:HA	2.37	0.54
1:B:227:ARG:HA	1:B:230:TRP:CD1	2.42	0.54
1:B:102:MET:HE2	1:B:105:VAL:HG21	1.87	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:322:SER:HA	1:C:328:THR:HG22	1.89	0.54
1:A:344:ASN:C	1:A:344:ASN:HD22	2.11	0.54
1:B:43:ARG:HB2	1:B:43:ARG:NH2	2.22	0.54
1:A:227:ARG:HA	1:A:230:TRP:CE2	2.43	0.54
1:A:324:GLU:O	1:A:328:THR:HG23	2.07	0.54
1:B:79:ILE:HG21	1:B:83:PHE:CD2	2.42	0.54
1:B:88:LEU:HB2	1:B:89:PRO:HD3	1.88	0.54
1:C:205:LYS:O	1:C:209:ILE:HG13	2.08	0.54
1:D:312:ARG:HA	1:D:315:THR:CG2	2.37	0.54
1:A:314:ALA:O	1:A:318:ILE:HG13	2.07	0.54
1:B:102:MET:HE3	1:B:105:VAL:HG21	1.90	0.54
1:B:179:TYR:CE1	1:B:279:VAL:HG13	2.43	0.54
1:B:180:VAL:HG21	1:B:190:ALA:HB2	1.89	0.54
1:B:34:CYS:O	1:B:37:ILE:HG22	2.08	0.54
1:D:296:LEU:HD22	1:D:310:THR:HG22	1.88	0.54
1:D:210:ARG:O	1:D:210:ARG:HD2	2.08	0.53
1:A:210:ARG:HD2	1:A:210:ARG:O	2.08	0.53
1:A:80:PRO:HB3	1:A:82:GLU:OE2	2.08	0.53
1:D:76:ASP:OD1	1:D:79:ILE:HG13	2.08	0.53
1:D:86:ARG:HB3	1:D:86:ARG:HH11	1.73	0.53
1:A:87:GLU:O	1:A:90:LYS:HG3	2.08	0.53
1:C:263:HIS:O	1:C:267:VAL:HG23	2.09	0.53
1:D:188:ARG:HA	1:D:188:ARG:NE	2.22	0.53
1:A:312:ARG:HA	1:A:315:THR:CG2	2.39	0.53
1:B:196:ALA:O	1:B:199:MET:HB2	2.09	0.53
1:C:227:ARG:HA	1:C:230:TRP:NE1	2.25	0.52
1:D:89:PRO:HB3	1:D:144:ASN:HD21	1.74	0.52
1:C:42:SER:HB2	1:C:64:TYR:OH	2.09	0.52
1:B:270:TYR:O	1:B:273:SER:HB3	2.10	0.52
1:A:37:ILE:O	1:A:41:VAL:HG23	2.10	0.52
1:D:300:ASN:ND2	1:D:302:ASP:HB2	2.23	0.52
1:D:37:ILE:O	1:D:41:VAL:HG23	2.09	0.52
1:D:43:ARG:HB2	1:D:43:ARG:CZ	2.39	0.52
1:C:111:ARG:O	1:C:115:GLU:HG3	2.09	0.52
1:A:179:TYR:CE1	1:A:279:VAL:HG13	2.44	0.52
1:B:184:LEU:HD22	1:B:276:ASP:OD2	2.10	0.52
1:C:145:GLY:HA3	1:C:166:TYR:CD1	2.45	0.52
1:C:210:ARG:C	1:C:210:ARG:HD2	2.31	0.52
1:C:58:ASP:O	1:C:62:ILE:HG12	2.10	0.52
1:D:74:GLU:HG3	1:D:146:MET:HB3	1.92	0.51
1:D:166:TYR:O	1:D:170:LEU:HD12	2.09	0.51
1:D:79:ILE:HD11	1:D:105:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:239:ALA:HB1	1:B:245:HIS:CD2	2.45	0.51
1:B:91:PHE:HA	1:B:94:HIS:CD2	2.46	0.51
1:C:186:ASP:OD2	1:C:188:ARG:HB2	2.10	0.51
1:C:236:ASP:OD2	1:C:238:HIS:HB2	2.11	0.51
1:D:203:LEU:HD23	1:D:290:ALA:HB2	1.93	0.51
1:D:88:LEU:HB2	1:D:89:PRO:HD3	1.91	0.51
