



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:05 AM UTC

PDB ID : 3SY2 / pdb_00003sy2
Title : Crystal structure of the Salmonella E3 ubiquitin ligase SopA in complex with the human E2 UbcH7
Authors : Diao, J.; Lin, D.Y.; Chen, J.
Deposited on : 2011-07-15
Resolution : 3.27 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

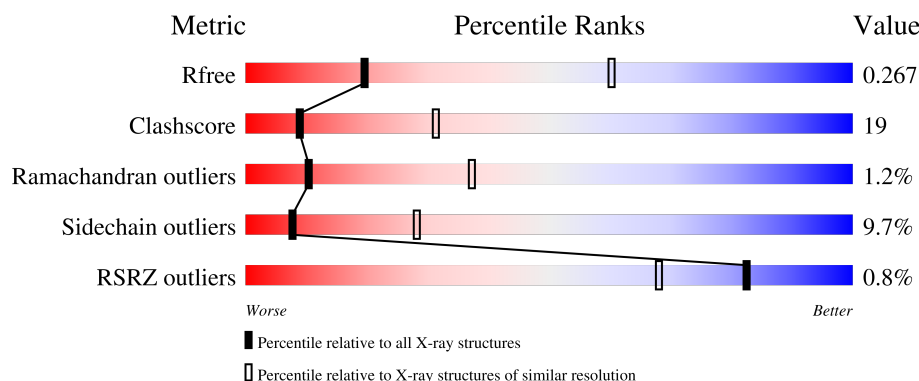
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.27 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1303 (3.30-3.26)
Clashscore	190562	1354 (3.30-3.26)
Ramachandran outliers	187476	1334 (3.30-3.26)
Sidechain outliers	187428	1333 (3.30-3.26)
RSRZ outliers	180081	1303 (3.30-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	621	% 61% 33% ..
1	B	621	% 62% 34% ..
2	C	156	60% 36% ..
2	D	156	% 53% 38% 7% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11660 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 E3 ubiquitin-protein ligase SopA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	609	Total	C	N	O	S	0	0	0
			4631	2935	794	882	20			
1	B	616	Total	C	N	O	S	0	0	0
			4667	2965	796	886	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	162	SER	-	expression tag	UNP Q8ZNR3
A	163	ASN	-	expression tag	UNP Q8ZNR3
A	164	ALA	-	expression tag	UNP Q8ZNR3
B	162	SER	-	expression tag	UNP Q8ZNR3
B	163	ASN	-	expression tag	UNP Q8ZNR3
B	164	ALA	-	expression tag	UNP Q8ZNR3

- Molecule 2 is a protein called Ubiquitin-conjugating enzyme E2 L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	154	Total	C	N	O	S	0	0	0
			1175	753	206	212	4			
2	D	154	Total	C	N	O	S	0	0	0
			1167	751	202	209	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP P68036
C	0	SER	-	expression tag	UNP P68036
D	-1	GLY	-	expression tag	UNP P68036
D	0	SER	-	expression tag	UNP P68036

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

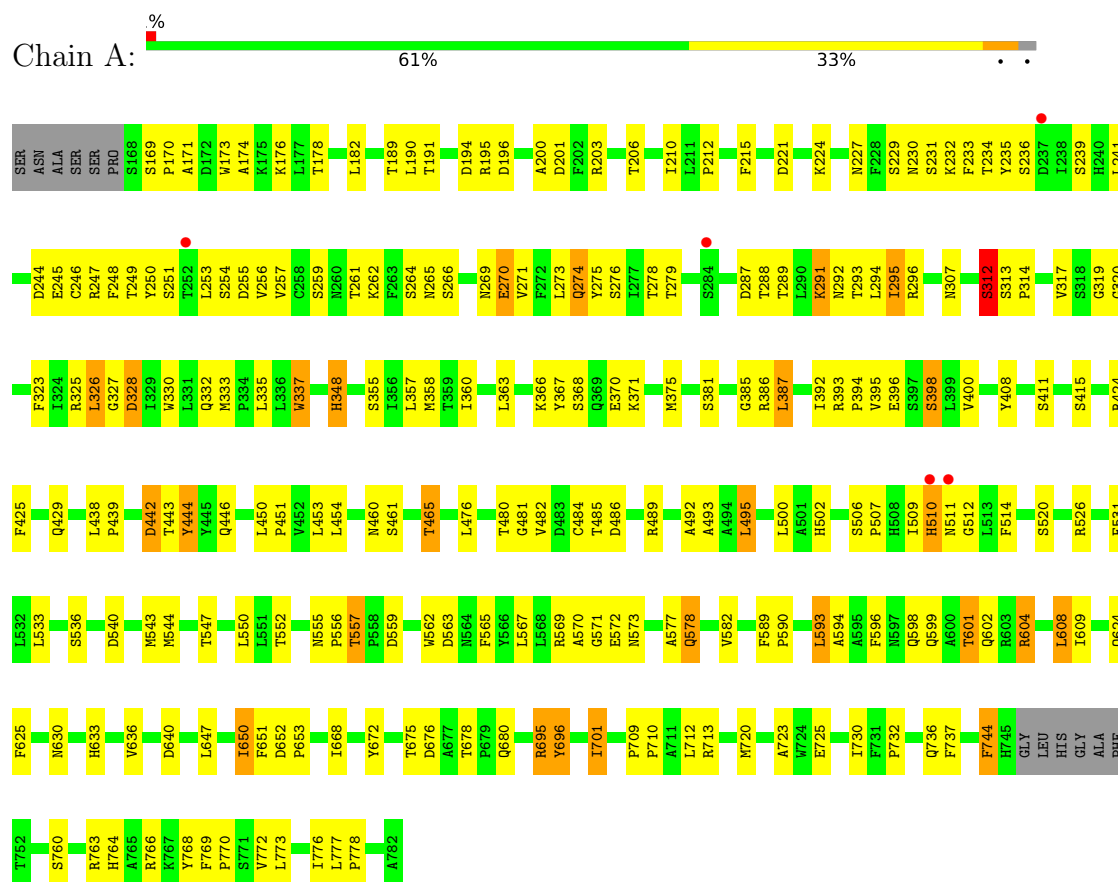
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		
4	B	6	Total	O	0	0
			6	6		
4	D	1	Total	O	0	0
			1	1		

