Full wwPDB X-ray Structure Validation Report (i)

Sep 3, 2023 – 02:41 PM EDT

PDB ID	:	3SY2
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 (i) 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 (i)) were used in the production of this report:

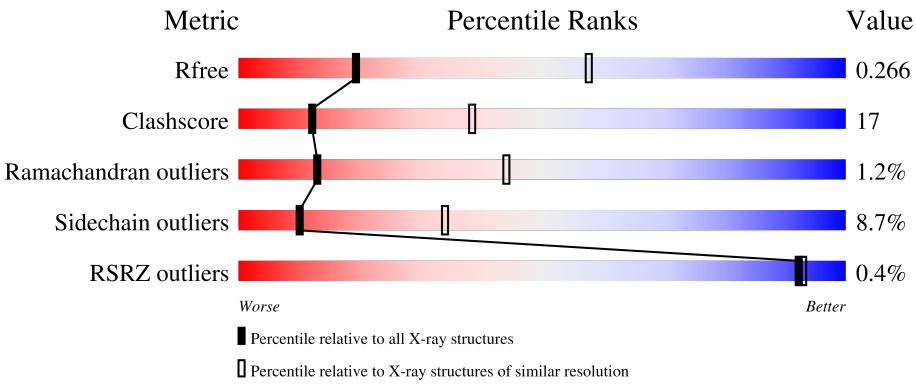
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

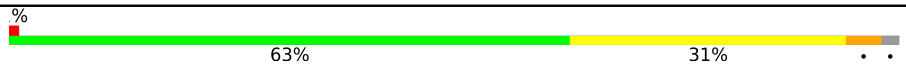
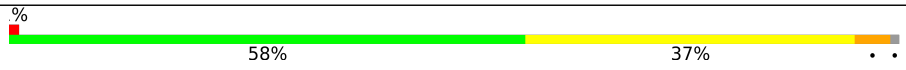
The reported resolution of this entry is 3.27 Å.

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}	130704	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

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 <=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	
1	B	621	
2	C	156	
2	D	156	

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	609	4631	2935	794	882	20	0	0	0
1	B	616	4667	2965	796	886	20	0	0	0

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

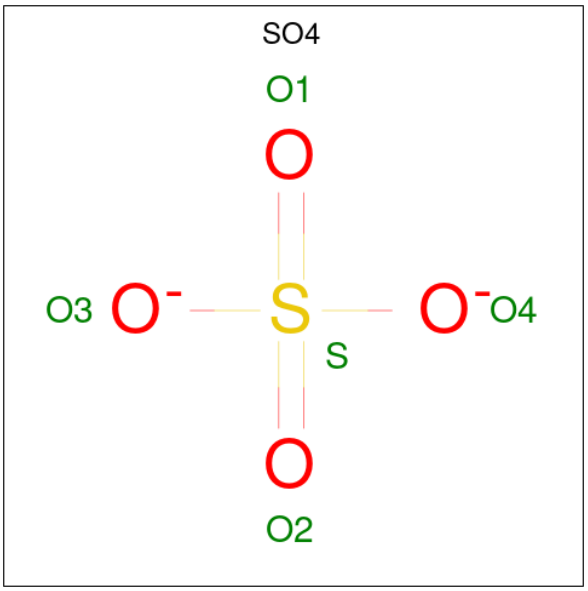
- Molecule 2 is a protein called Ubiquitin-conjugating enzyme E2 L3.

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

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 (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

