



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:28 AM UTC

PDB ID : 3DC2 / pdb_00003dc2
Title : Crystal structure of serine bound D-3-phosphoglycerate dehydrogenase from Mycobacterium tuberculosis
Authors : Dey, S.; Sacchettini, J.C.
Deposited on : 2008-06-03
Resolution : 2.70 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

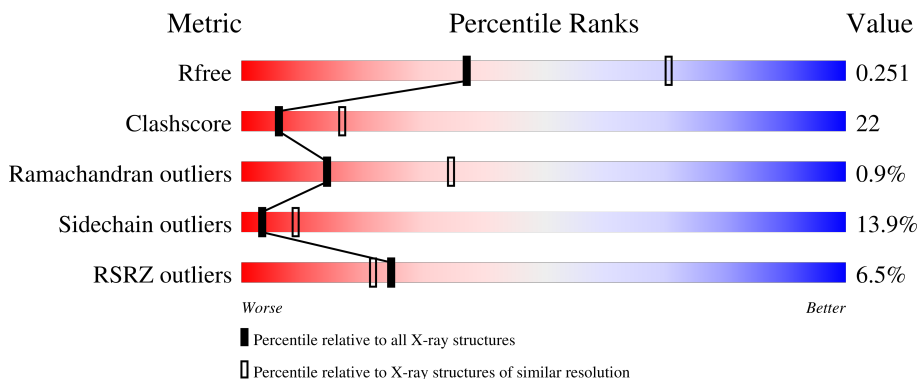
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	529	 5% 59% 33% 6% ..
1	B	529	 8% 56% 35% 8% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7761 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.

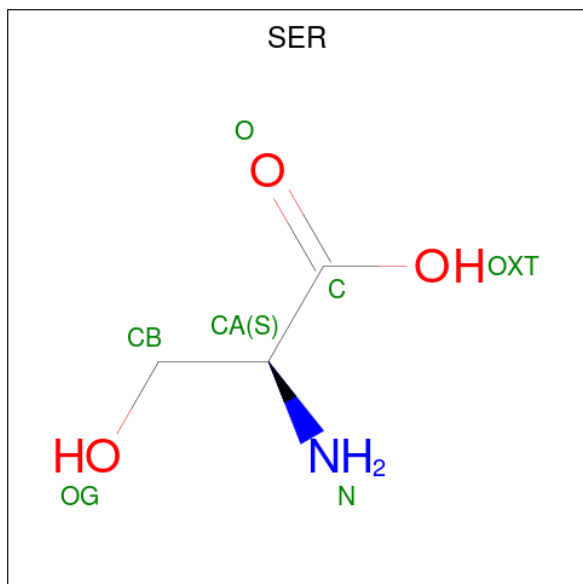
- Molecule 1 is a protein called D-3-phosphoglycerate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	526	Total 3830	C 2413	N 672	O 743	S 2	0	0	0
1	B	523	Total 3810	C 2401	N 669	O 738	S 2	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

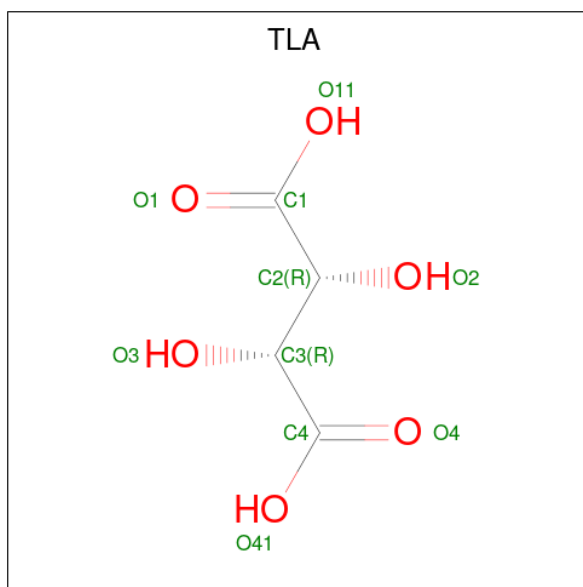
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P0A544
A	2	VAL	-	expression tag	UNP P0A544
B	1	MET	-	expression tag	UNP P0A544
B	2	VAL	-	expression tag	UNP P0A544

