



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 04:05 PM GMT

PDB ID : 2C5D  
Title : STRUCTURE OF A MINIMAL GAS6-AXL COMPLEX  
Authors : Sasaki, T.; Knyazev, P.G.; Clout, N.J.; Cheburkin, Y.; Goehring, W.; Ullrich, A.; Timpl, R.; Hohenester, E.  
Deposited on : 2005-10-26  
Resolution : 3.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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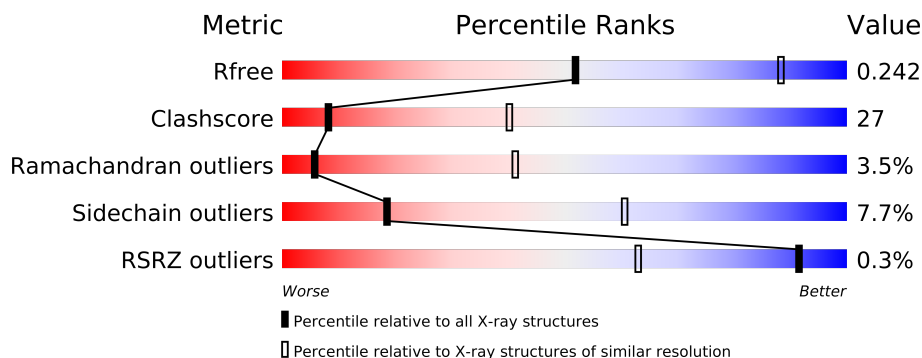
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
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) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.30 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	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)

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  $\geq 3$ , 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	422	
1	B	422	
2	C	195	
2	D	195	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8879 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 GROWTH-ARREST-SPECIFICPROTEIN 6 PRECURSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	1
			2953	1882	518	539	14			
1	B	381	Total	C	N	O	S	0	0	1
			2953	1882	518	539	14			

- Molecule 2 is a protein called TYROSINE-PROTEIN KINASE RECEPTOR UFO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	192	Total	C	N	O	S	0	0	1
			1454	911	251	288	4			
2	D	192	Total	C	N	O	S	0	0	1
			1454	911	251	288	4			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		

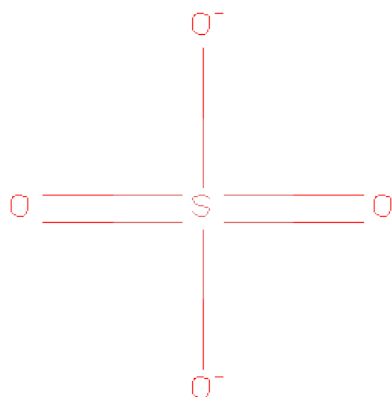
- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Ni	0	0
			1	1		
5	C	1	Total	Ni	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



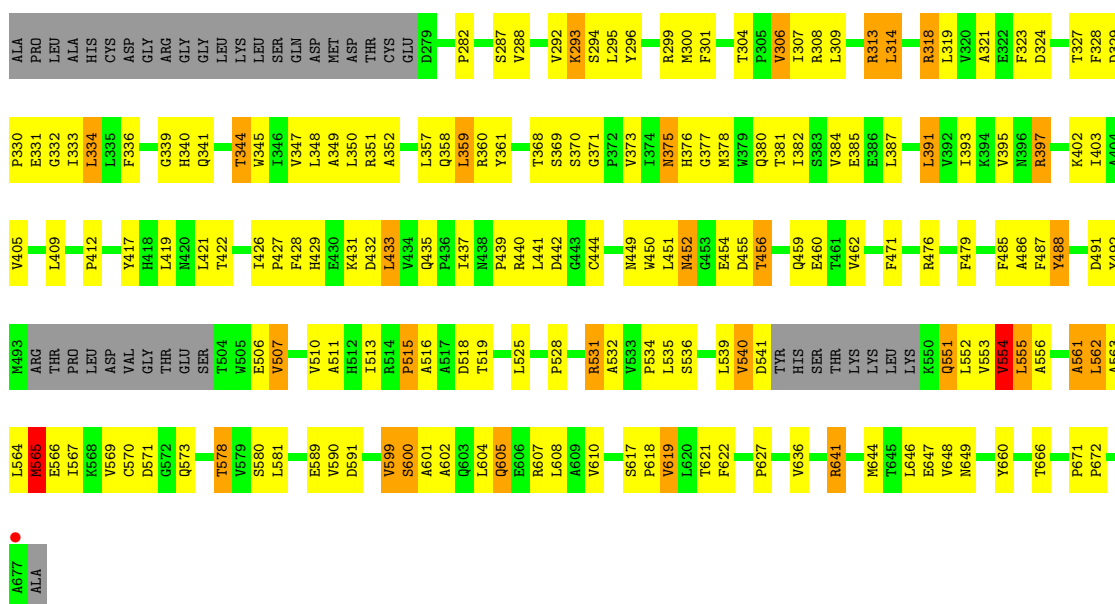
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	S	0	0
			5	4	1		

### 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.

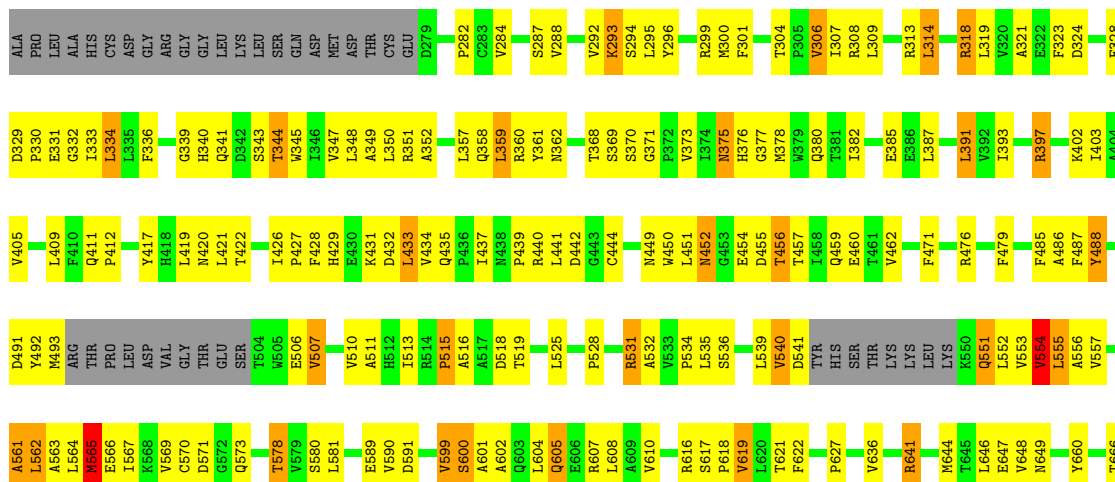
#### • Molecule 1: GROWTH-ARREST-SPECIFICPROTEIN 6 PRECURSOR

Chain A:



#### • Molecule 1: GROWTH-ARREST-SPECIFICPROTEIN 6 PRECURSOR

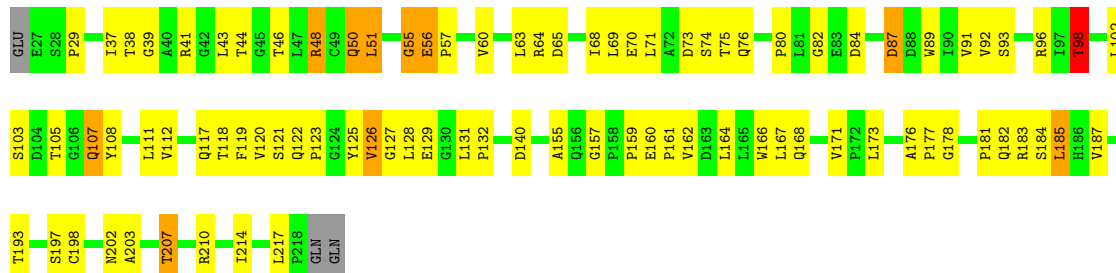
Chain B:





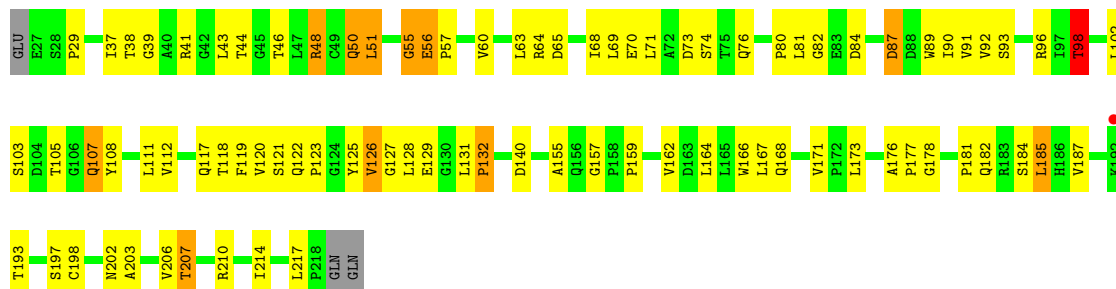
• Molecule 2: TYROSINE-PROTEIN KINASE RECEPTOR UFO

Chain C:



• Molecule 2: TYROSINE-PROTEIN KINASE RECEPTOR UFO

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	292.95Å 292.95Å 63.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.30 19.89 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-3.30) 99.9 (19.89-3.30)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.10 (at 3.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.241 , 0.265 0.218 , 0.242	Depositor DCC
$R_{free}$ test set	2383 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	85.0	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 14.7	EDS
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 47647 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8879	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: NI, CA, NAG, 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	0.45	0/3017	0.70	0/4107
1	B	0.45	0/3017	0.70	0/4107
2	C	0.52	0/1489	0.69	0/2041
2	D	0.52	0/1489	0.69	0/2041
All	All	0.48	0/9012	0.70	0/12296

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	2953	0	2951	151	0
1	B	2953	0	2951	156	0
2	C	1454	0	1401	86	0
2	D	1454	0	1401	85	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	28	0	25	1	0
4	B	28	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	C	5	0	0	0	0
All	All	8879	0	8754	468	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 27.