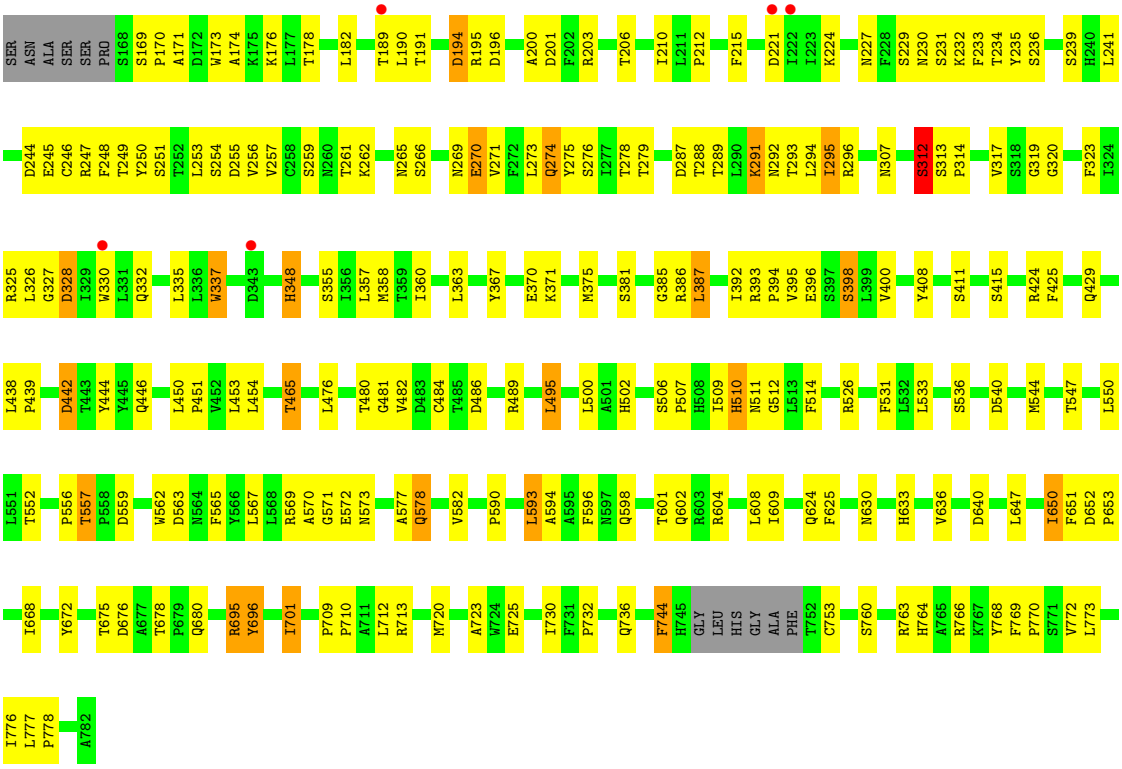
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	8	8	8	0	0
			Total	O		
4	B	6	6	6	0	0
			Total	O		
4	D	1	1	1	0	0

3 Residue-property plots (i)

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

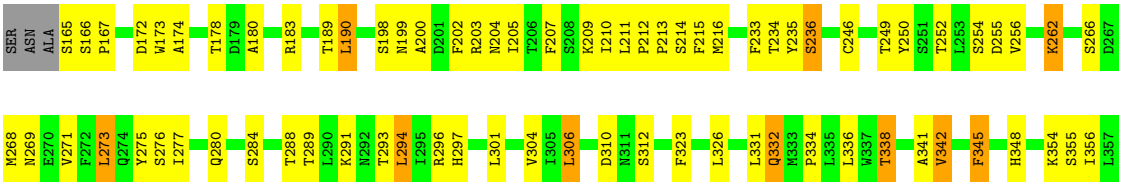
• Molecule 1: E3 ubiquitin-protein ligase SopA

Chain A:



• Molecule 1: E3 ubiquitin-protein ligase SopA

Chain B:



M358 T359 I360 L363 P364 D365 K366 Y367 S368 Q369 E370 K371 V372 Q373 A374 M375 V379 R383 L387 T388 I392 R393 P394 P407 Y408 T409 Q410 W417 L418 V421 Y433 L438 P439 D442 Y445 Q446 I449 L450 L454 D458 A462 A463 M464 T465

T466 L476 C484 T485 D486 R489 L500 V505 S506 P507 H508 I509 H510 N511 N516 Y517 D518 L532 S535 S536 Q537 D538 S539 D540 T541 A542 M543 D548 T549 L550 L551 T552 M553 L554 N555 P556 T557 L567 L568 R569 T576 A577 Q578 I579 S580 P581 F589

L593 F596 N597 Q598 T601 R604 L608 I609 I612 L613 F625 N630 S634 I639 D640 D641 A642 R646 L647 A648 T649 D652 P653 H664 Y665 Q666 H667 S670 T675 L686 F693 A694 R695 Y696 S697 S698 S699 A700 I701 F702 G703 H706 D707

P710 A711 L712 R713 G714 Y715 Q721 S727 I730 F731 P732 S733 Q736 S741 D742 R743 F744 H745 G746 L747 HIS GLY A750 F751 T752 C753 R763 H764 S771 V772 L773 S774 S775 I776 L777 P778 A782

- Molecule 2: Ubiquitin-conjugating enzyme E2 L3

Chain C:

GLY SER M1 A2 A3 L7 M8 K9 E13 F22 R23 N24 I25 Q26 V27 D28 E29 A30 N31 L32 L33 Q36 I39 V40 P41 D47 K48 G49 R52 I53 P58 A59 E60 Y61 P62 F63 K64 P65 P66 F70 K71 I74 Y75 H76 P77 N78 I79 D80 Q84

V85 C86 L87 P88 V89 E93 K100 T101 D102 Q103 V104 I105 I109 A110 L111 Q116 R122 E127 E128 Y129 K138 E142 F143 T144 R151 P152 V153 D154