- Molecule 2 is SERINE (CCD ID: SER) (formula: C₃H₇NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			7	3	1	3		
2	B	1	Total	C	N	O	0	0
			7	3	1	3		

- Molecule 3 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	4	6		
3	B	1	Total	C	O	0	0
			10	4	6		
3	B	1	Total	C	O	0	0
			10	4	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total	O	0	0
			40	40		
4	B	37	Total	O	0	0
			37	37		

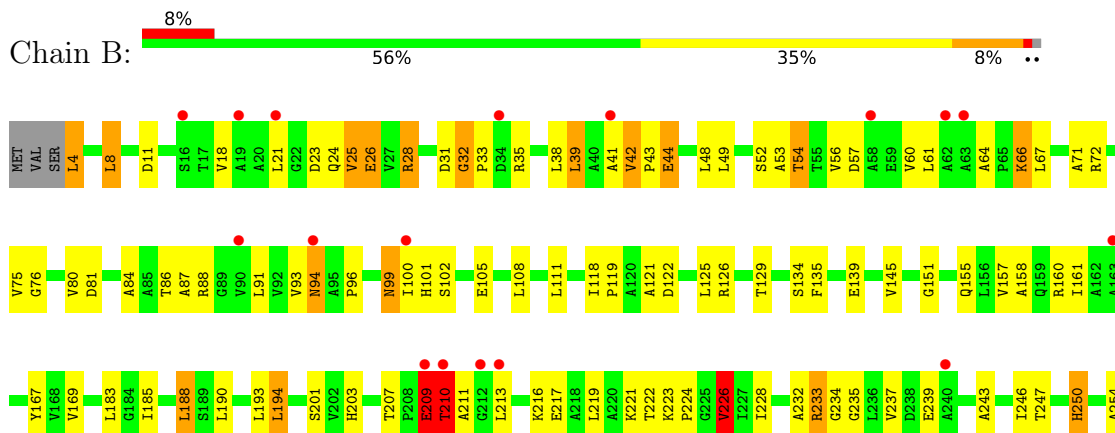
3 Residue-property plots i

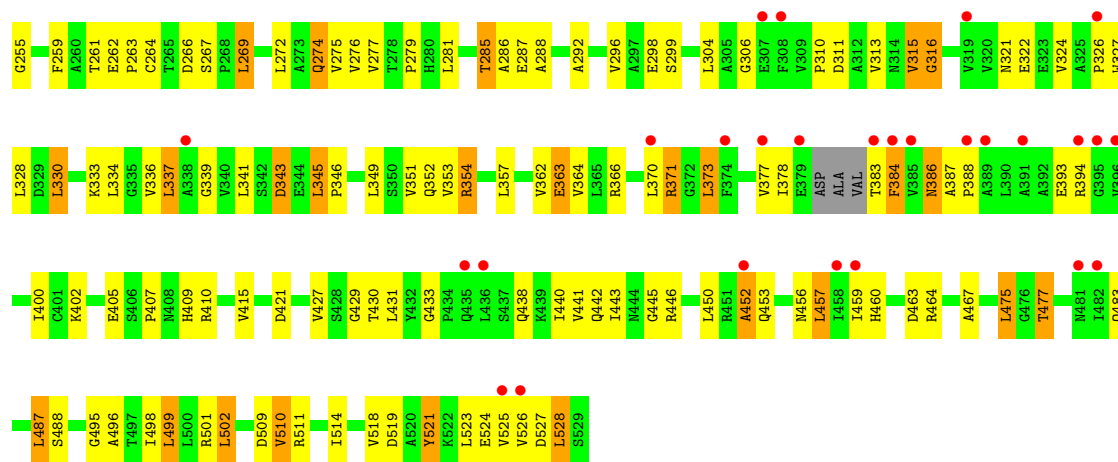
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: D-3-phosphoglycerate dehydrogenase



- Molecule 1: D-3-phosphoglycerate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	165.19Å 165.19Å 218.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.57 – 2.70 46.57 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.57-2.70) 99.1 (46.57-2.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.263 0.210 , 0.251	Depositor DCC
R_{free} test set	2452 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	67.7	Xtrriage
Anisotropy	0.632	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 66.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7761	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.10% 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 i