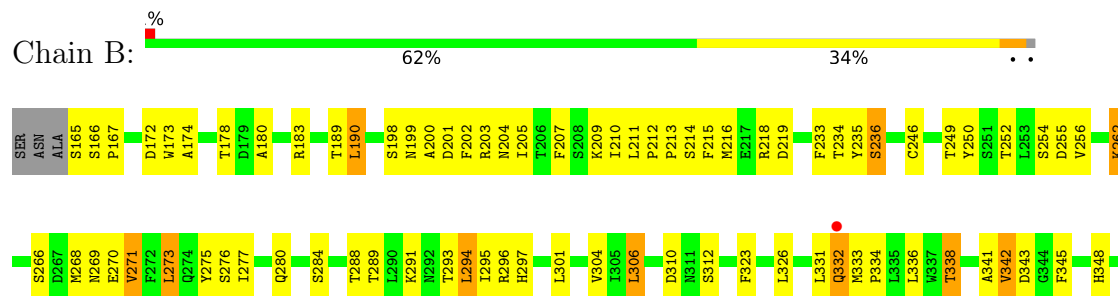
3 Residue-property plots

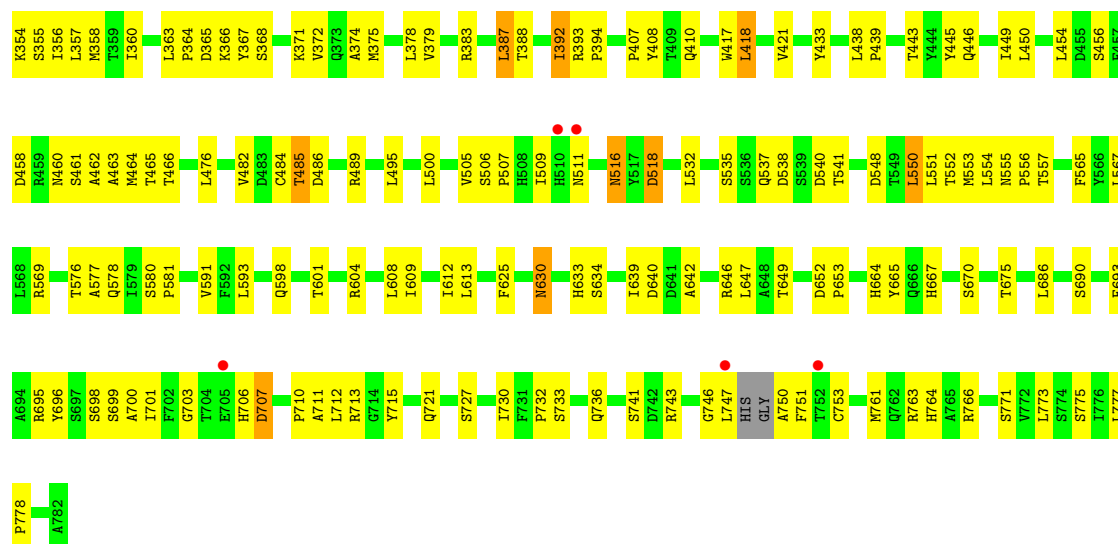
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: E3 ubiquitin-protein ligase SopA



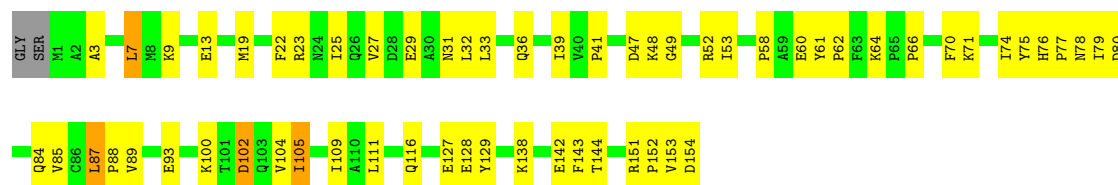
• Molecule 1: E3 ubiquitin-protein ligase SopA





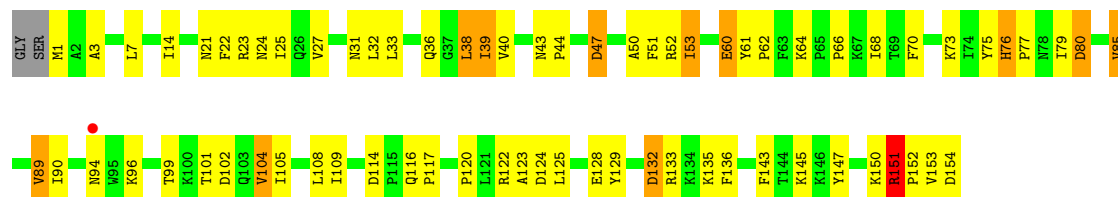
• Molecule 2: Ubiquitin-conjugating enzyme E2 L3

Chain C: 60% 36% ..



• Molecule 2: Ubiquitin-conjugating enzyme E2 L3

Chain D: 53% 38% 7% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.12Å 118.36Å 241.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.42 – 3.27 45.42 – 3.27	Depositor EDS
% Data completeness (in resolution range)	93.8 (45.42-3.27) 93.7 (45.42-3.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.211 , 0.275 0.205 , 0.267	Depositor DCC
R_{free} test set	1572 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	85.2	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 75.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11660	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.38	0/4752	0.79	4/6493 (0.1%)
1	B	0.37	0/4790	0.79	2/6548 (0.0%)
2	C	0.37	0/1206	0.87	2/1646 (0.1%)
2	D	0.40	0/1197	0.93	9/1635 (0.6%)
All	All	0.38	0/11945	0.82	17/16322 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	87	LEU	CA-C-N	7.94	127.50	119.24
2	C	87	LEU	C-N-CA	7.94	127.50	119.24
1	A	555	ASN	CA-C-N	6.11	126.12	119.89
1	A	555	ASN	C-N-CA	6.11	126.12	119.89
1	B	555	ASN	CA-C-N	6.06	125.82	119.76
1	B	555	ASN	C-N-CA	6.06	125.82	119.76
2	D	94	ASN	N-CA-C	-5.30	106.31	114.16
1	A	589	PHE	CA-C-N	5.26	125.07	119.28
1	A	589	PHE	C-N-CA	5.26	125.07	119.28
2	D	76	HIS	CA-C-N	5.22	124.89	119.56
2	D	76	HIS	C-N-CA	5.22	124.89	119.56
2	D	43	ASN	CA-C-N	5.17	123.44	119.66
2	D	43	ASN	C-N-CA	5.17	123.44	119.66
2	D	114	ASP	CA-C-N	5.14	125.06	119.76
2	D	114	ASP	C-N-CA	5.14	125.06	119.76
2	D	151	ARG	CA-C-N	5.01	124.92	119.76
2	D	151	ARG	C-N-CA	5.01	124.92	119.76

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	4631	0	4322	174	0
1	B	4667	0	4363	149	0
2	C	1175	0	1107	46	0
2	D	1167	0	1110	52	0
3	A	5	0	0	0	0
4	A	8	0	0	0	0
4	B	6	0	0	0	0
4	D	1	0	0	0	0
All	All	11660	0	10902	418	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 19.