- Molecule 2: Ubiquitin-conjugating enzyme E2 L3

Chain D:

GLY SER M1 A2 A3 L7 N21 F22 R23 N24 V27 N31 L32 L33 Q36 G37 L38 I39 V40 P44 D47 A50 F51 R52 I53 E60 Y61 P62 F63 K64 P65 P66 K67 I68 T69 F70 K73 I74 Y75 H76 P77 N78 I79 D80 V85 V89 I90

K96 T99 K100 T101 D102 Q103 V104 I105 L108 I109 Q116 P117 P120 L121 R122 L125 E128 Y129 D132 R133 K134 K135 F136 F143 T144 K145 K146 Y147 K150 R151 P152 V153 D154

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.13 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.211 , 0.275 0.204 , 0.266	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)	0.30 , 61.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.28	0/4752	0.46	0/6493
1	B	0.29	0/4790	0.46	0/6548
2	C	0.29	0/1206	0.49	0/1646
2	D	0.30	0/1197	0.54	0/1635
All	All	0.29	0/11945	0.47	0/16322

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4631	0	4322	160	0
1	B	4667	0	4363	134	0
2	C	1175	0	1107	44	0
2	D	1167	0	1110	50	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	385	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 17.

All (385) 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
1:A:593:LEU:HD23	1:A:594:ALA:H	1.44	0.78
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:165:SER:C	1:B:167:PRO:HD3	2.18	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:554:LEU:C	1:B:556:PRO:HD3	2.24	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
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:D:31:ASN:O	2:D:32:LEU:HB3	2.05	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: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:C:53:ILE:HD11	2:C:70:PHE:CE1	2.41	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
1:B:516:ASN:C	1:B:516:ASN:HD22	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:337:TRP:HZ2	1:A:381:SER:HG	1.56	0.53
1:B:273:LEU:HD23	1:B:273:LEU:O	2.09	0.53
1:A:276:SER:C	1:A:278:THR:H	2.12	0.53
1:A:393:ARG:HA	1:A:396:GLU:HG3	1.91	0.53
1:A:557:THR:CG2	1:A:559:ASP:H	2.21	0.52
1:B:293:THR:HG22	1:B:294:LEU:N	2.24	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
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
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:A:392:ILE:HG21	1:A:424:ARG:HH21	1.75	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:ARG:O	1:B:204:ASN:HB2	2.10	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: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
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
1:A:189:THR:O	1:A:190:LEU:HD23	2.12	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
2:D:31:ASN:C	2:D:33:LEU:H	2.15	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: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:348:HIS:CD2	1:A:398:SER:HB3	2.48	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: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
1:A:288:THR:CG2	1:A:289:THR:N	2.76	0.48
2:D:22:PHE:CE2	2:D:105:ILE:HD13	2.48	0.48
1:A:652:ASP:N	1:A:653:PRO:CD	2.76	0.48
1:A:276:SER:C	1:A:278:THR:N	2.64	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:THR:HG22	1:B:211:LEU:CD2	2.44	0.48
2:D:60:GLU:CD	2:D:60:GLU:H	2.16	0.48
1:A:173:TRP:CZ2	1:A:200:ALA:HA	2.49	0.47
1:A:357:LEU:HA	1:A:375:MET:HE1	1.95	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: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:348:HIS:HB3	1:B:355:SER:CB	2.45	0.46
1:B:698:SER:C	1:B:700:ALA:H	2.19	0.46
1:B:751:PHE:C	1:B:753:CYS:N	2.69	0.46
1:A:273:LEU:HD12	1:A:293:THR:HG21	1.97	0.46
1:B:751:PHE:C	1:B:753:CYS:H	2.18	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
2:C:60:GLU:OE2	2:C:64:LYS:HD3	2.15	0.46
1:A:256:VAL:CG1	1:A:257:VAL:N	2.78	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: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:332:GLN:CD	1:B:332:GLN:H	2.19	0.46
1:B:647:LEU:HB3	1:B:711:ALA:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:127:GLU:C	2:C:129:TYR:H	2.20	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:207:PHE:C	1:B:209:LYS:H	2.20	0.45
1:B:348:HIS:CD2	1:B:358:MET:HE3	2.52	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
1:A:328:ASP:O	1:A:328:ASP:CG	2.54	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
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:306:LEU:HD22	1:B:367:TYR:CD2	2.52	0.44
1:B:506:SER:N	1:B:507:PRO:CD	2.81	0.44
1:A:236:SER:O	1:A:256:VAL:HG13	2.18	0.44
1:B:543:MET:HE3	1:B:589:PHE:CD1	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:B:202:PHE:O	1:B:205:ILE:HG12	2.18	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
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:B:577:ALA:O	1:B:578:GLN:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:31:ASN:C	2:C:33:LEU:H	2.22	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: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:60:GLU:CD	2:C:60:GLU:H	2.21	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:233:PHE:O	1:A:234:THR:C	2.56	0.43
1:A:251:SER:N	1:A:271:VAL:HG12	2.32	0.43
1:A:269:ASN:O	1:A:270:GLU:C	2.57	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: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: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:570:ALA:C	1:A:572:GLU:H	2.21	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
1:A:174:ALA:C	1:A:176:LYS:H	2.23	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
2:C:49:GLY:HA3	2:C:144:THR:CG2	2.49	0.42
1:A:201:ASP:OD2	1:A:201:ASP:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:A:248:PHE:O	1:A:249:THR:C	2.59	0.41
1:B:212:PRO:HA	1:B:213:PRO:HD3	1.88	0.41
1:B:551:LEU:HD23	1:B:551:LEU:HA	1.81	0.41
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:B:212:PRO:C	1:B:214:SER:H	2.23	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:348:HIS:HB3	1:A:355:SER:OG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:B:310:ASP:C	1:B:312:SER:H	2.25	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 (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	605/621 (97%)	519 (86%)	74 (12%)	12 (2%)	7	34
1	B	612/621 (99%)	537 (88%)	71 (12%)	4 (1%)	22	56
2	C	152/156 (97%)	135 (89%)	16 (10%)	1 (1%)	22	56
2	D	152/156 (97%)	135 (89%)	16 (10%)	1 (1%)	22	56
All	All	1521/1554 (98%)	1326 (87%)	177 (12%)	18 (1%)	13	44