5.1 Standard geometry i

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

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	1.23	10/3884 (0.3%)	1.23	16/5308 (0.3%)
1	B	1.16	21/3863 (0.5%)	1.23	26/5277 (0.5%)
All	All	1.20	31/7747 (0.4%)	1.23	42/10585 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	HIS	CE1-NE2	36.00	1.68	1.32
1	A	128	HIS	CG-ND1	20.74	1.61	1.38
1	B	250	HIS	CE1-NE2	19.03	1.51	1.32
1	B	250	HIS	CG-CD2	13.34	1.50	1.35
1	A	446	ARG	CZ-NH1	11.25	1.48	1.32
1	B	250	HIS	CG-ND1	10.48	1.49	1.38
1	B	393	GLU	CD-OE1	9.80	1.44	1.25
1	A	477	THR	CB-OG1	9.03	1.58	1.43
1	B	66	LYS	CE-NZ	7.97	1.73	1.49
1	B	217	GLU	CD-OE2	7.70	1.40	1.25
1	B	393	GLU	CD-OE2	6.90	1.38	1.25
1	A	159	GLN	CD-OE1	6.62	1.36	1.23
1	B	250	HIS	ND1-CE1	6.59	1.39	1.32
1	B	185	ILE	CA-CB	-6.49	1.46	1.54
1	B	44	GLU	CD-OE2	6.40	1.37	1.25
1	A	128	HIS	CG-CD2	6.35	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	28	ARG	NE-CZ	6.25	1.40	1.33
1	B	226	VAL	CB-CG2	6.15	1.72	1.52
1	A	168	VAL	CA-CB	-6.13	1.47	1.54
1	B	44	GLU	CG-CD	5.78	1.66	1.52
1	B	44	GLU	CD-OE1	5.75	1.36	1.25
1	B	217	GLU	CD-OE1	5.57	1.35	1.25
1	B	221	LYS	CE-NZ	5.55	1.66	1.49
1	A	477	THR	CB-CG2	5.52	1.70	1.52
1	B	216	LYS	C-O	5.50	1.30	1.24
1	A	446	ARG	NE-CZ	5.48	1.39	1.33
1	B	477	THR	C-O	5.46	1.30	1.24
1	B	26	GLU	CG-CD	5.45	1.65	1.52
1	A	417	ALA	CA-CB	-5.19	1.46	1.53
1	B	28	ARG	CG-CD	5.07	1.67	1.52
1	B	216	LYS	CB-CG	5.06	1.67	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	HIS	ND1-CG-CD2	10.30	116.41	106.10
1	B	433	GLY	CA-C-N	8.94	128.53	119.24
1	B	433	GLY	C-N-CA	8.94	128.53	119.24
1	B	210	THR	N-CA-C	-8.78	101.64	111.82
1	B	223	LYS	CA-C-N	-8.01	111.75	119.76
1	B	223	LYS	C-N-CA	-8.01	111.75	119.76
1	A	430	THR	CB-CA-C	-7.24	94.26	111.65
1	A	446	ARG	NE-CZ-NH2	-7.13	112.78	119.20
1	B	44	GLU	CB-CG-CD	-7.01	100.69	112.60
1	B	42	VAL	CA-C-N	6.58	127.10	119.47
1	B	42	VAL	C-N-CA	6.58	127.10	119.47
1	A	441	VAL	CB-CA-C	-6.51	104.25	110.70
1	B	100	ILE	N-CA-C	6.21	116.38	110.42
1	B	223	LYS	O-C-N	6.07	127.55	121.30
1	A	417	ALA	CA-C-N	-6.00	115.37	122.93
1	A	417	ALA	C-N-CA	-6.00	115.37	122.93
1	A	226	VAL	CB-CA-C	-5.84	101.88	111.51
1	B	99	ASN	N-CA-CB	-5.84	101.57	110.33
1	B	86	THR	N-CA-C	-5.83	104.93	111.28
1	B	233	ARG	N-CA-C	5.74	117.83	108.76
1	B	345	LEU	CA-C-N	-5.73	114.41	120.66
1	B	345	LEU	C-N-CA	-5.73	114.41	120.66
1	B	250	HIS	N-CA-C	5.68	117.56	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	521	TYR	N-CA-C	-5.52	105.27	112.23
1	B	185	ILE	CB-CA-C	-5.50	102.43	110.62
1	A	508	ASP	N-CA-C	5.40	116.86	110.97
1	A	462	VAL	N-CA-C	5.37	116.45	108.23
1	B	211	ALA	N-CA-C	5.37	117.87	110.35
1	A	69	ILE	CB-CA-C	-5.37	102.49	111.29
1	A	514	ILE	CB-CA-C	-5.35	104.92	112.14
1	A	95	ALA	CA-C-N	-5.28	114.23	119.56
1	A	95	ALA	C-N-CA	-5.28	114.23	119.56
1	A	396	VAL	CB-CA-C	-5.27	102.77	110.62
1	B	167	TYR	CA-C-N	-5.26	116.28	123.12
1	B	167	TYR	C-N-CA	-5.26	116.28	123.12
1	B	510	VAL	N-CA-C	-5.26	105.41	110.72
1	B	250	HIS	ND1-CG-CD2	5.23	111.33	106.10
1	B	75	VAL	N-CA-C	-5.21	107.68	111.90
1	B	32	GLY	N-CA-C	5.18	121.80	115.22
1	A	393	GLU	N-CA-C	-5.12	105.87	112.68
1	B	405	GLU	N-CA-C	5.12	116.52	109.15
1	A	418	VAL	N-CA-C	5.08	115.62	108.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	209	GLU	Peptide