All (468) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:622:PHE:CE2	1:A:627:PRO:HD3	2.02	0.94
2:D:51:LEU:HD23	2:D:51:LEU:H	1.32	0.94
2:C:51:LEU:H	2:C:51:LEU:HD23	1.33	0.93
1:B:622:PHE:CE2	1:B:627:PRO:HD3	2.04	0.93
1:B:332:GLY:HA3	1:B:441:LEU:HB2	1.54	0.89
1:B:519:THR:HG22	1:B:540:VAL:HA	1.54	0.87
1:A:519:THR:HG22	1:A:540:VAL:HA	1.55	0.86
1:A:332:GLY:HA3	1:A:441:LEU:HB2	1.56	0.86
1:A:555:LEU:HD11	1:A:581:LEU:HD21	1.61	0.82
1:A:397:ARG:HH11	1:A:397:ARG:HG2	1.45	0.82
2:D:44:THR:HG22	2:D:98:THR:O	1.79	0.82
1:A:429:HIS:HD2	1:A:431:LYS:HB2	1.44	0.82
2:C:44:THR:HG22	2:C:98:THR:O	1.80	0.81
1:B:397:ARG:HH11	1:B:397:ARG:HG2	1.46	0.81
1:B:429:HIS:HD2	1:B:431:LYS:HB2	1.44	0.80
1:B:555:LEU:HD11	1:B:581:LEU:HD21	1.61	0.80
1:A:376:HIS:HD2	1:A:378:MET:H	1.29	0.80
1:A:555:LEU:HD23	1:A:556:ALA:H	1.49	0.78
2:D:60:VAL:HG11	2:D:93:SER:HB2	1.66	0.77
1:B:376:HIS:HD2	1:B:378:MET:H	1.29	0.77
1:B:555:LEU:HD23	1:B:556:ALA:H	1.50	0.76
1:B:300:MET:HE3	1:B:304:THR:HB	1.68	0.76
2:C:60:VAL:HG11	2:C:93:SER:HB2	1.68	0.75
1:A:300:MET:HE3	1:A:304:THR:HB	1.69	0.73
2:D:51:LEU:CD2	2:D:51:LEU:H	2.02	0.73
1:B:397:ARG:CG	1:B:397:ARG:HH11	2.01	0.72
1:A:397:ARG:HH11	1:A:397:ARG:CG	2.01	0.72
2:C:51:LEU:H	2:C:51:LEU:CD2	2.03	0.71
2:D:181:PRO:O	2:D:182:GLN:HG2	1.91	0.70
2:C:168:GLN:HB2	2:C:173:LEU:HD11	1.72	0.70
2:C:181:PRO:O	2:C:182:GLN:HG2	1.91	0.70
2:C:50:GLN:HB2	2:C:92:VAL:HG22	1.73	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:168:GLN:HB2	2:D:173:LEU:HD11	1.74	0.70
1:A:319:LEU:HD12	1:A:451:LEU:HD11	1.73	0.70
1:A:607:ARG:HA	1:A:607:ARG:HE	1.58	0.69
1:B:319:LEU:HD12	1:B:451:LEU:HD11	1.74	0.68
1:A:314:LEU:HB2	2:C:73:ASP:OD1	1.92	0.68
2:D:50:GLN:HB2	2:D:92:VAL:HG22	1.75	0.67
1:B:507:VAL:HG11	1:B:535:LEU:CD2	2.25	0.67
1:A:507:VAL:HG11	1:A:535:LEU:CD2	2.24	0.67
2:D:166:TRP:C	2:D:167:LEU:HD12	2.15	0.67
1:A:599:VAL:HG21	1:A:604:LEU:HB2	1.76	0.67
1:A:299:ARG:NH2	2:C:80:PRO:O	2.29	0.66
1:A:344:THR:HB	1:A:361:TYR:HA	1.76	0.66
1:B:607:ARG:HE	1:B:607:ARG:HA	1.60	0.66
1:B:600:SER:C	1:B:602:ALA:H	1.98	0.66
2:C:166:TRP:C	2:C:167:LEU:HD12	2.16	0.65
1:A:531:ARG:HH11	1:A:531:ARG:HG3	1.60	0.65
1:B:599:VAL:HG21	1:B:604:LEU:HB2	1.78	0.65
1:B:344:THR:HB	1:B:361:TYR:HA	1.77	0.65
1:B:454:GLU:O	1:B:456:THR:N	2.30	0.65
1:A:454:GLU:O	1:A:456:THR:N	2.31	0.64
1:A:563:ALA:O	1:A:564:LEU:HD23	1.98	0.64
1:A:511:ALA:O	1:A:513:ILE:HG23	1.98	0.64
1:B:531:ARG:HG3	1:B:531:ARG:HH11	1.62	0.63
2:C:44:THR:HG22	2:C:98:THR:C	2.18	0.63
1:A:300:MET:CE	1:A:304:THR:HB	2.27	0.63
2:C:50:GLN:HG3	2:C:50:GLN:O	1.99	0.63
2:D:44:THR:HG22	2:D:98:THR:C	2.17	0.63
1:A:600:SER:C	1:A:602:ALA:H	1.99	0.63
1:B:563:ALA:O	1:B:564:LEU:HD23	1.98	0.62
1:B:318:ARG:HH11	1:B:318:ARG:CB	2.12	0.62
1:B:357:LEU:HD13	1:B:393:ILE:HD11	1.80	0.62
1:A:318:ARG:HH11	1:A:318:ARG:CB	2.12	0.62
1:B:336:PHE:HB3	1:B:422:THR:OG1	1.99	0.62
1:A:336:PHE:HB3	1:A:422:THR:OG1	2.00	0.62
1:A:553:VAL:CG2	1:A:567:ILE:HD12	2.29	0.62
1:B:553:VAL:CG2	1:B:567:ILE:HD12	2.30	0.62
1:A:357:LEU:HD13	1:A:393:ILE:HD11	1.82	0.61
1:B:300:MET:CE	1:B:304:THR:HB	2.30	0.61
1:B:301:PHE:O	1:B:440:ARG:NH1	2.33	0.61
2:C:181:PRO:C	2:C:182:GLN:HG2	2.21	0.61
2:D:43:LEU:HD23	2:D:43:LEU:C	2.20	0.61
1:B:299:ARG:NH2	2:D:80:PRO:O	2.34	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:578:THR:HG23	1:B:589:GLU:HB2	1.83	0.61
2:D:181:PRO:C	2:D:182:GLN:HG2	2.21	0.60
2:D:166:TRP:O	2:D:167:LEU:HD12	2.01	0.60
1:B:555:LEU:HD23	1:B:556:ALA:N	2.16	0.60
2:D:50:GLN:O	2:D:50:GLN:HG3	2.00	0.60
1:B:345:TRP:CZ3	1:B:347:VAL:HG23	2.37	0.60
1:B:604:LEU:O	1:B:608:LEU:HG	2.02	0.60
2:C:102:LEU:O	2:C:105:THR:HG22	2.02	0.60
2:C:132:PRO:O	2:C:207:THR:HG21	2.02	0.60
1:B:607:ARG:HH21	1:B:610:VAL:HG21	1.67	0.60
2:C:43:LEU:HD23	2:C:43:LEU:C	2.22	0.60
1:A:555:LEU:HD23	1:A:556:ALA:N	2.15	0.60
1:B:516:ALA:HB3	1:B:641:ARG:O	2.02	0.59
1:B:541:ASP:HA	1:B:551:GLN:H	1.68	0.59
1:A:552:LEU:HD12	1:A:564:LEU:HB3	1.84	0.59
1:A:604:LEU:O	1:A:608:LEU:HG	2.02	0.59
2:D:162:VAL:HG12	2:D:202:ASN:HB3	1.85	0.59
1:B:535:LEU:HD11	1:B:555:LEU:HD21	1.83	0.59
1:A:607:ARG:HH21	1:A:610:VAL:HG21	1.67	0.59
1:A:344:THR:HA	1:A:360:ARG:O	2.03	0.58