1:B:79:ILE:HD11	1:B:105:VAL:HG13	1.92	0.51
1:D:314:ALA:HA	1:D:317:ARG:HH12	1.74	0.51
1:C:300:ASN:OD1	1:C:302:ASP:HB2	2.11	0.51
1:A:88:LEU:HB2	1:A:89:PRO:HD3	1.93	0.51
1:B:142:MET:O	1:B:146:MET:HG3	2.11	0.51
1:D:253:LEU:HD21	1:D:297:VAL:O	2.11	0.51
1:B:294:LEU:HA	1:B:297:VAL:HG22	1.92	0.50
1:D:30:ASP:O	1:D:33:PHE:HB3	2.11	0.50
1:C:332:LEU:O	1:C:336:THR:HG23	2.10	0.50
1:B:142:MET:HG3	1:B:166:TYR:O	2.11	0.50
1:D:240:PHE:CE1	1:D:249:ALA:HA	2.47	0.50
1:B:274:LEU:HD13	1:B:280:PHE:HA	1.94	0.49
1:C:352:ARG:HG2	1:C:352:ARG:HH11	1.77	0.49
1:C:98:THR:O	1:C:118:THR:HG23	2.11	0.49
1:D:250:VAL:O	1:D:253:LEU:HB3	2.11	0.49
1:A:102:MET:CE	1:A:105:VAL:HG21	2.42	0.49
1:D:92:HIS:CG	1:D:140:GLU:HB2	2.47	0.49
1:C:339:LEU:HD23	1:C:339:LEU:C	2.32	0.49
1:C:227:ARG:HA	1:C:230:TRP:CE2	2.48	0.49
1:D:102:MET:O	1:D:115:GLU:HA	2.12	0.49
1:B:339:LEU:C	1:B:339:LEU:HD23	2.32	0.49
1:A:352:ARG:HG2	1:A:352:ARG:HH11	1.77	0.49
1:A:41:VAL:HG12	1:A:68:ARG:NH1	2.27	0.49
1:A:353:ILE:O	1:A:357:VAL:HG23	2.13	0.49
1:A:42:SER:HB2	1:A:64:TYR:OH	2.12	0.49
1:D:111:ARG:O	1:D:115:GLU:HG3	2.13	0.49
1:B:180:VAL:CG1	1:B:187:VAL:HA	2.41	0.49
1:B:280:PHE:CE1	1:B:328:THR:HG21	2.48	0.48
1:B:58:ASP:O	1:B:62:ILE:HG12	2.14	0.48
1:A:338:ARG:O	1:A:342:ARG:HG3	2.13	0.48
1:B:162:LEU:O	1:B:165:HIS:HB3	2.13	0.48
1:B:63:PHE:HD1	1:B:135:ILE:HG23	1.77	0.48
1:A:32:ARG:NH1	1:C:301:LYS:HZ1	2.09	0.48
1:B:343:MET:HE3	1:B:353:ILE:HG21	1.95	0.48
1:C:87:GLU:OE1	1:C:90:LYS:HE2	2.13	0.48
1:A:239:ALA:HB1	1:A:245:HIS:CD2	2.48	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:111:ARG:NH2	1:D:362:ARG:HH11	2.11	0.48
1:C:80:PRO:HG2	1:C:83:PHE:HB2	1.96	0.48
1:A:339:LEU:C	1:A:339:LEU:HD23	2.34	0.48
1:B:46:ALA:O	1:B:49:ILE:HG22	2.14	0.48
1:C:137:GLY:O	1:C:141:ARG:HG3	2.14	0.48
1:C:274:LEU:HD13	1:C:280:PHE:HA	1.96	0.48
1:B:169:GLY:HA3	1:B:197:ASN:OD1	2.13	0.48
1:D:249:ALA:HB1	1:D:304:PHE:CE2	2.48	0.48
1:D:77:MET:C	1:D:79:ILE:H	2.17	0.48
1:A:264:VAL:HG11	1:A:360:ALA:HB1	1.96	0.48
1:C:34:CYS:O	1:C:37:ILE:HG22	2.13	0.48
1:A:300:ASN:HD22	1:A:342:ARG:HH22	1.62	0.48
1:C:336:THR:HG21	1:C:364:MET:HE1	1.96	0.48
1:D:210:ARG:C	1:D:210:ARG:HD2	2.33	0.48
1:B:312:ARG:O	1:B:315:THR:HG23	2.14	0.47