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	3830	0	3916	169	0
1	B	3810	0	3897	186	0
2	A	7	0	4	0	0
2	B	7	0	4	0	0
3	A	10	0	4	0	0
3	B	20	0	8	0	0
4	A	40	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	37	0	0	5	0
All	All	7761	0	7833	347	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 22.

All (347) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:LYS:CE	1:B:66:LYS:NZ	1.73	1.49
1:A:128:HIS:CE1	1:A:128:HIS:NE2	1.68	1.45
1:A:285:THR:HG22	1:A:288:ALA:H	1.06	1.20
1:A:332:ARG:HG2	1:A:332:ARG:HH21	1.18	1.08
1:B:285:THR:HG22	1:B:288:ALA:H	1.16	1.07
1:B:352:GLN:HE21	1:B:354:ARG:HD3	1.12	1.06
1:B:42:VAL:HG12	1:B:64:ALA:HB2	1.38	1.03
1:A:246:ILE:HD12	1:A:251:VAL:HG22	1.44	0.99
1:B:42:VAL:N	1:B:43:PRO:HD2	1.79	0.97
1:B:345:LEU:HD12	1:B:346:PRO:HD3	1.44	0.97
1:B:345:LEU:HD12	1:B:346:PRO:CD	2.01	0.91
1:B:511:ARG:NH2	1:B:525:VAL:HB	1.88	0.89
1:B:352:GLN:NE2	1:B:354:ARG:HD3	1.87	0.88
1:B:407:PRO:HD2	4:B:829:HOH:O	1.74	0.87
1:B:118:ILE:HB	1:B:119:PRO:HD3	1.57	0.87
1:B:430:THR:HG22	1:B:431:LEU:N	1.89	0.85
1:A:285:THR:CG2	1:A:288:ALA:H	1.88	0.85
1:A:332:ARG:HG2	1:A:332:ARG:NH2	1.85	0.85
1:B:371:ARG:HH12	1:B:384:PHE:HE1	1.26	0.84
1:B:315:VAL:HG13	1:B:316:GLY:N	1.91	0.84
1:A:285:THR:HG22	1:A:288:ALA:N	1.90	0.84
1:A:490:ASP:O	1:A:491:ALA:C	2.23	0.82
1:A:411:SER:O	1:A:430:THR:HG23	1.80	0.81
1:A:205:PRO:O	1:A:210:THR:HG21	1.82	0.80
1:B:285:THR:CG2	1:B:288:ALA:H	1.94	0.80
1:B:371:ARG:NH1	1:B:384:PHE:HE1	1.80	0.80
1:A:246:ILE:CD1	1:A:251:VAL:HG22	2.10	0.80
1:A:69:ILE:HD12	1:A:303:ALA:HB3	1.65	0.79
1:B:41:ALA:C	1:B:43:PRO:HD2	2.08	0.78
1:A:88:ARG:HH21	1:A:88:ARG:HB3	1.48	0.78
1:B:285:THR:HG22	1:B:288:ALA:N	1.98	0.76
1:A:69:ILE:HD13	1:A:303:ALA:HB1	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ASP:OD2	1:B:84:ALA:HB2	1.87	0.75
1:B:386:ASN:OD1	1:B:386:ASN:C	2.28	0.75
1:B:315:VAL:HG13	1:B:316:GLY:H	1.50	0.75
1:B:274:GLN:H	1:B:274:GLN:HE21	1.35	0.74
1:A:72:ARG:NH2	1:A:74:GLY:HA3	2.03	0.74
1:A:102:SER:HG	1:A:285:THR:HG21	1.52	0.73