1:B:552:LEU:HD12	1:B:564:LEU:HB3	1.86	0.58
1:B:331:GLU:HA	1:B:350:LEU:O	2.02	0.58
1:A:578:THR:HG23	1:A:589:GLU:HB2	1.85	0.58
1:A:402:LYS:HB3	2:D:207:THR:HB	1.83	0.58
1:B:295:LEU:HD21	1:B:307:ILE:HD12	1.85	0.58
1:A:301:PHE:O	1:A:440:ARG:NH1	2.37	0.58
1:B:314:LEU:HB2	2:D:73:ASP:OD1	2.04	0.58
2:C:51:LEU:N	2:C:51:LEU:HD23	2.13	0.58
1:A:535:LEU:HD11	1:A:555:LEU:HD21	1.86	0.58
2:D:132:PRO:O	2:D:207:THR:HG21	2.03	0.58
1:A:541:ASP:HA	1:A:551:GLN:H	1.69	0.58
2:C:166:TRP:O	2:C:167:LEU:HD12	2.04	0.57
1:B:345:TRP:CE3	1:B:347:VAL:HG23	2.39	0.57
1:A:506:GLU:O	1:A:507:VAL:HG23	2.04	0.57
1:B:293:LYS:H	1:B:293:LYS:HD2	1.68	0.57
1:A:295:LEU:HD21	1:A:307:ILE:HD12	1.85	0.57
2:D:102:LEU:O	2:D:105:THR:HG22	2.05	0.57
1:A:580:SER:O	1:A:581:LEU:HD23	2.05	0.57
1:B:429:HIS:CD2	1:B:431:LYS:H	2.23	0.57
1:A:345:TRP:CZ3	1:A:347:VAL:HG23	2.40	0.57
1:A:293:LYS:HD2	1:A:293:LYS:H	1.68	0.57
1:B:580:SER:O	1:B:581:LEU:HD23	2.05	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:456:THR:O	1:A:456:THR:HG22	2.05	0.57
2:C:162:VAL:HG12	2:C:202:ASN:HB3	1.86	0.57
1:B:511:ALA:O	1:B:513:ILE:HG23	2.04	0.57
1:A:507:VAL:HG12	1:A:507:VAL:O	2.05	0.57
1:A:429:HIS:CD2	1:A:431:LYS:HB2	2.33	0.57
2:D:107:GLN:NE2	2:D:125:TYR:HE2	2.03	0.56
1:A:429:HIS:CD2	1:A:431:LYS:H	2.24	0.56
2:C:44:THR:HA	2:C:98:THR:O	2.06	0.56
1:B:429:HIS:CD2	1:B:431:LYS:HB2	2.33	0.56
2:D:44:THR:HA	2:D:98:THR:O	2.06	0.56
1:A:345:TRP:CE3	1:A:347:VAL:HG23	2.40	0.56
1:A:569:VAL:HG23	1:A:570:CYS:SG	2.46	0.56
1:B:391:LEU:HD12	1:B:405:VAL:HG11	1.87	0.56
1:A:426:ILE:HD12	1:A:428:PHE:CE1	2.41	0.56
1:A:516:ALA:HB3	1:A:641:ARG:O	2.06	0.56
1:B:525:LEU:HD12	1:B:535:LEU:HB3	1.87	0.55
1:B:456:THR:HG22	1:B:456:THR:O	2.06	0.55
1:B:552:LEU:HB2	1:B:565:MET:O	2.06	0.55
1:A:525:LEU:HD12	1:A:535:LEU:HB3	1.88	0.55
1:B:426:ILE:HD12	1:B:428:PHE:CE1	2.42	0.55
1:A:391:LEU:HD12	1:A:405:VAL:HG11	1.88	0.55
2:D:51:LEU:HD23	2:D:51:LEU:N	2.12	0.55
1:A:513:ILE:HG13	1:A:515:PRO:HD3	1.86	0.55
1:A:331:GLU:HA	1:A:350:LEU:O	2.06	0.55
1:A:552:LEU:HB2	1:A:565:MET:O	2.05	0.55
2:D:182:GLN:C	2:D:184:SER:H	2.08	0.55
1:B:324:ASP:HA	1:B:380:GLN:O	2.06	0.55
2:C:46:THR:HG22	2:C:96:ARG:HG3	1.89	0.55
1:B:553:VAL:HG12	1:B:554:VAL:N	2.22	0.55
1:B:344:THR:HA	1:B:360:ARG:O	2.06	0.55
2:C:129:GLU:HG3	2:C:159:PRO:HD3	1.88	0.54
1:B:648:VAL:O	1:B:649:ASN:HB2	2.06	0.54
2:C:182:GLN:C	2:C:184:SER:H	2.09	0.54
1:A:339:GLY:HA2	4:A:1678:NAG:O7	2.07	0.54
1:A:552:LEU:N	1:A:552:LEU:HD23	2.23	0.54
2:D:46:THR:HG22	2:D:96:ARG:HG3	1.90	0.54
1:B:397:ARG:NH1	1:B:397:ARG:CG	2.67	0.54
1:A:403:ILE:N	1:A:403:ILE:HD12	2.22	0.54
2:D:129:GLU:HG3	2:D:159:PRO:HD3	1.90	0.54
1:B:426:ILE:HD12	1:B:428:PHE:CD1	2.43	0.54
1:A:590:VAL:O	1:A:591:ASP:HB2	2.08	0.54
1:A:648:VAL:O	1:A:649:ASN:HB2	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:69:LEU:HD11	2:C:108:TYR:HE2	1.74	0.53
1:B:507:VAL:O	1:B:507:VAL:HG12	2.07	0.53
1:B:555:LEU:CD2	1:B:556:ALA:N	2.71	0.53
1:B:457:THR:CG2	2:D:92:VAL:HG11	2.38	0.53
1:B:513:ILE:HG13	1:B:515:PRO:HD3	1.89	0.53
1:A:373:VAL:HG13	1:A:375:ASN:ND2	2.23	0.53
1:B:644:MET:HE3	1:B:646:LEU:HD11	1.90	0.53
1:A:306:VAL:O	1:A:307:ILE:HG13	2.09	0.53
2:C:48:ARG:HG3	2:C:48:ARG:O	2.09	0.53
1:B:552:LEU:HD23	1:B:552:LEU:N	2.24	0.53
1:B:532:ALA:C	1:B:534:PRO:HD3	2.29	0.53
1:B:569:VAL:HG23	1:B:570:CYS:SG	2.49	0.53
1:A:324:ASP:HA	1:A:380:GLN:O	2.09	0.53
1:A:553:VAL:HG12	1:A:554:VAL:N	2.24	0.53
1:A:555:LEU:CD2	1:A:556:ALA:N	2.72	0.53
1:B:561:ALA:O	1:B:562:LEU:HD23	2.09	0.53
1:A:375:ASN:HD22	1:A:375:ASN:N	2.07	0.53
1:A:471:PHE:CE1	1:A:671:PRO:HD3	2.44	0.53
1:B:605:GLN:C	1:B:607:ARG:H	2.11	0.53
1:A:426:ILE:HD12	1:A:428:PHE:CD1	2.44	0.53
2:C:122:GLN:HG3	2:C:123:PRO:HD2	1.91	0.53
1:B:373:VAL:HG13	1:B:375:ASN:ND2	2.25	0.52
2:D:60:VAL:CG1	2:D:93:SER:HB2	2.37	0.52
1:A:385:GLU:OE1	1:A:387:LEU:HG	2.09	0.52
1:B:385:GLU:OE1	1:B:387:LEU:HG	2.09	0.52
1:B:506:GLU:O	1:B:507:VAL:HG23	2.08	0.52
1:B:402:LYS:HB3	2:C:207:THR:HB	1.91	0.52
1:B:306:VAL:O	1:B:307:ILE:HG13	2.09	0.52
2:D:122:GLN:HG3	2:D:123:PRO:HD2	1.91	0.52
1:A:561:ALA:O	1:A:562:LEU:HD23	2.09	0.52
1:B:449:ASN:HD21	1:B:452:ASN:HA	1.74	0.52