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 (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	484/541 (90%)	448 (93%)	36 (7%)	13 40
1	B	487/541 (90%)	439 (90%)	48 (10%)	8 28
2	C	115/139 (83%)	106 (92%)	9 (8%)	12 38
2	D	115/139 (83%)	104 (90%)	11 (10%)	8 29
All	All	1201/1360 (88%)	1097 (91%)	104 (9%)	10 34

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	ASP
1	A	196	ASP

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Mol	Chain	Res	Type
1	A	270	GLU
1	A	295	ILE
1	A	312	SER
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	444	TYR
1	A	465	THR
1	A	482	VAL
1	A	486	ASP
1	A	495	LEU
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	609	ILE
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	753	CYS
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

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Mol	Chain	Res	Type
1	B	273	LEU
1	B	294	LEU
1	B	306	LEU
1	B	332	GLN
1	B	336	LEU
1	B	338	THR
1	B	342	VAL
1	B	345	PHE
1	B	369	GLN
1	B	379	VAL
1	B	387	LEU
1	B	388	THR
1	B	392	ILE
1	B	418	LEU
1	B	442	ASP
1	B	465	THR
1	B	484	CYS
1	B	485	THR
1	B	486	ASP
1	B	516	ASN
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	593	LEU
1	B	596	PHE
1	B	604	ARG
1	B	608	LEU
1	B	630	ASN
1	B	670	SER
1	B	675	THR
1	B	707	ASP
1	B	721	GLN
1	B	741	SER
1	B	744	PHE
1	B	771	SER
1	B	775	SER
2	C	7	LEU
2	C	25	ILE

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Mol	Chain	Res	Type
2	C	31	ASN
2	C	60	GLU
2	C	100	LYS
2	C	102	ASP
2	C	104	VAL
2	C	105	ILE
2	C	122	ARG
2	D	1	MET
2	D	36	GLN
2	D	38	LEU
2	D	47	ASP
2	D	67	LYS
2	D	80	ASP
2	D	102	ASP
2	D	104	VAL
2	D	132	ASP
2	D	150	LYS
2	D	151	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	292	ASN
1	A	573	ASN
1	A	631	GLN
1	A	764	HIS
1	B	516	ASN
1	B	664	HIS
1	B	764	HIS
2	C	76	HIS
2	C	78	ASN
2	C	139	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	0.14	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%)	-0.13	5 (0%)	86	86	40, 87, 146, 314	0
1	B	616/621 (99%)	-0.28	0	100	100	45, 79, 124, 187	0
2	C	154/156 (98%)	-0.24	0	100	100	46, 77, 116, 158	0
2	D	154/156 (98%)	-0.21	1 (0%)	89	90	46, 74, 115, 150	0
All	All	1533/1554 (98%)	-0.21	6 (0%)	92	93	40, 81, 136, 314	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	ILE	4.1
1	A	221	ASP	2.3
1	A	343	ASP	2.2
1	A	189	THR	2.2
1	A	330	TRP	2.1
2	D	147	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	A	1	5/5	0.93	0.37	138,138,138,138	0

6.5 Other polymers (i)

There are no such residues in this entry.