1:A:226:VAL:HG23	1:A:251:VAL:HB	1.71	0.73
1:B:101:HIS:O	1:B:105:GLU:HG3	1.88	0.73
1:A:88:ARG:HB3	1:A:88:ARG:NH2	2.03	0.72
1:A:460:HIS:HD2	1:A:497:THR:HG23	1.55	0.72
1:A:411:SER:O	1:A:430:THR:CG2	2.37	0.72
1:A:72:ARG:HH21	1:A:74:GLY:HA3	1.53	0.72
1:B:274:GLN:HE21	1:B:274:GLN:N	1.88	0.72
1:A:49:LEU:HD22	1:A:71:ALA:HB3	1.72	0.71
1:B:352:GLN:HE21	1:B:354:ARG:CD	2.00	0.70
1:B:371:ARG:NH2	4:B:819:HOH:O	2.22	0.70
1:B:52:SER:HB3	1:B:72:ARG:NH1	2.06	0.70
1:A:461:TYR:O	1:A:495:GLY:HA2	1.92	0.70
1:B:11:ASP:OD2	1:B:54:THR:HG23	1.90	0.70
1:A:361:GLU:HA	4:A:808:HOH:O	1.90	0.69
1:B:362:VAL:HG22	1:B:402:LYS:HD3	1.72	0.69
1:A:206:LYS:CB	4:A:832:HOH:O	2.41	0.69
1:B:38:LEU:O	1:B:42:VAL:HG23	1.93	0.68
1:A:310:PRO:O	1:A:384:PHE:CE1	2.45	0.68
1:B:334:LEU:HB3	1:B:415:VAL:CG2	2.24	0.68
1:B:23:ASP:HB3	1:B:24:GLN:NE2	2.08	0.68
1:A:69:ILE:CD1	1:A:303:ALA:CB	2.71	0.68
1:B:209:GLU:OE2	1:B:209:GLU:HA	1.93	0.68
1:B:42:VAL:N	1:B:43:PRO:CD	2.57	0.68
1:A:12:LYS:HB2	4:A:821:HOH:O	1.94	0.68
1:B:334:LEU:HB3	1:B:415:VAL:HG21	1.74	0.67
1:B:349:LEU:HD13	1:B:373:LEU:HG	1.77	0.67
1:B:11:ASP:CG	1:B:54:THR:HG23	2.20	0.67
1:A:69:ILE:CD1	1:A:303:ALA:HB1	2.25	0.67
1:B:169:VAL:HB	1:B:188:LEU:HD22	1.75	0.66
1:A:21:LEU:O	1:A:22:GLY:O	2.14	0.66
1:A:514:ILE:O	1:A:518:VAL:HG22	1.97	0.65
1:B:457:LEU:HD11	1:B:459:ILE:HD11	1.79	0.65
1:B:23:ASP:HB3	1:B:24:GLN:HE21	1.62	0.65
1:B:371:ARG:NH1	1:B:384:PHE:CE1	2.63	0.65
1:B:121:ALA:HA	1:B:135:PHE:CZ	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:LYS:HE2	1:B:528:LEU:O	1.97	0.65
1:A:255:GLY:HA2	1:A:276:VAL:O	1.96	0.64
1:B:457:LEU:HD11	1:B:459:ILE:CG1	2.26	0.64
1:B:315:VAL:CG1	1:B:316:GLY:N	2.59	0.64
1:A:310:PRO:O	1:A:384:PHE:HE1	1.80	0.64
1:A:457:LEU:HD23	1:A:500:LEU:HD13	1.78	0.64
1:B:430:THR:HG22	1:B:431:LEU:H	1.61	0.64
1:A:102:SER:OG	1:B:139:GLU:HG3	1.98	0.64
1:B:430:THR:CG2	1:B:431:LEU:N	2.61	0.64
1:A:230:ASN:ND2	1:A:232:ALA:H	1.96	0.63
1:A:69:ILE:HD12	1:A:303:ALA:CB	2.29	0.63
1:B:145:VAL:HG11	1:B:161:ILE:HD12	1.81	0.63