1:A:535:LEU:HD12	1:A:536:SER:H	1.74	0.52
1:B:294:SER:O	1:B:462:VAL:HG11	2.09	0.52
1:B:403:ILE:HD12	1:B:403:ILE:N	2.24	0.52
1:A:644:MET:HE3	1:A:646:LEU:HD11	1.90	0.52
2:C:60:VAL:CG1	2:C:93:SER:HB2	2.38	0.52
1:B:590:VAL:O	1:B:591:ASP:HB2	2.09	0.52
2:C:41:ARG:HH11	2:C:41:ARG:HG3	1.75	0.52
1:A:294:SER:O	1:A:462:VAL:HG11	2.09	0.52
2:C:185:LEU:HD23	2:C:185:LEU:O	2.09	0.52
2:D:193:THR:HG23	2:D:214:ILE:O	2.09	0.52
1:A:449:ASN:HD21	1:A:452:ASN:HA	1.75	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:107:GLN:NE2	2:C:125:TYR:HE2	2.07	0.51
2:D:185:LEU:O	2:D:185:LEU:HD23	2.10	0.51
1:A:605:GLN:C	1:A:607:ARG:H	2.13	0.51
1:B:336:PHE:CE2	1:B:427:PRO:HG2	2.46	0.51
1:B:471:PHE:CE1	1:B:671:PRO:HD3	2.45	0.51
1:A:318:ARG:HB2	1:A:318:ARG:HH11	1.75	0.51
2:D:48:ARG:O	2:D:48:ARG:HG3	2.09	0.51
1:A:571:ASP:O	1:A:573:GLN:HG2	2.10	0.51
2:D:69:LEU:HD11	2:D:108:TYR:HE2	1.75	0.51
1:B:528:PRO:O	1:B:531:ARG:HD2	2.10	0.51
2:C:178:GLY:HA2	2:C:182:GLN:HE22	1.76	0.51
1:B:607:ARG:NE	1:B:607:ARG:HA	2.25	0.51
1:A:370:SER:OG	1:A:371:GLY:N	2.44	0.50
2:C:155:ALA:O	2:C:162:VAL:HG21	2.11	0.50
2:C:193:THR:HG23	2:C:214:ILE:O	2.11	0.50
1:B:535:LEU:HD12	1:B:536:SER:H	1.76	0.50
1:B:318:ARG:HH11	1:B:318:ARG:HB2	1.76	0.50
1:B:375:ASN:N	1:B:375:ASN:HD22	2.09	0.50
1:B:510:VAL:HB	1:B:647:GLU:HB2	1.93	0.50
1:A:532:ALA:C	1:A:534:PRO:HD3	2.31	0.50
1:A:318:ARG:NH1	1:A:318:ARG:HB2	2.27	0.50
1:B:339:GLY:HA2	4:B:1678:NAG:H81	1.93	0.50
1:B:318:ARG:HB2	1:B:318:ARG:NH1	2.27	0.50
2:D:131:LEU:HB3	2:D:207:THR:HG22	1.94	0.50
1:B:487:PHE:HA	1:B:621:THR:O	2.12	0.50
1:B:294:SER:HB2	1:B:444:CYS:SG	2.52	0.49
1:B:351:ARG:O	1:B:352:ALA:HB3	2.10	0.49
1:B:555:LEU:CD2	1:B:556:ALA:H	2.23	0.49
1:A:607:ARG:NE	1:A:607:ARG:HA	2.24	0.49
1:B:571:ASP:O	1:B:573:GLN:HG2	2.11	0.49
1:A:555:LEU:CD2	1:A:556:ALA:H	2.23	0.49
1:B:456:THR:HG22	1:B:460:GLU:HG3	1.94	0.49
1:A:599:VAL:CG2	1:A:604:LEU:HB2	2.43	0.49
1:A:294:SER:HB2	1:A:444:CYS:SG	2.52	0.49
2:D:39:GLY:HA3	2:D:43:LEU:HD13	1.94	0.49
1:B:513:ILE:HD12	1:B:515:PRO:HG3	1.95	0.49
2:C:51:LEU:CD1	2:C:112:VAL:HG11	2.43	0.49
1:A:600:SER:C	1:A:602:ALA:N	2.65	0.49
1:A:528:PRO:O	1:A:531:ARG:HD2	2.12	0.49
2:D:178:GLY:HA2	2:D:182:GLN:HE22	1.78	0.48
1:A:513:ILE:HD12	1:A:515:PRO:HG3	1.95	0.48
1:B:567:ILE:HD11	1:B:590:VAL:CG1	2.43	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:532:ALA:O	1:B:534:PRO:HD3	2.13	0.48
1:B:518:ASP:OD1	1:B:519:THR:HG23	2.13	0.48
1:B:486:ALA:HA	1:B:660:TYR:O	2.13	0.48
1:A:567:ILE:HD11	1:A:590:VAL:CG1	2.44	0.48
1:A:510:VAL:HB	1:A:647:GLU:HB2	1.93	0.48
2:C:39:GLY:HA3	2:C:43:LEU:HD13	1.95	0.48
1:B:516:ALA:HB3	1:B:641:ARG:HD3	1.95	0.48
1:A:351:ARG:O	1:A:352:ALA:HB3	2.14	0.48
1:B:600:SER:C	1:B:602:ALA:N	2.65	0.48
2:D:63:LEU:CD2	2:D:68:ILE:HD13	2.44	0.48
1:B:599:VAL:CG2	1:B:604:LEU:HB2	2.44	0.48
1:A:336:PHE:CE2	1:A:427:PRO:HG2	2.48	0.48
1:B:331:GLU:HG3	1:B:437:ILE:HD11	1.96	0.48
1:B:359:LEU:HD12	1:B:359:LEU:N	2.28	0.48
1:A:456:THR:HG22	1:A:460:GLU:HG3	1.94	0.48
2:C:132:PRO:HB2	2:C:207:THR:HG23	1.95	0.48
1:B:457:THR:HG23	2:D:92:VAL:HG11	1.96	0.48
2:D:51:LEU:CD1	2:D:112:VAL:HG11	2.44	0.47
1:A:375:ASN:H	1:A:375:ASN:ND2	2.12	0.47
2:D:55:GLY:O	2:D:56:GLU:C	2.51	0.47
2:C:131:LEU:HB3	2:C:207:THR:HG22	1.96	0.47
2:D:164:LEU:HD22	2:D:198:CYS:SG	2.55	0.47
1:A:309:LEU:HD12	1:A:421:LEU:HD22	1.96	0.47
2:D:70:GLU:C	2:D:71:LEU:HD23	2.34	0.47
1:A:456:THR:HG23	1:A:459:GLN:HB3	1.96	0.47
1:B:309:LEU:HD12	1:B:421:LEU:HD22	1.96	0.47
1:A:487:PHE:HA	1:A:621:THR:O	2.15	0.47
1:A:518:ASP:OD1	1:A:519:THR:HG23	2.15	0.47
2:D:43:LEU:O	2:D:43:LEU:HD23	2.15	0.47
1:A:516:ALA:HB3	1:A:641:ARG:HD3	1.96	0.47
1:A:486:ALA:HA	1:A:660:TYR:O	2.15	0.47
2:C:117:GLN:HG2	2:C:119:PHE:CE1	2.49	0.47
2:C:29:PRO:HD2	2:C:119:PHE:CD2	2.50	0.47
2:D:37:ILE:O	2:D:37:ILE:HG13	2.14	0.47
2:D:126:VAL:O	2:D:126:VAL:CG2	2.63	0.47
1:B:476:ARG:HH11	1:B:476:ARG:HG2	1.79	0.47
2:D:41:ARG:HG3	2:D:41:ARG:HH11	1.79	0.47
2:C:64:ARG:HG3	2:C:108:TYR:CZ	2.50	0.47
2:C:41:ARG:HG2	2:C:128:LEU:HD21	1.97	0.47
2:C:70:GLU:C	2:C:71:LEU:HD23	2.35	0.47
1:A:532:ALA:O	1:A:534:PRO:HD3	2.15	0.47