1:C:122:ARG:NH1	1:C:122:ARG:HG3	2.29	0.47
1:D:339:LEU:HD23	1:D:339:LEU:C	2.34	0.47
1:C:80:PRO:HG2	1:C:83:PHE:CB	2.45	0.47
1:C:188:ARG:NE	1:C:188:ARG:HA	2.26	0.47
1:D:137:GLY:O	1:D:141:ARG:HG3	2.14	0.47
1:D:283:SER:O	1:D:287:GLN:HG2	2.14	0.47
1:D:314:ALA:HA	1:D:317:ARG:NH1	2.30	0.47
1:B:227:ARG:O	1:B:231:GLU:HG2	2.15	0.47
1:C:31:LEU:HD21	1:C:58:ASP:OD1	2.13	0.47
1:A:102:MET:O	1:A:115:GLU:HA	2.14	0.47
1:A:142:MET:O	1:A:146:MET:HG3	2.14	0.47
1:D:106:GLY:HA3	1:D:111:ARG:HA	1.97	0.47
1:D:171:VAL:O	1:D:175:LEU:HG	2.14	0.47
1:D:188:ARG:O	1:D:190:ALA:N	2.47	0.47
1:C:76:ASP:OD1	1:C:79:ILE:HG12	2.15	0.47
1:A:73:VAL:CG2	1:A:102:MET:HE1	2.35	0.47
1:A:114:LEU:O	1:A:117:TYR:HB2	2.15	0.47
1:C:128:GLY:O	1:C:132:GLN:HG3	2.15	0.47
1:C:257:VAL:HG13	1:C:294:LEU:CD1	2.45	0.47
1:C:327:ALA:O	1:C:330:GLN:HG3	2.15	0.47
1:C:41:VAL:HG11	1:C:68:ARG:HG2	1.96	0.47
1:A:296:LEU:HD22	1:A:310:THR:HG22	1.96	0.47
1:C:156:THR:O	1:C:159:ASP:HB2	2.15	0.46
1:C:227:ARG:O	1:C:231:GLU:HB3	2.15	0.46
1:D:34:CYS:HB3	1:D:65:LEU:HD11	1.97	0.46
1:B:265:PRO:O	1:B:269:GLU:HG2	2.15	0.46
1:B:43:ARG:O	1:B:47:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:210:ARG:HD2	1:A:210:ARG:C	2.35	0.46
1:B:188:ARG:HA	1:B:191:ASP:OD2	2.16	0.46
1:B:210:ARG:HD2	1:B:210:ARG:C	2.36	0.46
1:A:334:THR:O	1:A:338:ARG:HG3	2.16	0.46
1:C:240:PHE:CE1	1:C:249:ALA:HA	2.49	0.46
1:A:81:VAL:HG12	1:A:85:LEU:CD1	2.46	0.46
1:B:43:ARG:CB	1:B:43:ARG:HH21	2.29	0.46
1:B:102:MET:HB3	1:B:114:LEU:HB3	1.98	0.46
1:B:197:ASN:O	1:B:201:LEU:HD13	2.16	0.46
1:C:156:THR:HA	1:C:228:GLU:HB2	1.98	0.46
1:C:246:GLU:O	1:C:249:ALA:HB3	2.16	0.46
1:A:32:ARG:NH1	1:C:301:LYS:CE	2.79	0.46
1:D:300:ASN:HB2	1:D:342:ARG:HH22	1.81	0.46
1:B:34:CYS:HA	1:B:37:ILE:HG22	1.97	0.46
1:B:63:PHE:CZ	1:B:67:LEU:HD11	2.51	0.46
1:D:69:ALA:HB1	1:D:114:LEU:CD2	2.46	0.46
1:A:265:PRO:O	1:A:269:GLU:HG2	2.16	0.46
1:D:236:ASP:OD2	1:D:238:HIS:HB2	2.16	0.46
1:A:344:ASN:HD21	1:A:346:GLN:HG3	1.81	0.45
1:D:246:GLU:OE2	1:D:301:LYS:HD2	2.17	0.45
1:C:122:ARG:HG3	1:C:122:ARG:HH11	1.80	0.45
1:C:246:GLU:CD	1:C:301:LYS:HD2	2.35	0.45
1:D:176:THR:HA	1:D:179:TYR:CD2	2.51	0.45
1:C:34:CYS:HB3	1:C:65:LEU:HD11	1.98	0.45
1:B:257:VAL:HG13	1:B:294:LEU:HD11	1.99	0.45