All (418) 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)
2:D:151:ARG:HD3	2:D:152:PRO:HD2	1.45	0.97
2:C:52:ARG:HH12	2:C:71:LYS:HD3	1.37	0.88
1:A:375:MET:HG3	1:A:408:TYR:HE2	1.37	0.88
1:A:274:GLN:HG3	1:A:294:LEU:HD22	1.53	0.87
1:A:593:LEU:HD23	1:A:594:ALA:N	1.89	0.87
2:D:96:LYS:O	2:D:99:THR:HG23	1.76	0.85
2:D:23:ARG:O	2:D:38:LEU:HB3	1.75	0.85
2:C:78:ASN:HD21	2:C:116:GLN:H	1.25	0.84
1:B:438:LEU:HD12	1:B:439:PRO:HD2	1.59	0.84
1:B:174:ALA:HB1	1:B:210:ILE:HD12	1.60	0.84
1:A:375:MET:HG3	1:A:408:TYR:CE2	2.12	0.84
2:C:76:HIS:HD2	2:C:78:ASN:H	1.26	0.83
1:B:387:LEU:HD12	1:B:387:LEU:H	1.42	0.83
1:A:590:PRO:O	1:A:593:LEU:HD22	1.78	0.83
1:A:680:GLN:HG3	1:A:730:ILE:HD11	1.61	0.83
1:B:732:PRO:HD3	1:B:764:HIS:CE1	2.14	0.82
1:B:695:ARG:HG3	1:B:695:ARG:HH11	1.46	0.80
2:D:101:THR:HA	2:D:104:VAL:HG13	1.63	0.79
1:A:244:ASP:OD2	1:A:245:GLU:HG3	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:LEU:HD23	1:A:594:ALA:H	1.44	0.78
1:A:357:LEU:HA	1:A:375:MET:HE1	1.66	0.76
2:C:78:ASN:ND2	2:C:111:LEU:HD11	1.99	0.76
2:C:52:ARG:NH1	2:C:71:LYS:HD3	2.00	0.76
1:A:582:VAL:HG22	1:A:596:PHE:CE2	2.20	0.75
2:C:76:HIS:CD2	2:C:78:ASN:H	2.05	0.75
2:D:7:LEU:HD11	2:D:33:LEU:HD23	1.71	0.72
1:B:743:ARG:HD2	1:B:753:CYS:SG	2.29	0.72
1:B:357:LEU:HA	1:B:375:MET:HE1	1.72	0.72
1:A:393:ARG:CZ	1:A:763:ARG:HD3	2.20	0.72
1:A:325:ARG:HH21	1:A:330:TRP:HE1	1.38	0.71
1:A:557:THR:HG23	1:A:559:ASP:H	1.56	0.71
1:A:319:GLY:N	1:A:320:GLY:HA3	2.06	0.70
1:B:727:SER:O	1:B:730:ILE:HG12	1.91	0.70
1:A:307:ASN:O	1:A:328:ASP:HB3	1.92	0.69
1:B:233:PHE:O	1:B:236:SER:HB3	1.91	0.69
1:A:438:LEU:HD12	1:A:439:PRO:HD2	1.73	0.69
1:B:165:SER:C	1:B:167:PRO:HD3	2.18	0.69
1:A:190:LEU:HB3	1:A:194:ASP:HB2	1.75	0.68
1:B:277:ILE:HD12	1:B:706:HIS:CD2	2.28	0.68
1:A:540:ASP:HB2	1:A:569:ARG:NH1	2.09	0.68
2:C:3:ALA:O	2:C:7:LEU:HB2	1.94	0.68
1:A:732:PRO:HG2	1:A:736:GLN:HG2	1.76	0.67
1:A:500:LEU:HD22	1:A:509:ILE:HD11	1.76	0.67
1:B:288:THR:HG22	1:B:289:THR:H	1.58	0.67
1:A:190:LEU:HB3	1:A:194:ASP:CB	2.25	0.67
1:A:577:ALA:O	1:A:578:GLN:HB2	1.94	0.67
2:D:22:PHE:HD1	2:D:39:ILE:HG22	1.58	0.67
2:C:79:ILE:HG12	2:C:85:VAL:HG22	1.77	0.66
1:A:573:ASN:ND2	2:D:96:LYS:HB2	2.10	0.66
1:A:251:SER:H	1:A:271:VAL:HG12	1.60	0.66
1:A:732:PRO:HD3	1:A:764:HIS:CE1	2.31	0.65
1:A:292:ASN:HD21	1:A:312:SER:CB	2.09	0.65
1:A:269:ASN:O	1:A:271:VAL:HG13	1.96	0.65
1:A:271:VAL:O	1:A:293:THR:HG23	1.96	0.65
1:B:598:GLN:HA	1:B:601:THR:HB	1.79	0.65
2:D:22:PHE:CD1	2:D:39:ILE:HG22	2.31	0.64
2:C:80:ASP:HB3	2:C:84:GLN:H	1.62	0.64
1:B:306:LEU:HB2	1:B:367:TYR:CE2	2.31	0.64
1:A:174:ALA:HB1	1:A:210:ILE:CD1	2.28	0.64
1:B:198:SER:O	1:B:199:ASN:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:61:TYR:CD1	2:C:62:PRO:HA	2.33	0.64
2:D:79:ILE:HG12	2:D:85:VAL:HG22	1.79	0.64
1:A:385:GLY:O	1:A:386:ARG:HB2	1.97	0.63
2:D:117:PRO:O	2:D:120:PRO:HD3	1.99	0.63
1:B:364:PRO:HG2	1:B:367:TYR:CD1	2.34	0.62
1:A:254:SER:O	1:A:255:ASP:HB2	1.99	0.62
1:B:554:LEU:C	1:B:556:PRO:HD3	2.24	0.62
2:C:22:PHE:HD1	2:C:39:ILE:HG22	1.63	0.62
1:B:713:ARG:HH12	1:B:746:GLY:HA3	1.63	0.62
2:D:21:ASN:HB3	2:D:109:ILE:HD13	1.81	0.62
1:B:341:ALA:O	1:B:345:PHE:HB2	1.99	0.62
1:B:269:ASN:ND2	1:B:291:LYS:HB3	2.15	0.62
1:A:540:ASP:HB2	1:A:569:ARG:HH12	1.65	0.62
1:B:345:PHE:O	1:B:356:ILE:HG22	2.00	0.62
1:B:166:SER:N	1:B:167:PRO:HD3	2.15	0.61
1:A:695:ARG:HG3	1:A:695:ARG:HH11	1.65	0.61
1:A:348:HIS:HB3	1:A:355:SER:HB3	1.83	0.61
1:B:695:ARG:HG3	1:B:695:ARG:NH1	2.14	0.61
1:B:500:LEU:HA	1:B:505:VAL:HG11	1.82	0.60
2:D:27:VAL:CG2	2:D:32:LEU:HA	2.31	0.60
1:B:476:LEU:HD21	1:B:551:LEU:HD23	1.82	0.60
1:A:773:LEU:HD11	1:A:777:LEU:HD12	1.83	0.60
2:D:75:TYR:HB2	2:D:143:PHE:CD1	2.36	0.60
1:B:348:HIS:HB3	1:B:355:SER:HB3	1.83	0.60
1:A:768:TYR:OH	2:C:127:GLU:HG2	2.01	0.60
1:A:246:CYS:H	1:A:266:SER:CB	2.15	0.59
2:C:58:PRO:HD3	2:C:66:PRO:HA	1.82	0.59
2:C:74:ILE:HG12	2:C:75:TYR:N	2.17	0.59
1:B:516:ASN:C	1:B:516:ASN:HD22	2.11	0.59
1:A:169:SER:HB3	1:A:170:PRO:HD2	1.85	0.59
1:A:313:SER:HB2	1:A:314:PRO:HD2	1.84	0.59
2:D:61:TYR:CD1	2:D:62:PRO:HA	2.37	0.59
1:A:442:ASP:O	1:A:446:GLN:HG3	2.01	0.59
1:B:485:THR:O	1:B:489:ARG:HG3	2.03	0.59
1:A:234:THR:O	1:A:235:TYR:HB2	2.02	0.59
1:B:334:PRO:HD3	1:B:345:PHE:CZ	2.38	0.58
1:B:634:SER:HB3	1:B:701:ILE:HA	1.85	0.58
1:B:553:MET:HE1	1:B:565:PHE:CD1	2.39	0.58
2:D:60:GLU:HG3	2:D:64:LYS:HD2	1.86	0.57
1:A:604:ARG:HG2	1:A:672:TYR:CE2	2.39	0.57
1:A:481:GLY:HA3	1:A:484:CYS:SG	2.45	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:HIS:HD1	1:A:358:MET:HG2	1.68	0.57
1:A:326:LEU:HD11	1:A:363:LEU:HD11	1.87	0.57
2:C:78:ASN:ND2	2:C:116:GLN:H	1.98	0.57