2:D:41:ARG:NH2	2:D:157:GLY:O	2.48	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:332:GLY:O	1:B:349:ALA:HB1	2.15	0.47
1:B:456:THR:HG23	1:B:459:GLN:HB3	1.95	0.47
1:A:333:ILE:HD13	1:A:426:ILE:HG23	1.96	0.47
2:C:37:ILE:HG13	2:C:37:ILE:O	2.13	0.47
1:A:567:ILE:HG12	1:A:590:VAL:HG11	1.98	0.46
1:A:476:ARG:HH11	1:A:476:ARG:HG2	1.80	0.46
1:B:411:GLN:HA	1:B:412:PRO:HD3	1.75	0.46
2:C:140:ASP:CG	2:C:210:ARG:HH22	2.18	0.46
2:D:41:ARG:HG2	2:D:128:LEU:HD21	1.97	0.46
2:C:55:GLY:O	2:C:56:GLU:C	2.54	0.46
1:B:351:ARG:HG3	1:B:351:ARG:HH11	1.81	0.46
1:B:479:PHE:HB3	1:B:666:THR:OG1	2.15	0.46
2:D:167:LEU:HB2	2:D:197:SER:HB2	1.97	0.46
1:B:437:ILE:O	1:B:439:PRO:HD3	2.15	0.46
2:D:132:PRO:HB2	2:D:207:THR:HG23	1.96	0.46
2:D:64:ARG:HG3	2:D:108:TYR:CZ	2.51	0.46
2:D:111:LEU:HD12	2:D:119:PHE:O	2.16	0.46
2:C:178:GLY:CA	2:C:182:GLN:HE22	2.28	0.46
1:A:437:ILE:O	1:A:439:PRO:HD3	2.16	0.46
1:B:412:PRO:HG3	1:B:417:TYR:CE2	2.50	0.46
1:A:375:ASN:ND2	1:A:375:ASN:N	2.64	0.46
1:B:476:ARG:HG2	1:B:476:ARG:NH1	2.31	0.46
1:B:333:ILE:HD13	1:B:426:ILE:HG23	1.98	0.46
2:C:41:ARG:NH1	2:C:41:ARG:HG3	2.31	0.46
2:C:185:LEU:HD21	2:C:187:VAL:HG22	1.97	0.46
1:B:368:THR:HG22	1:B:369:SER:N	2.31	0.46
2:D:82:GLY:HA3	2:D:87:ASP:HB2	1.98	0.45
2:D:162:VAL:O	2:D:162:VAL:HG23	2.16	0.45
2:D:182:GLN:O	2:D:184:SER:N	2.49	0.45
2:C:132:PRO:HD2	2:C:207:THR:CG2	2.46	0.45
2:C:43:LEU:HD23	2:C:43:LEU:O	2.17	0.45
1:A:359:LEU:N	1:A:359:LEU:HD12	2.31	0.45
1:A:567:ILE:CG1	1:A:590:VAL:HG11	2.47	0.45
1:A:282:PRO:HA	1:A:516:ALA:O	2.16	0.45
2:D:140:ASP:CG	2:D:210:ARG:HH22	2.19	0.45
1:B:375:ASN:H	1:B:375:ASN:ND2	2.14	0.45
1:A:479:PHE:HB3	1:A:666:THR:OG1	2.15	0.45
2:C:63:LEU:CD2	2:C:68:ILE:HD13	2.46	0.45
2:D:60:VAL:HG12	2:D:76:GLN:OE1	2.17	0.45
1:A:332:GLY:O	1:A:349:ALA:HB1	2.17	0.45
1:B:567:ILE:HG12	1:B:590:VAL:HG11	1.98	0.45
2:D:155:ALA:O	2:D:162:VAL:HG21	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:82:GLY:HA3	2:C:87:ASP:HB2	1.98	0.45
2:D:178:GLY:CA	2:D:182:GLN:HE22	2.30	0.45
1:A:368:THR:HG22	1:A:369:SER:N	2.31	0.45
1:A:412:PRO:HG3	1:A:417:TYR:CE2	2.51	0.45
2:C:57:PRO:HD3	2:C:89:TRP:CD1	2.51	0.44
1:B:567:ILE:CG1	1:B:590:VAL:HG11	2.47	0.44
1:A:331:GLU:HG3	1:A:437:ILE:HD11	1.98	0.44
2:C:103:SER:C	2:C:105:THR:H	2.20	0.44
1:B:370:SER:OG	1:B:371:GLY:N	2.47	0.44
1:B:488:TYR:CD1	1:B:488:TYR:N	2.86	0.44
1:A:519:THR:HA	1:A:539:LEU:O	2.17	0.44
2:C:38:THR:HA	2:C:127:GLY:O	2.17	0.44
1:A:340:HIS:CD2	1:A:341:GLN:N	2.85	0.44
2:C:60:VAL:HG12	2:C:76:GLN:OE1	2.17	0.44
1:B:420:ASN:ND2	4:B:1678:NAG:H82	2.32	0.44
1:A:358:GLN:C	1:A:359:LEU:HD12	2.38	0.44
2:D:38:THR:HA	2:D:127:GLY:O	2.17	0.44
1:A:351:ARG:HG3	1:A:351:ARG:HH11	1.82	0.44
1:A:476:ARG:NH1	1:A:476:ARG:HG2	2.32	0.44
2:D:140:ASP:OD2	2:D:210:ARG:NH2	2.51	0.44
1:B:321:ALA:HB1	1:B:450:TRP:CZ3	2.53	0.44
2:C:167:LEU:HB2	2:C:197:SER:HB2	1.99	0.44
1:B:358:GLN:C	1:B:359:LEU:HD12	2.38	0.44
1:A:617:SER:O	1:A:619:VAL:HG22	2.17	0.44
1:B:340:HIS:CD2	1:B:341:GLN:N	2.86	0.44
2:C:46:THR:CG2	2:C:96:ARG:HG3	2.48	0.44
1:B:287:SER:HB2	1:B:672:PRO:HG2	2.00	0.43
2:C:167:LEU:HA	2:C:171:VAL:O	2.18	0.43
2:D:185:LEU:HD21	2:D:187:VAL:HG22	1.99	0.43
2:D:117:GLN:HG2	2:D:119:PHE:CE1	2.53	0.43
2:C:80:PRO:HD3	2:C:89:TRP:CZ3	2.53	0.43
2:D:57:PRO:HD3	2:D:89:TRP:CD1	2.53	0.43
2:C:140:ASP:OD2	2:C:210:ARG:NH2	2.51	0.43
1:A:397:ARG:NH1	1:A:397:ARG:CG	2.67	0.43
2:C:57:PRO:HD3	2:C:89:TRP:CG	2.53	0.43
1:A:308:ARG:HG2	1:A:422:THR:HG22	1.98	0.43
2:D:103:SER:C	2:D:105:THR:H	2.22	0.43
2:D:64:ARG:O	2:D:65:ASP:HB2	2.19	0.43
2:C:182:GLN:O	2:C:184:SER:N	2.51	0.43
1:B:336:PHE:HB2	1:B:426:ILE:HG22	1.99	0.43
2:C:162:VAL:HG23	2:C:162:VAL:O	2.18	0.43
2:D:29:PRO:HD2	2:D:119:PHE:CD2	2.54	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:432:ASP:O	1:A:433:LEU:O	2.37	0.43
1:B:329:ASP:HA	1:B:330:PRO:HD3	1.80	0.43
1:B:328:PHE:CE2	1:B:377:GLY:HA3	2.53	0.43
1:A:321:ALA:HB1	1:A:450:TRP:CZ3	2.53	0.43
2:C:51:LEU:N	2:C:51:LEU:CD2	2.76	0.43
1:A:562:LEU:O	1:A:563:ALA:HB2	2.18	0.43
1:B:433:LEU:HB3	1:B:434:VAL:H	1.56	0.43
1:B:590:VAL:HG12	1:B:590:VAL:O	2.19	0.43
2:D:80:PRO:HD3	2:D:89:TRP:CZ3	2.54	0.43
1:B:562:LEU:O	1:B:563:ALA:HB2	2.19	0.42
2:D:107:GLN:HE21	2:D:125:TYR:HE2	1.66	0.42