1:D:98:THR:O	1:D:118:THR:HG23	2.17	0.45
1:C:162:LEU:O	1:C:165:HIS:HB3	2.17	0.45
1:A:162:LEU:HG	1:A:166:TYR:CE2	2.51	0.45
1:C:37:ILE:HD12	1:C:109:ARG:HG3	1.98	0.45
1:C:240:PHE:C	1:C:242:ASP:H	2.21	0.45
1:D:153:LYS:HB2	1:D:155:GLU:OE2	2.17	0.45
1:D:302:ASP:O	1:D:306:THR:HG22	2.16	0.45
1:A:338:ARG:HH11	1:A:338:ARG:HG2	1.82	0.44
1:D:173:HIS:CD2	1:D:193:LEU:HB3	2.52	0.44
1:A:83:PHE:CE1	1:A:87:GLU:HG3	2.52	0.44
1:A:349:CYS:O	1:A:350:TYR:C	2.55	0.44
1:A:34:CYS:O	1:A:37:ILE:HG22	2.17	0.44
1:A:49:ILE:HG12	1:A:57:ARG:HG3	1.99	0.44
1:B:222:ARG:HG3	1:B:222:ARG:HH11	1.81	0.44
1:D:169:GLY:HA3	1:D:197:ASN:OD1	2.17	0.44
1:B:128:GLY:O	1:B:132:GLN:HG3	2.18	0.44
1:C:105:VAL:HG12	1:C:106:GLY:N	2.32	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:122:ARG:HH11	1:D:122:ARG:HG3	1.81	0.44
1:D:49:ILE:HG12	1:D:57:ARG:HG3	2.00	0.44
1:A:352:ARG:NH1	1:A:352:ARG:HG2	2.33	0.44
1:C:100:TRP:O	1:C:101:CYS:HB3	2.18	0.44
1:C:88:LEU:CB	1:C:89:PRO:HD3	2.38	0.44
1:A:63:PHE:HD1	1:A:135:ILE:HG23	1.82	0.44
1:D:222:ARG:NH1	1:D:222:ARG:HG3	2.31	0.44
1:D:83:PHE:HA	1:D:86:ARG:HH12	1.82	0.44
1:A:176:THR:HA	1:A:179:TYR:CD2	2.52	0.44
1:D:242:ASP:OD2	1:D:243:GLU:N	2.51	0.44
1:A:249:ALA:HB1	1:A:304:PHE:CE2	2.52	0.43
1:B:111:ARG:O	1:B:115:GLU:HG3	2.18	0.43
1:D:201:LEU:HD23	1:D:263:HIS:CE1	2.53	0.43
1:A:236:ASP:OD1	1:A:238:HIS:HB2	2.18	0.43
1:A:311:THR:O	1:A:315:THR:HG22	2.18	0.43
1:B:76:ASP:OD1	1:B:79:ILE:HG13	2.17	0.43
1:C:174:GLY:O	1:C:178:LEU:HG	2.19	0.43
1:C:84:LYS:C	1:C:86:ARG:H	2.22	0.43
1:A:180:VAL:HG21	1:A:190:ALA:HB2	2.00	0.43
1:B:160:TYR:CD1	1:B:226:PRO:HD3	2.54	0.43
1:C:324:GLU:O	1:C:328:THR:HG23	2.18	0.43
1:B:147:CYS:HA	1:B:150:LEU:HD12	2.01	0.43
1:B:344:ASN:HB3	1:B:345:ALA:H	1.67	0.43
1:B:41:VAL:HG12	1:B:68:ARG:CZ	2.48	0.43
1:C:300:ASN:O	1:C:303:VAL:HG23	2.19	0.43
1:C:249:ALA:HB1	1:C:304:PHE:CE2	2.53	0.43
1:C:56:MET:HE1	1:C:178:LEU:HB3	2.00	0.43
1:C:102:MET:O	1:C:115:GLU:HA	2.18	0.43
1:D:82:GLU:OE1	1:D:83:PHE:N	2.51	0.43
1:A:240:PHE:CE1	1:A:249:ALA:HA	2.53	0.43
1:C:37:ILE:CD1	1:C:109:ARG:HG3	2.48	0.43
1:D:324:GLU:O	1:D:328:THR:HG23	2.18	0.43
1:A:361:ILE:O	1:A:365:GLU:HG3	2.18	0.43
1:D:43:ARG:HH21	1:D:43:ARG:CB	2.31	0.43