1:B:277:ILE:HD12	1:B:706:HIS:CG	2.40	0.56
1:A:203:ARG:HG3	1:A:232:LYS:O	2.04	0.56
1:A:327:GLY:HA2	1:A:370:GLU:HG2	1.87	0.56
2:C:128:GLU:O	2:C:128:GLU:HG2	2.05	0.56
1:B:256:VAL:O	1:B:275:TYR:HB2	2.05	0.56
1:A:276:SER:C	1:A:278:THR:H	2.12	0.56
1:A:360:ILE:HB	1:A:375:MET:HE2	1.88	0.56
1:B:207:PHE:HA	1:B:210:ILE:HG12	1.88	0.56
2:C:74:ILE:HG12	2:C:75:TYR:H	1.70	0.56
2:D:31:ASN:O	2:D:32:LEU:HB3	2.05	0.56
2:C:53:ILE:HD11	2:C:70:PHE:CE1	2.41	0.55
2:D:31:ASN:C	2:D:33:LEU:H	2.15	0.55
1:B:577:ALA:HB1	2:C:93:GLU:HA	1.89	0.55
2:D:27:VAL:HG21	2:D:32:LEU:HD12	1.89	0.55
1:A:625:PHE:HD2	1:A:696:TYR:CZ	2.24	0.55
1:B:275:TYR:CE1	1:B:296:ARG:HD3	2.41	0.55
1:B:732:PRO:HG2	1:B:736:GLN:HG2	1.87	0.55
2:C:9:LYS:HE3	2:C:13:GLU:OE2	2.07	0.55
1:B:255:ASP:O	1:B:276:SER:HB2	2.07	0.55
2:D:61:TYR:CG	2:D:62:PRO:HA	2.42	0.55
1:A:224:LYS:HA	1:A:244:ASP:O	2.07	0.54
1:A:249:THR:HG23	1:A:269:ASN:HB2	1.89	0.54
1:A:348:HIS:HB3	1:A:355:SER:CB	2.38	0.54
1:B:446:GLN:HA	1:B:450:LEU:HD12	1.89	0.54
1:B:407:PRO:O	1:B:410:GLN:HG2	2.07	0.54
1:B:393:ARG:N	1:B:394:PRO:HD2	2.22	0.54
1:A:396:GLU:O	1:A:400:VAL:HG22	2.08	0.53
2:C:76:HIS:CD2	2:C:77:PRO:HD2	2.43	0.53
1:B:294:LEU:HD21	1:B:332:GLN:HG3	1.91	0.53
1:B:273:LEU:HD23	1:B:273:LEU:O	2.09	0.53
1:A:393:ARG:HA	1:A:396:GLU:HG3	1.91	0.53
1:A:276:SER:C	1:A:278:THR:N	2.64	0.53
1:A:557:THR:CG2	1:A:559:ASP:H	2.21	0.52
2:D:3:ALA:O	2:D:7:LEU:HG	2.08	0.52
2:C:61:TYR:CG	2:C:62:PRO:HA	2.43	0.52
1:B:476:LEU:HD22	1:B:550:LEU:HD13	1.91	0.52
1:B:535:SER:HB3	1:B:538:ASP:O	2.10	0.52
1:B:609:ILE:HD13	1:B:625:PHE:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:129:TYR:O	2:D:133:ARG:HG2	2.10	0.52
1:A:348:HIS:ND1	1:A:358:MET:HG2	2.25	0.52
1:B:463:ALA:HA	1:B:466:THR:OG1	2.09	0.52
1:A:476:LEU:HD22	1:A:550:LEU:HD23	1.91	0.52
1:B:207:PHE:HB3	1:B:211:LEU:HD12	1.91	0.52
2:D:60:GLU:CD	2:D:60:GLU:H	2.16	0.52
1:B:167:PRO:HA	1:B:173:TRP:NE1	2.25	0.51
1:B:271:VAL:O	1:B:293:THR:HG23	2.10	0.51
1:B:368:SER:HB2	1:B:407:PRO:HG3	1.92	0.51
1:A:465:THR:HG21	1:A:502:HIS:ND1	2.26	0.51
1:A:604:ARG:HG2	1:A:672:TYR:CD2	2.46	0.51
2:D:75:TYR:HB2	2:D:143:PHE:HD1	1.76	0.51
1:B:698:SER:C	1:B:700:ALA:H	2.19	0.51
1:A:392:ILE:HG21	1:A:424:ARG:HH21	1.75	0.51
1:B:293:THR:HG22	1:B:294:LEU:N	2.24	0.51
1:B:249:THR:O	1:B:250:TYR:HB2	2.10	0.51
2:C:22:PHE:CD1	2:C:39:ILE:HG22	2.45	0.51
1:B:751:PHE:C	1:B:753:CYS:H	2.18	0.51
1:A:730:ILE:O	1:A:764:HIS:HE1	1.94	0.50
2:C:75:TYR:HB2	2:C:143:PHE:CD1	2.46	0.50
2:D:128:GLU:HG2	2:D:136:PHE:HB2	1.92	0.50
1:A:294:LEU:HD23	1:A:295:ILE:N	2.27	0.50
1:B:288:THR:HG22	1:B:289:THR:N	2.25	0.50
1:B:332:GLN:CD	1:B:332:GLN:H	2.19	0.50
1:B:462:ALA:O	1:B:466:THR:HG23	2.11	0.50
1:A:215:PHE:CE2	1:A:221:ASP:HB2	2.47	0.50
1:A:288:THR:HG22	1:A:289:THR:N	2.27	0.50
1:B:203:ARG:O	1:B:204:ASN:HB2	2.10	0.50
1:B:360:ILE:HB	1:B:375:MET:HE2	1.93	0.50
1:B:277:ILE:HB	1:B:706:HIS:CE1	2.46	0.50
1:B:516:ASN:ND2	1:B:518:ASP:H	2.09	0.50
1:B:639:ILE:HG21	1:B:707:ASP:HB3	1.93	0.50
1:B:690:SER:OG	1:B:761:MET:HE1	2.11	0.50
1:A:174:ALA:HB1	1:A:210:ILE:HD11	1.93	0.50
1:B:548:ASP:O	1:B:552:THR:HG23	2.11	0.50
1:A:261:THR:HG22	1:A:262:LYS:N	2.26	0.50
1:B:207:PHE:C	1:B:209:LYS:H	2.20	0.50
2:C:151:ARG:HG3	2:C:152:PRO:HD2	1.94	0.50
1:B:178:THR:HG22	1:B:211:LEU:HD23	1.94	0.50
1:B:375:MET:HG3	1:B:408:TYR:CE2	2.46	0.50
2:D:38:LEU:CD2	2:D:50:ALA:HB1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:THR:O	1:A:190:LEU:HD23	2.12	0.50
2:C:127:GLU:C	2:C:129:TYR:H	2.20	0.50
2:D:38:LEU:HD21	2:D:50:ALA:HB1	1.94	0.50
1:B:433:TYR:CG	1:B:438:LEU:HD13	2.47	0.49
1:A:174:ALA:O	1:A:178:THR:HG23	2.12	0.49
1:A:249:THR:HG22	1:A:250:TYR:CD1	2.47	0.49
1:A:328:ASP:O	1:A:328:ASP:CG	2.54	0.49
1:A:570:ALA:C	1:A:572:GLU:H	2.21	0.49
1:A:732:PRO:CG	1:A:736:GLN:HG2	2.40	0.49
1:B:713:ARG:HH12	1:B:746:GLY:CA	2.26	0.49
1:B:540:ASP:HB2	1:B:569:ARG:NH1	2.27	0.49
2:C:41:PRO:O	2:C:151:ARG:NH2	2.42	0.49
2:C:138:LYS:O	2:C:142:GLU:HG3	2.12	0.49
1:A:357:LEU:HD23	1:A:375:MET:HE1	1.95	0.49
1:A:348:HIS:CD2	1:A:398:SER:HB3	2.48	0.49
1:B:553:MET:HE1	1:B:565:PHE:HD1	1.77	0.49
1:B:554:LEU:O	1:B:556:PRO:HD3	2.13	0.49
1:A:476:LEU:HA	1:A:531:PHE:HZ	1.78	0.49
2:D:122:ARG:HH11	2:D:125:LEU:HG	1.78	0.49
1:A:249:THR:O	1:A:250:TYR:HB2	2.13	0.49
1:A:720:MET:HE3	1:A:737:PHE:CD1	2.48	0.49
1:B:234:THR:O	1:B:235:TYR:HB2	2.11	0.49
1:A:766:ARG:O	1:A:770:PRO:HB3	2.12	0.48
2:D:22:PHE:CE2	2:D:105:ILE:HD13	2.48	0.48
1:A:288:THR:CG2	1:A:289:THR:N	2.76	0.48
1:A:652:ASP:N	1:A:653:PRO:CD	2.76	0.48
1:A:582:VAL:HG22	1:A:596:PHE:HE2	1.77	0.48
1:A:190:LEU:HB2	1:A:195:ARG:HG3	1.94	0.48