1:B:375:ASN:N	1:B:375:ASN:ND2	2.66	0.42
2:C:41:ARG:NH2	2:C:157:GLY:O	2.50	0.42
1:B:540:VAL:HG13	1:B:636:VAL:HG22	2.01	0.42
1:A:601:ALA:HA	1:A:604:LEU:HB3	2.01	0.42
2:D:57:PRO:HD3	2:D:89:TRP:CG	2.53	0.42
2:C:111:LEU:HD12	2:C:119:PHE:O	2.18	0.42
1:A:488:TYR:CD1	1:A:488:TYR:N	2.86	0.42
1:A:492:TYR:CD2	1:A:507:VAL:HG22	2.54	0.42
1:B:282:PRO:HA	1:B:516:ALA:O	2.18	0.42
1:A:287:SER:HB2	1:A:672:PRO:HG2	2.01	0.42
1:A:323:PHE:CE1	1:A:382:ILE:HB	2.55	0.42
1:A:336:PHE:HB2	1:A:426:ILE:HG22	2.01	0.42
1:A:590:VAL:HG12	1:A:590:VAL:O	2.18	0.42
1:B:432:ASP:O	1:B:433:LEU:O	2.38	0.42
1:B:601:ALA:HA	1:B:604:LEU:HB3	2.00	0.42
1:A:329:ASP:HA	1:A:330:PRO:HD3	1.81	0.42
2:D:51:LEU:HD21	2:D:91:VAL:HB	2.02	0.42
2:D:167:LEU:HA	2:D:171:VAL:O	2.20	0.42
1:B:557:VAL:HG23	1:B:562:LEU:HD11	2.00	0.42
1:B:308:ARG:HG2	1:B:422:THR:HG22	2.02	0.42
1:B:329:ASP:OD1	1:B:331:GLU:O	2.37	0.42
1:A:350:LEU:HA	1:A:350:LEU:HD12	1.88	0.42
2:C:185:LEU:HD21	2:C:187:VAL:CG2	2.50	0.42
1:B:617:SER:HB3	1:B:618:PRO:CD	2.50	0.42
2:D:80:PRO:HB3	2:D:89:TRP:CH2	2.55	0.42
2:D:125:TYR:N	2:D:125:TYR:CD1	2.88	0.42
1:A:334:LEU:HD23	1:A:348:LEU:CD2	2.50	0.42
1:A:334:LEU:HD23	1:A:348:LEU:HD23	2.02	0.42
1:B:519:THR:HA	1:B:539:LEU:O	2.20	0.42
1:A:552:LEU:HB3	1:A:566:GLU:HA	2.01	0.42
1:A:336:PHE:CE1	1:A:345:TRP:HB2	2.55	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:617:SER:HB3	1:A:618:PRO:CD	2.49	0.42
1:B:617:SER:O	1:B:619:VAL:HG22	2.18	0.42
1:B:492:TYR:CD2	1:B:507:VAL:HG22	2.55	0.41
1:B:341:GLN:HA	1:B:428:PHE:CE2	2.55	0.41
2:C:125:TYR:CD1	2:C:125:TYR:N	2.87	0.41
2:D:176:ALA:HB1	2:D:177:PRO:HD2	2.02	0.41
2:D:51:LEU:HD11	2:D:112:VAL:HG11	2.02	0.41
2:C:51:LEU:HD11	2:C:112:VAL:HG11	2.02	0.41
2:C:126:VAL:CG2	2:C:126:VAL:O	2.68	0.41
1:B:552:LEU:HB3	1:B:566:GLU:HA	2.01	0.41
1:B:328:PHE:O	1:B:375:ASN:HB2	2.19	0.41
2:C:29:PRO:CD	2:C:119:PHE:CD2	3.03	0.41
1:B:485:PHE:CD1	1:B:485:PHE:C	2.94	0.41
1:A:296:TYR:CE2	1:A:299:ARG:HA	2.55	0.41
2:D:81:LEU:HD11	2:D:90:ILE:HG13	2.02	0.41
1:A:328:PHE:CE2	1:A:377:GLY:HA3	2.55	0.41
2:C:164:LEU:HD22	2:C:198:CYS:SG	2.60	0.41
1:B:336:PHE:CE1	1:B:345:TRP:HB2	2.56	0.41
1:B:296:TYR:CE2	1:B:299:ARG:HA	2.55	0.41
1:A:660:TYR:C	1:A:660:TYR:CD2	2.93	0.41
2:D:41:ARG:NH1	2:D:41:ARG:HG3	2.36	0.41
1:A:531:ARG:NH1	1:A:531:ARG:HG3	2.30	0.41
1:B:284:VAL:HG21	1:B:570:CYS:HA	2.03	0.41
1:A:617:SER:HB3	1:A:618:PRO:HD2	2.01	0.41
1:B:334:LEU:HD23	1:B:348:LEU:CD2	2.50	0.41
1:B:409:LEU:HD23	1:B:409:LEU:HA	1.85	0.41
1:A:485:PHE:CD1	1:A:485:PHE:C	2.93	0.41
2:C:182:GLN:O	2:C:183:ARG:HB2	2.21	0.41
2:C:64:ARG:O	2:C:65:ASP:HB2	2.20	0.41
2:C:48:ARG:CG	2:C:48:ARG:O	2.69	0.41
2:D:185:LEU:HD21	2:D:187:VAL:CG2	2.51	0.41
2:D:126:VAL:O	2:D:126:VAL:HG23	2.20	0.41
2:D:182:GLN:C	2:D:184:SER:N	2.73	0.41
1:A:296:TYR:HE1	1:A:442:ASP:OD1	2.04	0.41
2:D:56:GLU:HA	2:D:57:PRO:HD2	1.80	0.41
1:B:343:SER:O	1:B:362:ASN:HA	2.21	0.41
2:C:51:LEU:HD21	2:C:91:VAL:HB	2.03	0.41
1:A:314:LEU:N	2:C:73:ASP:OD1	2.54	0.41
2:C:185:LEU:C	2:C:185:LEU:HD23	2.41	0.41
1:B:323:PHE:CE1	1:B:382:ILE:HB	2.56	0.41
1:A:409:LEU:HA	1:A:409:LEU:HD23	1.85	0.41
1:A:540:VAL:HG13	1:A:636:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:296:TYR:HE1	1:B:442:ASP:OD1	2.04	0.40
2:D:120:VAL:HG12	2:D:121:SER:O	2.21	0.40
2:D:51:LEU:CD2	2:D:91:VAL:HB	2.51	0.40
1:B:600:SER:O	1:B:602:ALA:N	2.55	0.40
2:C:160:GLU:HB3	2:C:161:PRO:HA	2.02	0.40
2:D:206:VAL:CG2	2:D:207:THR:N	2.83	0.40
1:A:327:THR:O	1:A:375:ASN:HA	2.21	0.40
2:D:63:LEU:HD23	2:D:68:ILE:HD13	2.02	0.40
1:B:493:MET:HE2	1:B:616:ARG:HA	2.03	0.40
2:C:202:ASN:C	2:C:202:ASN:OD1	2.60	0.40
2:C:63:LEU:HD23	2:C:68:ILE:HD13	2.03	0.40
1:B:617:SER:HB3	1:B:618:PRO:HD2	2.03	0.40
2:C:176:ALA:HB1	2:C:177:PRO:HD2	2.04	0.40
1:A:381:THR:O	1:A:395:VAL:HA	2.21	0.40
1:A:313:ARG:NH2	2:C:75:THR:OG1	2.51	0.40
2:C:120:VAL:HG12	2:C:121:SER:O	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	375/422 (89%)	296 (79%)	64 (17%)	15 (4%)	5	36
1	B	375/422 (89%)	297 (79%)	63 (17%)	15 (4%)	5	36
2	C	190/195 (97%)	171 (90%)	14 (7%)	5 (3%)	8	50
2	D	190/195 (97%)	171 (90%)	14 (7%)	5 (3%)	8	50
All	All	1130/1234 (92%)	935 (83%)	155 (14%)	40 (4%)	6	41