1:D:79:ILE:HG23	1:D:80:PRO:HD2	2.00	0.43
1:A:75:ASP:CG	1:A:222:ARG:HH21	2.21	0.43
1:A:315:THR:HA	1:A:318:ILE:HD12	2.01	0.43
1:C:342:ARG:HG2	1:C:342:ARG:HH11	1.83	0.43
1:B:32:ARG:NH2	1:D:301:LYS:HE2	2.34	0.42
1:C:353:ILE:O	1:C:357:VAL:HG23	2.18	0.42
1:A:280:PHE:CZ	1:A:325:LEU:HA	2.55	0.42
1:B:276:ASP:HA	1:B:277:PRO:HD3	1.88	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:237:LEU:HD12	1:D:240:PHE:CE2	2.54	0.42
1:B:311:THR:O	1:B:315:THR:HG22	2.20	0.42
1:C:165:HIS:O	1:C:170:LEU:HG	2.19	0.42
1:C:250:VAL:O	1:C:253:LEU:HB3	2.19	0.42
1:A:302:ASP:O	1:A:306:THR:HG22	2.19	0.42
1:B:280:PHE:HZ	1:B:328:THR:HG21	1.81	0.42
1:B:68:ARG:HD2	1:B:68:ARG:HA	1.82	0.42
1:D:56:MET:O	1:D:60:VAL:HG23	2.20	0.42
1:D:343:MET:HE2	1:D:350:TYR:HA	2.01	0.42
1:A:276:ASP:HA	1:A:277:PRO:HD3	1.89	0.42
1:B:219:VAL:HA	1:B:220:PRO:HA	1.94	0.42
1:C:41:VAL:HG12	1:C:42:SER:N	2.34	0.42
1:D:122:ARG:NH1	1:D:122:ARG:HG3	2.35	0.42
1:A:32:ARG:NH1	1:C:301:LYS:HE3	2.34	0.42
1:C:173:HIS:O	1:C:177:LEU:HG	2.19	0.42
1:C:276:ASP:HA	1:C:277:PRO:HD3	1.92	0.42
1:A:32:ARG:NH2	1:C:302:ASP:OD1	2.53	0.42
1:D:106:GLY:HA3	1:D:111:ARG:CA	2.50	0.42
1:D:145:GLY:HA3	1:D:166:TYR:CD1	2.55	0.42
1:D:205:LYS:O	1:D:209:ILE:HG13	2.20	0.42
1:D:261:LEU:HA	1:D:264:VAL:HG23	2.01	0.42
1:B:349:CYS:O	1:B:350:TYR:C	2.58	0.41
1:B:79:ILE:CG2	1:B:80:PRO:HD2	2.50	0.41
1:C:40:ALA:CB	1:C:109:ARG:HG2	2.50	0.41
1:C:142:MET:O	1:C:146:MET:HG3	2.19	0.41
1:B:307:LYS:HD3	1:B:309:LYS:HE3	2.02	0.41
1:B:268:VAL:HG13	1:B:329:LEU:HD21	2.02	0.41
1:B:32:ARG:HG3	1:B:32:ARG:HH11	1.85	0.41
1:B:250:VAL:O	1:B:253:LEU:HB3	2.20	0.41
1:C:253:LEU:HD21	1:C:297:VAL:O	2.20	0.41
1:C:314:ALA:O	1:C:318:ILE:HG13	2.20	0.41
1:A:74:GLU:OE1	1:A:74:GLU:C	2.59	0.41
1:D:69:ALA:HB1	1:D:114:LEU:HD23	2.03	0.41
1:D:118:THR:O	1:D:122:ARG:HG2	2.19	0.41
1:B:82:GLU:HG2	1:B:83:PHE:N	2.34	0.41
1:C:222:ARG:NH1	1:C:222:ARG:HG3	2.36	0.41
1:C:56:MET:O	1:C:60:VAL:HG23	2.20	0.41
1:D:280:PHE:CZ	1:D:325:LEU:HA	2.56	0.41
1:B:95:LEU:HB3	1:B:124:TYR:CE2	2.55	0.41
1:B:227:ARG:HH11	1:B:227:ARG:HG3	1.86	0.41
1:C:242:ASP:OD1	1:C:244:LEU:HB3	2.20	0.41
1:D:119:HIS:O	1:D:122:ARG:HB2	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:97:ASP:C	1:D:99:THR:H	2.23	0.41