1:B:387:LEU:H	1:B:387:LEU:CD1	2.21	0.48
2:C:31:ASN:C	2:C:33:LEU:H	2.22	0.48
2:D:7:LEU:CD1	2:D:33:LEU:HD23	2.42	0.48
1:A:266:SER:O	1:A:288:THR:HG23	2.13	0.48
1:B:664:HIS:HE1	1:B:715:TYR:OH	1.96	0.48
1:A:244:ASP:OD2	1:A:245:GLU:N	2.47	0.48
1:A:178:THR:O	1:A:182:LEU:HG	2.13	0.48
1:B:178:THR:HG22	1:B:211:LEU:CD2	2.44	0.48
1:B:751:PHE:C	1:B:753:CYS:N	2.69	0.48
2:C:60:GLU:CD	2:C:60:GLU:H	2.21	0.48
1:A:173:TRP:CZ2	1:A:200:ALA:HA	2.49	0.47
1:A:333:MET:HA	1:A:333:MET:HE2	1.96	0.47
1:A:233:PHE:O	1:A:234:THR:C	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ASN:O	1:A:270:GLU:C	2.57	0.47
1:B:699:SER:HA	1:B:703:GLY:O	2.15	0.47
1:B:750:ALA:O	1:B:753:CYS:HB3	2.13	0.47
1:B:665:TYR:HE1	1:B:686:LEU:HD11	1.79	0.47
1:A:647:LEU:O	1:A:650:ILE:HG13	2.14	0.47
1:A:772:VAL:O	1:A:776:ILE:HD13	2.15	0.47
2:D:117:PRO:HG3	2:D:129:TYR:CD1	2.50	0.47
1:B:174:ALA:O	1:B:178:THR:HG23	2.14	0.47
1:B:418:LEU:HD22	1:B:421:VAL:HB	1.96	0.47
2:C:27:VAL:CG1	2:C:32:LEU:HA	2.44	0.47
1:A:174:ALA:C	1:A:176:LYS:H	2.23	0.47
1:A:577:ALA:O	1:A:578:GLN:CB	2.62	0.47
1:A:720:MET:O	1:A:723:ALA:HB3	2.15	0.47
1:B:640:ASP:OD2	1:B:642:ALA:HB3	2.15	0.47
1:B:773:LEU:HD11	1:B:777:LEU:HD12	1.97	0.47
2:D:70:PHE:CE2	2:D:85:VAL:HG21	2.49	0.47
1:A:253:LEU:HD12	1:A:253:LEU:N	2.30	0.47
1:A:489:ARG:HH11	1:A:489:ARG:HG2	1.80	0.47
1:B:190:LEU:HD12	1:B:190:LEU:H	1.80	0.47
1:B:630:ASN:OD1	1:B:630:ASN:N	2.48	0.47
1:A:171:ALA:O	1:A:174:ALA:HB3	2.14	0.47
2:D:23:ARG:NH1	2:D:154:ASP:OD1	2.41	0.47
1:B:464:MET:HE2	1:B:495:LEU:HD13	1.97	0.46
1:A:201:ASP:OD2	1:A:201:ASP:C	2.58	0.46
1:B:348:HIS:HB3	1:B:355:SER:CB	2.45	0.46
1:A:273:LEU:HD12	1:A:293:THR:HG21	1.97	0.46
2:C:74:ILE:HG21	2:C:79:ILE:HD12	1.98	0.46
1:A:227:ASN:HA	1:A:247:ARG:HB3	1.96	0.46
1:A:327:GLY:HA2	1:A:370:GLU:CG	2.44	0.46
1:B:212:PRO:C	1:B:214:SER:H	2.23	0.46
2:C:60:GLU:OE2	2:C:64:LYS:HD3	2.15	0.46
1:A:323:PHE:HD2	1:A:332:GLN:HA	1.81	0.46
1:B:746:GLY:HA3	1:B:747:LEU:HA	1.50	0.46
1:A:256:VAL:CG1	1:A:257:VAL:N	2.78	0.46
1:A:393:ARG:N	1:A:394:PRO:HD2	2.31	0.46
2:C:87:LEU:CD1	2:C:89:VAL:HG12	2.46	0.46
1:A:510:HIS:O	1:A:512:GLY:N	2.49	0.46
1:B:647:LEU:HB3	1:B:711:ALA:CB	2.46	0.46
2:C:19:MET:HE1	2:C:102:ASP:HA	1.97	0.46
1:A:231:SER:HB2	1:A:233:PHE:CE1	2.51	0.45
1:A:651:PHE:CZ	1:A:712:LEU:HD23	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:ARG:NH1	1:A:744:PHE:O	2.49	0.45
2:D:38:LEU:HD21	2:D:50:ALA:CB	2.46	0.45
1:A:234:THR:O	1:A:235:TYR:CB	2.64	0.45
1:A:248:PHE:O	1:A:249:THR:C	2.59	0.45
1:A:563:ASP:HA	1:A:565:PHE:CE1	2.52	0.45
1:A:212:PRO:HG2	1:A:215:PHE:CD1	2.51	0.45
1:A:696:TYR:HD2	1:A:701:ILE:HG21	1.81	0.45
1:B:393:ARG:CZ	1:B:763:ARG:HD2	2.47	0.45
2:D:40:VAL:HG21	2:D:152:PRO:HG3	1.97	0.45
1:B:293:THR:CG2	1:B:294:LEU:N	2.80	0.45
1:A:495:LEU:HD23	1:A:495:LEU:HA	1.77	0.45
1:A:604:ARG:HD2	1:A:672:TYR:HA	1.99	0.45
1:B:310:ASP:C	1:B:312:SER:H	2.25	0.45
1:B:646:ARG:O	1:B:649:THR:HB	2.17	0.45
1:B:268:MET:HG3	1:B:288:THR:HG21	1.99	0.45
1:B:368:SER:O	1:B:372:VAL:HG23	2.17	0.45
2:D:145:LYS:HE2	2:D:145:LYS:HB3	1.84	0.45
1:A:506:SER:N	1:A:507:PRO:CD	2.80	0.44
1:B:201:ASP:C	1:B:201:ASP:OD2	2.60	0.44
1:B:333:MET:HE1	1:B:378:LEU:HD13	1.98	0.44
2:D:24:ASN:OD1	2:D:24:ASN:O	2.35	0.44
2:D:68:ILE:HD13	2:D:108:LEU:HD12	1.99	0.44
1:B:269:ASN:CG	1:B:291:LYS:HB3	2.43	0.44
1:B:306:LEU:HD22	1:B:367:TYR:CD2	2.52	0.44
1:B:348:HIS:NE2	1:B:358:MET:HE2	2.32	0.44
1:B:506:SER:N	1:B:507:PRO:CD	2.81	0.44
2:D:50:ALA:C	2:D:51:PHE:CD1	2.96	0.44
1:A:236:SER:O	1:A:256:VAL:HG13	2.18	0.44
1:A:543:MET:HE2	1:A:565:PHE:CE2	2.53	0.44
1:B:203:ARG:HA	1:B:234:THR:O	2.17	0.44
1:B:454:LEU:O	1:B:458:ASP:HB2	2.16	0.44
1:A:367:TYR:O	1:A:371:LYS:HG3	2.18	0.44
1:A:393:ARG:NH1	1:A:763:ARG:HD3	2.32	0.44
1:A:460:ASN:O	1:A:461:SER:C	2.61	0.44
1:B:202:PHE:O	1:B:205:ILE:HG12	2.18	0.44
1:B:365:ASP:C	1:B:367:TYR:H	2.25	0.44
2:D:44:PRO:HG3	2:D:47:ASP:OD2	2.18	0.44
2:D:153:VAL:O	2:D:154:ASP:HB2	2.18	0.44
1:B:710:PRO:HA	1:B:713:ARG:HE	1.82	0.44
1:A:450:LEU:HB2	1:A:451:PRO:HD3	2.00	0.44
1:A:695:ARG:HG3	1:A:695:ARG:NH1	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:652:ASP:N	1:B:653:PRO:CD	2.80	0.44
1:A:273:LEU:O	1:A:275:TYR:N	2.47	0.43
1:A:366:LYS:C	1:A:368:SER:H	2.27	0.43
1:B:577:ALA:O	1:B:578:GLN:CB	2.66	0.43
1:A:189:THR:C	1:A:190:LEU:HD23	2.43	0.43
1:A:296:ARG:HG3	1:A:296:ARG:HH11	1.83	0.43
1:A:317:VAL:HG22	1:A:320:GLY:HA3	1.99	0.43
1:A:562:TRP:CZ2	1:A:596:PHE:HA	2.53	0.43
1:A:425:PHE:O	1:A:429:GLN:HG2	2.18	0.43
1:A:476:LEU:HD22	1:A:550:LEU:CD2	2.48	0.43
1:B:338:THR:O	1:B:342:VAL:HB	2.18	0.43
1:A:387:LEU:CD2	1:A:387:LEU:H	2.31	0.43