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	433	LEU
1	A	455	ASP

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Mol	Chain	Res	Type
1	A	456	THR
1	B	433	LEU
1	B	455	ASP
1	B	456	THR
1	A	507	VAL
1	A	599	VAL
1	B	507	VAL
1	B	599	VAL
2	C	55	GLY
2	C	98	THR
2	C	203	ALA
2	D	55	GLY
2	D	98	THR
2	D	203	ALA
1	B	600	SER
1	A	292	VAL
1	A	551	GLN
1	A	561	ALA
1	A	562	LEU
1	A	600	SER
1	B	562	LEU
1	A	452	ASN
1	A	515	PRO
1	A	565	MET
1	B	292	VAL
1	B	452	ASN
1	B	551	GLN
1	B	565	MET
2	C	56	GLU
2	D	56	GLU
1	B	515	PRO
1	B	561	ALA
2	C	217	LEU
2	D	217	LEU
1	A	554	VAL
1	B	554	VAL
1	A	288	VAL
1	B	288	VAL

### 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	320/356 (90%)	295 (92%)	25 (8%)	18	60
1	B	320/356 (90%)	296 (92%)	24 (8%)	19	62
2	C	162/166 (98%)	150 (93%)	12 (7%)	20	63
2	D	162/166 (98%)	149 (92%)	13 (8%)	17	58
All	All	964/1044 (92%)	890 (92%)	74 (8%)	18	60

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	293	LYS
1	A	306	VAL
1	A	313	ARG
1	A	314	LEU
1	A	318	ARG
1	A	334	LEU
1	A	344	THR
1	A	359	LEU
1	A	375	ASN
1	A	384	VAL
1	A	391	LEU
1	A	397	ARG
1	A	419	LEU
1	A	435	GLN
1	A	488	TYR
1	A	491	ASP
1	A	531	ARG
1	A	540	VAL
1	A	554	VAL
1	A	555	LEU
1	A	565	MET
1	A	578	THR
1	A	605	GLN
1	A	619	VAL
1	A	641	ARG
1	B	293	LYS

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Mol	Chain	Res	Type
1	B	306	VAL
1	B	313	ARG
1	B	314	LEU
1	B	318	ARG
1	B	334	LEU
1	B	344	THR
1	B	359	LEU
1	B	375	ASN
1	B	391	LEU
1	B	397	ARG
1	B	419	LEU
1	B	435	GLN
1	B	488	TYR
1	B	491	ASP
1	B	531	ARG
1	B	540	VAL
1	B	554	VAL
1	B	555	LEU
1	B	565	MET
1	B	578	THR
1	B	605	GLN
1	B	619	VAL
1	B	641	ARG
2	C	48	ARG
2	C	50	GLN
2	C	51	LEU
2	C	74	SER
2	C	84	ASP
2	C	87	ASP
2	C	98	THR
2	C	107	GLN
2	C	118	THR
2	C	126	VAL
2	C	185	LEU
2	C	207	THR
2	D	48	ARG
2	D	50	GLN
2	D	51	LEU
2	D	74	SER
2	D	84	ASP
2	D	87	ASP
2	D	98	THR

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Mol	Chain	Res	Type
2	D	107	GLN
2	D	118	THR
2	D	126	VAL
2	D	132	PRO
2	D	185	LEU
2	D	207	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	340	HIS
1	A	375	ASN
1	A	376	HIS
1	A	429	HIS
1	A	449	ASN
1	A	465	ASN
1	A	573	GLN
1	B	340	HIS
1	B	375	ASN
1	B	376	HIS
1	B	429	HIS
1	B	449	ASN
1	B	465	ASN
1	B	573	GLN
2	C	101	GLN
2	C	107	GLN
2	C	109	GLN
2	C	182	GLN
2	D	94	GLN
2	D	101	GLN
2	D	107	GLN
2	D	109	GLN
2	D	182	GLN

### 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 ⓘ

4 carbohydrates 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
4	NAG	A	1678	1,4	12,14,15	0.71	0	15,19,21	0.86	1 (6%)
4	NAG	A	1679	4	12,14,15	0.52	0	15,19,21	0.73	1 (6%)
4	NAG	B	1678	1,4	12,14,15	0.62	0	15,19,21	0.88	1 (6%)
4	NAG	B	1679	4	12,14,15	0.69	0	15,19,21	0.80	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1678	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1679	4	-	0/6/23/26	0/1/1/1
4	NAG	B	1678	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1679	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1678	NAG	C2-N2-C7	-2.31	119.22	123.09
4	B	1679	NAG	C2-N2-C7	-2.21	119.38	123.09
4	A	1678	NAG	C3-C2-N2	-2.11	108.54	111.76
4	A	1679	NAG	C2-N2-C7	-2.07	119.61	123.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z  > 2$
6	SO4	C	1219	-	4,4,4	0.38	0	6,6,6	0.11	0

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
6	SO4	C	1219	-	-	0/0/0/0	0/0/0/0

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.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	381/422 (90%)	-0.19	1 (0%) 91 63	25, 60, 118, 144	2 (0%)
1	B	381/422 (90%)	-0.23	0 100 100	25, 60, 118, 144	2 (0%)
2	C	192/195 (98%)	-0.24	0 100 100	28, 56, 86, 101	0
2	D	192/195 (98%)	-0.20	1 (0%) 88 51	27, 56, 86, 101	0
All	All	1146/1234 (92%)	-0.21	2 (0%) 91 70	25, 59, 112, 144	4 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	677	ALA	2.7
2	D	192	LYS	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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
4	NAG	A	1679	14/15	0.55	8.97	86,91,94,95	0
4	NAG	B	1679	14/15	0.43	3.56	86,89,91,92	0
4	NAG	A	1678	14/15	0.22	0.11	65,73,77,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	B	1678	14/15	0.17	-0.52	62,68,72,80	0

## 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	CA	A	1677	1/1	0.18	0.67	40,40,40,40	0
3	CA	B	1677	1/1	0.16	0.20	45,45,45,45	0
5	NI	C	1218	1/1	0.04	-4.10	127,127,127,127	0
5	NI	D	1218	1/1	0.06	-4.82	134,134,134,134	0
6	SO4	C	1219	5/5	0.09	-7.34	103,103,104,104	0

## 6.5 Other polymers

There are no such residues in this entry.