1:A:228:GLU:O	1:A:232:LYS:HE3	2.21	0.41
1:A:32:ARG:NH2	1:C:302:ASP:CG	2.73	0.41
1:C:43:ARG:O	1:C:47:VAL:HG23	2.20	0.41
1:D:226:PRO:HD2	1:D:256:MET:CE	2.50	0.41
1:B:56:MET:HE2	1:B:178:LEU:HB3	2.02	0.41
1:C:261:LEU:HA	1:C:264:VAL:HG23	2.03	0.41
1:D:300:ASN:HB2	1:D:342:ARG:NH2	2.36	0.41
1:A:129:LYS:HB3	1:A:129:LYS:HE3	1.96	0.41
1:A:31:LEU:HD12	1:A:31:LEU:HA	1.83	0.41
1:B:293:THR:O	1:B:297:VAL:HG13	2.21	0.41
1:A:248:LYS:CE	1:A:248:LYS:HA	2.51	0.40
1:B:56:MET:CE	1:B:178:LEU:HB3	2.52	0.40
1:A:327:ALA:O	1:A:330:GLN:HG2	2.21	0.40
1:B:324:GLU:OE2	1:B:326:GLN:HB2	2.21	0.40
1:B:363:ALA:O	1:B:366:SER:HB3	2.21	0.40
1:B:43:ARG:CB	1:B:43:ARG:NH2	2.83	0.40
1:B:56:MET:O	1:B:60:VAL:HG23	2.21	0.40
1:C:361:ILE:O	1:C:365:GLU:HG3	2.21	0.40
1:C:82:GLU:CD	1:C:82:GLU:H	2.24	0.40
1:C:203:LEU:HD23	1:C:290:ALA:HB2	2.03	0.40
1:C:343:MET:HE2	1:C:350:TYR:HA	2.04	0.40
1:D:106:GLY:HA3	1:D:111:ARG:CB	2.51	0.40
1:A:281:ALA:O	1:A:285:ILE:HG13	2.21	0.40
1:A:95:LEU:HA	1:A:121:THR:HG22	2.03	0.40
1:D:174:GLY:O	1:D:178:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	339/365 (93%)	314 (93%)	24 (7%)	1 (0%)	50 84
1	B	339/365 (93%)	311 (92%)	23 (7%)	5 (2%)	15 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	339/365 (93%)	315 (93%)	21 (6%)	3 (1%)	25 63
1	D	339/365 (93%)	314 (93%)	20 (6%)	5 (2%)	15 46
All	All	1356/1460 (93%)	1254 (92%)	88 (6%)	14 (1%)	22 60

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	350	TYR
1	B	350	TYR
1	C	350	TYR
1	D	189	LEU
1	D	98	THR
1	C	348	ALA
1	B	54	GLU
1	B	98	THR
1	B	104	GLY
1	B	305	HIS
1	D	54	GLU
1	D	305	HIS
1	C	325	LEU
1	D	104	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	298/318 (94%)	282 (95%)	16 (5%)	31 66
1	B	298/318 (94%)	291 (98%)	7 (2%)	63 92
1	C	298/318 (94%)	287 (96%)	11 (4%)	45 81
1	D	298/318 (94%)	283 (95%)	15 (5%)	34 70
All	All	1192/1272 (94%)	1143 (96%)	49 (4%)	41 77

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	36	ASP
1	A	39	GLN
1	A	53	ASP
1	A	55	GLU
1	A	74	GLU
1	A	102	MET
1	A	109	ARG
1	A	161	ASP
1	A	188	ARG
1	A	231	GLU
1	A	235	ASP
1	A	315	THR
1	A	344	ASN
1	A	346	GLN
1	A	359	ASP
1	B	75	ASP
1	B	102	MET
1	B	109	ARG
1	B	129	LYS
1	B	161	ASP