1:B:392:ILE:C	1:B:394:PRO:HD2	2.43	0.43
1:B:445:TYR:CE1	1:B:449:ILE:HG21	2.54	0.43
1:B:301:LEU:O	1:B:304:VAL:HG13	2.18	0.43
1:B:693:PHE:HA	1:B:696:TYR:HB2	2.00	0.43
2:C:153:VAL:HG12	2:C:153:VAL:O	2.18	0.43
1:A:291:LYS:O	1:A:292:ASN:HB2	2.19	0.43
1:A:453:LEU:HD23	1:A:453:LEU:HA	1.91	0.43
1:A:178:THR:CG2	1:A:210:ILE:HD12	2.49	0.43
1:A:251:SER:N	1:A:271:VAL:HG12	2.32	0.43
1:A:444:TYR:C	1:A:444:TYR:CD2	2.96	0.43
1:B:246:CYS:O	1:B:266:SER:HB3	2.18	0.43
2:D:116:GLN:HA	2:D:117:PRO:HD2	1.86	0.43
1:A:411:SER:O	1:A:415:SER:OG	2.33	0.43
1:A:480:THR:HB	1:A:526:ARG:NH2	2.34	0.43
1:B:266:SER:C	1:B:288:THR:HG23	2.44	0.43
1:B:383:ARG:HD3	1:B:417:TRP:HD1	1.84	0.43
1:B:664:HIS:HA	1:B:667:HIS:ND1	2.34	0.43
1:A:275:TYR:CZ	1:A:296:ARG:HD3	2.53	0.42
1:B:178:THR:HG21	1:B:210:ILE:O	2.18	0.42
1:A:326:LEU:HD22	1:A:360:ILE:HG12	2.01	0.42
1:B:218:ARG:O	1:B:219:ASP:C	2.61	0.42
1:B:254:SER:O	1:B:255:ASP:HB2	2.19	0.42
1:A:229:SER:O	1:A:230:ASN:HB2	2.20	0.42
1:A:239:SER:O	1:A:241:LEU:HG	2.18	0.42
1:A:598:GLN:O	1:A:602:GLN:HG3	2.18	0.42
2:C:47:ASP:O	2:C:48:LYS:CB	2.68	0.42
2:C:60:GLU:CD	2:C:64:LYS:HD3	2.44	0.42
1:A:319:GLY:H	1:A:320:GLY:HA3	1.78	0.42
2:C:23:ARG:HH12	2:C:154:ASP:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:49:GLY:HA3	2:C:144:THR:CG2	2.49	0.42
1:A:514:PHE:HB2	1:A:544:MET:SD	2.60	0.42
1:B:280:GLN:O	1:B:354:LYS:HE2	2.19	0.42
2:C:58:PRO:HB2	2:C:60:GLU:OE2	2.20	0.42
1:A:212:PRO:HG2	1:A:215:PHE:HD1	1.85	0.42
1:A:274:GLN:HG3	1:A:294:LEU:CD2	2.36	0.42
1:B:326:LEU:HD22	1:B:360:ILE:HG12	2.01	0.42
1:B:450:LEU:HD23	1:B:450:LEU:HA	1.77	0.42
2:D:21:ASN:CB	2:D:109:ILE:HD13	2.49	0.42
1:A:454:LEU:HD22	1:A:495:LEU:HD12	2.01	0.42
1:A:625:PHE:CD2	1:A:696:TYR:CZ	3.07	0.42
1:B:343:ASP:C	1:B:345:PHE:H	2.27	0.42
1:B:516:ASN:ND2	1:B:518:ASP:N	2.68	0.42
1:A:572:GLU:OE1	1:A:572:GLU:HA	2.20	0.42
2:D:132:ASP:OD2	2:D:135:LYS:CB	2.68	0.42
1:A:720:MET:HE3	1:A:737:PHE:CE1	2.55	0.41
1:A:777:LEU:HA	1:A:778:PRO:HD3	1.89	0.41
1:B:262:LYS:HG3	1:B:284:SER:OG	2.20	0.41
1:B:612:ILE:HB	1:B:613:LEU:HD12	2.02	0.41
1:B:323:PHE:HA	1:B:331:LEU:O	2.21	0.41
1:B:516:ASN:ND2	1:B:518:ASP:HB2	2.35	0.41
1:B:777:LEU:CD2	1:B:778:PRO:HD2	2.50	0.41
2:D:70:PHE:HE2	2:D:85:VAL:HG21	1.85	0.41
2:D:73:LYS:HB2	2:D:147:TYR:HB3	2.02	0.41
1:A:169:SER:CB	1:A:170:PRO:HD2	2.48	0.41
1:A:598:GLN:HA	1:A:601:THR:HB	2.03	0.41
1:B:233:PHE:O	1:B:256:VAL:HG22	2.20	0.41
1:B:306:LEU:HD21	1:B:363:LEU:HD13	2.02	0.41
1:B:371:LYS:O	1:B:374:ALA:HB3	2.20	0.41
2:C:36:GLN:HE21	2:C:36:GLN:HB2	1.61	0.41
2:D:153:VAL:O	2:D:154:ASP:CB	2.67	0.41
1:A:337:TRP:HZ2	1:A:381:SER:HG	1.68	0.41
1:B:180:ALA:HB1	1:B:190:LEU:HD23	2.02	0.41
1:B:212:PRO:HG2	1:B:215:PHE:CD1	2.56	0.41
1:B:580:SER:HA	1:B:581:PRO:HD3	1.96	0.41
1:B:696:TYR:HB3	1:B:712:LEU:HD13	2.02	0.41
2:C:105:ILE:O	2:C:109:ILE:HG13	2.20	0.41
1:B:212:PRO:HA	1:B:213:PRO:HD3	1.88	0.41
1:B:456:SER:C	1:B:458:ASP:H	2.27	0.41
1:B:460:ASN:O	1:B:461:SER:C	2.64	0.41
1:B:551:LEU:HD23	1:B:551:LEU:HA	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:76:HIS:CD2	2:C:77:PRO:CD	3.02	0.41
2:D:89:VAL:HG13	2:D:90:ILE:HG23	2.03	0.41
1:A:234:THR:C	1:A:235:TYR:CD2	2.99	0.41
1:A:264:SER:C	1:A:266:SER:N	2.77	0.41
2:C:53:ILE:HD11	2:C:70:PHE:CD1	2.55	0.41
1:A:526:ARG:O	1:A:547:THR:HB	2.21	0.41
1:B:297:HIS:HB2	1:B:356:ILE:HB	2.02	0.41
1:A:325:ARG:HH21	1:A:330:TRP:NE1	2.12	0.41
1:A:348:HIS:HB3	1:A:355:SER:OG	2.21	0.41
1:A:492:ALA:O	1:A:493:ALA:C	2.64	0.41
1:A:624:GLN:NE2	1:A:636:VAL:HG11	2.36	0.41
1:B:364:PRO:HG2	1:B:367:TYR:HD1	1.79	0.41
2:D:52:ARG:O	2:D:53:ILE:HG13	2.21	0.41
2:D:123:ALA:O	2:D:124:ASP:C	2.62	0.41
1:A:265:ASN:HA	1:A:287:ASP:O	2.22	0.41
1:A:387:LEU:CD2	1:A:387:LEU:N	2.83	0.41
1:A:730:ILE:HG23	1:A:769:PHE:CE1	2.56	0.41
1:B:516:ASN:HD22	1:B:518:ASP:N	2.19	0.41
1:A:259:SER:N	1:A:279:THR:HG23	2.36	0.40
1:B:500:LEU:HD22	1:B:509:ILE:HD11	2.04	0.40
2:D:76:HIS:HA	2:D:77:PRO:HD2	1.81	0.40
1:B:366:LYS:HE3	1:B:367:TYR:CE1	2.56	0.40
2:C:87:LEU:HA	2:C:88:PRO:HD3	1.77	0.40
1:A:556:PRO:HG3	1:A:562:TRP:HH2	1.87	0.40
1:A:608:LEU:HD12	1:A:668:ILE:HG12	2.03	0.40
1:A:709:PRO:HA	1:A:710:PRO:HD3	1.76	0.40
2:D:117:PRO:HG3	2:D:129:TYR:HD1	1.86	0.40
1:A:173:TRP:CH2	1:A:200:ALA:HA	2.56	0.40
1:A:570:ALA:O	1:A:572:GLU:N	2.53	0.40
2:D:66:PRO:O	2:D:90:ILE:HD12	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	605/621 (97%)	519 (86%)	74 (12%)	12 (2%)	6	27
1	B	612/621 (99%)	537 (88%)	71 (12%)	4 (1%)	18	48
2	C	152/156 (97%)	135 (89%)	16 (10%)	1 (1%)	18	48
2	D	152/156 (97%)	135 (89%)	16 (10%)	1 (1%)	18	48
All	All	1521/1554 (98%)	1326 (87%)	177 (12%)	18 (1%)	10	37