1	B	315	THR
1	B	328	THR
1	C	79	ILE
1	C	102	MET
1	C	129	LYS
1	C	161	ASP
1	C	188	ARG
1	C	218	GLU
1	C	248	LYS
1	C	330	GLN
1	C	346	GLN
1	C	347	ASP
1	C	359	ASP
1	D	36	ASP
1	D	53	ASP
1	D	54	GLU
1	D	74	GLU
1	D	82	GLU
1	D	90	LYS
1	D	129	LYS
1	D	188	ARG
1	D	296	LEU

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Mol	Chain	Res	Type
1	D	315	THR
1	D	346	GLN
1	D	352	ARG
1	D	354	GLU
1	D	355	HIS
1	D	359	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	HIS
1	A	144	ASN
1	A	245	HIS
1	A	287	GLN
1	A	326	GLN
1	A	344	ASN
1	B	94	HIS
1	B	144	ASN
1	B	245	HIS
1	C	144	ASN
1	C	207	ASN
1	D	144	ASN
1	D	300	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 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	BH3	A	401	-	30,30,30	1.94	6 (20%)	39,39,39	1.05	3 (7%)
2	BH3	B	401	-	30,30,30	1.93	6 (20%)	39,39,39	1.06	3 (7%)
2	BH3	C	401	-	30,30,30	1.93	6 (20%)	39,39,39	1.05	3 (7%)
2	BH3	D	401	-	30,30,30	1.93	6 (20%)	39,39,39	1.06	3 (7%)

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	BH3	A	401	-	1/1/3/3	0/31/31/31	0/1/1/1
2	BH3	B	401	-	1/1/3/3	0/31/31/31	0/1/1/1
2	BH3	C	401	-	1/1/3/3	0/31/31/31	0/1/1/1
2	BH3	D	401	-	1/1/3/3	0/31/31/31	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	BH3	PBC-OAE	7.15	1.61	1.51
2	A	401	BH3	PBC-OAE	7.13	1.61	1.51
2	B	401	BH3	PBC-OAE	7.13	1.61	1.51
2	D	401	BH3	PBC-OAE	7.10	1.61	1.51
2	C	401	BH3	PBD-OAF	3.92	1.61	1.54
2	D	401	BH3	PBD-OAF	3.92	1.61	1.54
2	C	401	BH3	PBD-OAG	3.92	1.61	1.54
2	D	401	BH3	PBD-OAG	3.92	1.61	1.54
2	A	401	BH3	PBD-OAF	3.92	1.61	1.54
2	B	401	BH3	PBD-OAG	3.91	1.61	1.54
2	B	401	BH3	PBD-OAF	3.88	1.61	1.54
2	A	401	BH3	PBD-OAG	3.85	1.61	1.54
2	B	401	BH3	PBC-OAD	3.11	1.61	1.57
2	A	401	BH3	PBC-OAD	3.07	1.61	1.57
2	D	401	BH3	PBC-OAD	3.04	1.61	1.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	BH3	PBC-OAD	2.99	1.61	1.57
2	A	401	BH3	CAH-NBA	-2.32	1.33	1.37
2	A	401	BH3	CAI-NBB	-2.30	1.33	1.37
2	D	401	BH3	CAH-NBA	-2.26	1.33	1.37
2	C	401	BH3	CAI-NBB	-2.25	1.33	1.37
2	D	401	BH3	CAI-NBB	-2.24	1.33	1.37
2	B	401	BH3	CAI-NBB	-2.23	1.33	1.37
2	C	401	BH3	CAH-NBA	-2.18	1.33	1.37
2	B	401	BH3	CAH-NBA	-2.16	1.33	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	BH3	OAB-PBC-CAZ	2.90	113.45	108.99