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	GLN
1	A	511	ASN
1	A	291	LYS
1	B	511	ASN
1	B	733	SER
2	D	80	ASP
1	A	191	THR
1	A	206	THR
1	A	312	SER
1	A	442	ASP
1	B	200	ALA
1	B	537	GLN
1	A	337	TRP
1	A	510	HIS
1	A	578	GLN
2	C	29	GLU
1	A	571	GLY
1	A	701	ILE

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	484/541 (90%)	442 (91%)	42 (9%)	9	32
1	B	487/541 (90%)	436 (90%)	51 (10%)	6	25
2	C	115/139 (83%)	109 (95%)	6 (5%)	21	49
2	D	115/139 (83%)	98 (85%)	17 (15%)	3	14
All	All	1201/1360 (88%)	1085 (90%)	116 (10%)	8	28

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	ASP
1	A	270	GLU
1	A	295	ILE
1	A	312	SER
1	A	326	LEU
1	A	328	ASP
1	A	335	LEU
1	A	348	HIS
1	A	387	LEU
1	A	395	VAL
1	A	398	SER
1	A	443	THR
1	A	444	TYR
1	A	465	THR
1	A	482	VAL
1	A	485	THR
1	A	486	ASP
1	A	495	LEU
1	A	520	SER
1	A	533	LEU
1	A	536	SER
1	A	552	THR
1	A	557	THR
1	A	567	LEU
1	A	593	LEU
1	A	599	GLN
1	A	601	THR
1	A	604	ARG
1	A	608	LEU
1	A	609	ILE