2	D	401	BH3	OAB-PBC-CAZ	2.81	113.31	108.99
2	A	401	BH3	OAB-PBC-CAZ	2.73	113.19	108.99
2	C	401	BH3	OAB-PBC-CAZ	2.72	113.19	108.99
2	C	401	BH3	PBD-CAZ-PBC	-2.43	109.38	114.46
2	A	401	BH3	OAB-PBC-OAE	-2.33	112.28	115.90
2	B	401	BH3	OAB-PBC-OAE	-2.33	112.29	115.90
2	D	401	BH3	OAB-PBC-OAE	-2.32	112.30	115.90
2	C	401	BH3	OAB-PBC-OAE	-2.24	112.43	115.90
2	A	401	BH3	PBD-CAZ-PBC	-2.09	110.10	114.46
2	B	401	BH3	OAB-PBC-OAE	-2.07	105.62	109.84
2	D	401	BH3	OAB-PBC-OAE	-2.01	105.75	109.84

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	401	BH3	CAZ
2	C	401	BH3	CAZ
2	B	401	BH3	CAZ
2	D	401	BH3	CAZ

There are no torsion outliers.

There are no ring outliers.

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, 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	341/365 (93%)	-0.14	2 (0%) 86 88	35, 61, 88, 107	0
1	B	341/365 (93%)	0.06	6 (1%) 65 66	43, 74, 100, 113	0
1	C	341/365 (93%)	0.14	13 (3%) 38 38	42, 73, 106, 115	0
1	D	341/365 (93%)	0.39	23 (6%) 17 16	54, 99, 133, 151	0
All	All	1364/1460 (93%)	0.11	44 (3%) 45 46	35, 74, 118, 151	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	225	TRP	4.6
1	D	80	PRO	3.6
1	D	78	SER	3.6
1	D	81	VAL	3.5
1	D	66	VAL	3.1
1	D	65	LEU	3.1
1	B	346	GLN	3.0
1	D	256	MET	3.0
1	D	29	GLU	2.9
1	A	43	ARG	2.8
1	D	67	LEU	2.8
1	D	146	MET	2.7
1	B	188	ARG	2.7
1	C	69	ALA	2.7
1	C	107	VAL	2.6
1	D	55	GLU	2.5
1	C	252	CYS	2.5
1	D	151	THR	2.5
1	D	43	ARG	2.4
1	D	355	HIS	2.4
1	C	43	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	66	VAL	2.4
1	D	235	ASP	2.4
1	C	368	GLN	2.4
1	C	306	THR	2.3
1	D	107	VAL	2.3
1	C	67	LEU	2.3
1	D	69	ALA	2.2
1	D	102	MET	2.2
1	B	28	ASP	2.2
1	C	248	LYS	2.2
1	B	362	ARG	2.2
1	B	66	VAL	2.2
1	C	309	LYS	2.2
1	C	61	CYS	2.1
1	D	222	ARG	2.1
1	C	222	ARG	2.1
1	D	248	LYS	2.1
1	B	61	CYS	2.1
1	D	158	ALA	2.1
1	D	344	ASN	2.1
1	D	275	ARG	2.0
1	C	345	ALA	2.0
1	A	252	CYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	BH3	D	401	30/30	0.33	1.44	82,131,139,139	0
2	BH3	A	401	30/30	0.28	1.40	62,114,127,127	0
2	BH3	B	401	30/30	0.29	1.19	54,131,142,143	0
2	BH3	C	401	30/30	0.27	0.86	58,120,131,131	0

6.5 Other polymers

There are no such residues in this entry.