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Mol	Chain	Res	Type
1	A	630	ASN
1	A	633	HIS
1	A	640	ASP
1	A	650	ILE
1	A	675	THR
1	A	676	ASP
1	A	678	THR
1	A	695	ARG
1	A	696	TYR
1	A	725	GLU
1	A	744	PHE
1	A	760	SER
1	B	172	ASP
1	B	183	ARG
1	B	189	THR
1	B	190	LEU
1	B	216	MET
1	B	236	SER
1	B	252	THR
1	B	262	LYS
1	B	270	GLU
1	B	271	VAL
1	B	273	LEU
1	B	294	LEU
1	B	295	ILE
1	B	306	LEU
1	B	332	GLN
1	B	336	LEU
1	B	338	THR
1	B	342	VAL
1	B	379	VAL
1	B	387	LEU
1	B	388	THR
1	B	392	ILE
1	B	418	LEU
1	B	443	THR
1	B	465	THR
1	B	482	VAL
1	B	484	CYS
1	B	485	THR
1	B	486	ASP
1	B	516	ASN

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Mol	Chain	Res	Type
1	B	518	ASP
1	B	532	LEU
1	B	541	THR
1	B	550	LEU
1	B	557	THR
1	B	567	LEU
1	B	576	THR
1	B	591	VAL
1	B	593	LEU
1	B	604	ARG
1	B	608	LEU
1	B	630	ASN
1	B	633	HIS
1	B	670	SER
1	B	675	THR
1	B	707	ASP
1	B	721	GLN
1	B	741	SER
1	B	766	ARG
1	B	771	SER
1	B	775	SER
2	C	7	LEU
2	C	25	ILE
2	C	100	LYS
2	C	102	ASP
2	C	104	VAL
2	C	105	ILE
2	D	1	MET
2	D	14	ILE
2	D	25	ILE
2	D	36	GLN
2	D	38	LEU
2	D	39	ILE
2	D	47	ASP
2	D	53	ILE
2	D	60	GLU
2	D	80	ASP
2	D	85	VAL
2	D	89	VAL
2	D	102	ASP
2	D	104	VAL
2	D	132	ASP

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Mol	Chain	Res	Type
2	D	150	LYS
2	D	151	ARG

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

Mol	Chain	Res	Type
1	A	292	ASN
1	A	510	HIS
1	A	573	ASN
1	A	631	GLN
1	A	736	GLN
1	A	764	HIS
1	B	227	ASN
1	B	230	ASN
1	B	260	ASN
1	B	447	GLN
1	B	516	ASN
1	B	624	GLN
1	B	664	HIS
1	B	706	HIS
1	B	764	HIS
2	C	43	ASN
2	C	76	HIS
2	C	78	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
3	SO4	A	1	-	4,4,4	0.23	0	6,6,6	0.06	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	609/621 (98%)	-0.18	5 (0%) 82 68	40, 87, 146, 314	0
1	B	616/621 (99%)	-0.31	6 (0%) 79 63	45, 79, 124, 187	0
2	C	154/156 (98%)	-0.36	0 100 100	46, 77, 116, 158	0
2	D	154/156 (98%)	-0.33	1 (0%) 85 72	46, 74, 115, 150	0
All	All	1533/1554 (98%)	-0.27	12 (0%) 82 68	40, 81, 136, 314	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	510	HIS	3.7
1	A	252	THR	3.4
1	B	752	THR	3.3
1	A	511	ASN	2.7
1	B	747	LEU	2.4
1	A	237	ASP	2.4
2	D	94	ASN	2.3
1	A	284	SER	2.3
1	A	510	HIS	2.3
1	B	705	GLU	2.2
1	B	511	ASN	2.1
1	B	332	GLN	2.1

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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	1	5/5	0.94	0.07	138,138,138,138	0

6.5 Other polymers

There are no such residues in this entry.