1:B:364:VAL:HG22	1:B:384:PHE:HE2	1.63	0.62
1:B:327:TRP:CD2	1:B:357:LEU:HD11	2.34	0.62
1:B:409:HIS:NE2	1:B:441:VAL:HG11	2.14	0.62
1:A:102:SER:OG	1:A:285:THR:HG21	1.99	0.61
1:B:56:VAL:HB	1:B:80:VAL:HG22	1.82	0.61
1:B:151:GLY:O	1:B:155:GLN:HG3	2.00	0.61
1:B:194:LEU:O	1:B:222:THR:HA	2.00	0.61
1:B:336:VAL:HG12	1:B:526:VAL:HG21	1.81	0.61
1:A:63:ALA:O	1:A:65:PRO:HD3	2.00	0.61
1:A:246:ILE:HG22	1:A:247:THR:N	2.15	0.61
1:B:207:THR:O	1:B:210:THR:HG22	2.01	0.61
1:A:461:TYR:HB2	1:A:518:VAL:HB	1.83	0.61
1:B:145:VAL:HG11	1:B:161:ILE:CD1	2.31	0.61
1:B:363:GLU:OE1	1:B:366:ARG:NH1	2.35	0.60
1:A:387:ALA:HB3	1:A:388:PRO:HD3	1.84	0.60
1:B:42:VAL:HG12	1:B:64:ALA:CB	2.24	0.60
1:A:333:LYS:HE2	1:A:438:GLN:OE1	2.01	0.59
1:A:271:GLU:OE1	1:A:271:GLU:HA	2.01	0.59
1:B:274:GLN:H	1:B:274:GLN:NE2	1.98	0.59
1:B:35:ARG:O	1:B:39:LEU:HD13	2.02	0.59
1:B:354:ARG:HD2	4:B:836:HOH:O	2.01	0.59
1:A:49:LEU:HD21	1:A:300:VAL:HG21	1.85	0.59
1:A:386:ASN:HB3	1:A:389:ALA:HB3	1.85	0.59
1:A:125:LEU:HD12	1:B:277:VAL:HG23	1.84	0.59
1:A:207:THR:O	1:A:210:THR:N	2.24	0.58
1:A:459:ILE:HG12	1:A:523:LEU:HD22	1.84	0.58
1:B:31:ASP:OD1	1:B:33:PRO:HG2	2.03	0.58
1:B:457:LEU:HB3	1:B:502:LEU:HD21	1.85	0.58
1:A:56:VAL:HG13	1:A:80:VAL:HG13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:VAL:HG12	1:A:51:ARG:N	2.18	0.58
1:B:84:ALA:O	1:B:87:ALA:HB3	2.03	0.58
1:A:332:ARG:NH2	1:A:332:ARG:CG	2.60	0.58
1:A:324:VAL:CG2	1:A:360:GLU:HB3	2.34	0.57
1:B:310:PRO:HD2	4:B:811:HOH:O	2.02	0.57
1:B:269:LEU:HD12	1:B:272:LEU:HD12	1.87	0.57
1:A:116:ARG:NH1	1:B:102:SER:O	2.38	0.57
1:A:214:ILE:HB	1:A:237:VAL:HG22	1.87	0.57
1:A:206:LYS:N	4:A:832:HOH:O	2.25	0.57
1:B:122:ASP:O	1:B:126:ARG:HG2	2.04	0.57
1:B:190:LEU:O	1:B:194:LEU:HD22	2.04	0.57
1:A:35:ARG:HH22	1:A:60:VAL:HG23	1.70	0.56
1:B:243:ALA:HB2	1:B:269:LEU:CD1	2.35	0.56
1:A:204:LEU:HB2	1:A:236:LEU:HD13	1.88	0.56
1:B:193:LEU:C	1:B:193:LEU:HD23	2.31	0.56
1:A:259:PHE:HB2	1:A:262:GLU:HG2	1.88	0.55
1:A:370:LEU:HD21	1:A:398:ALA:HB2	1.88	0.55
1:A:332:ARG:HH21	1:A:332:ARG:CG	2.00	0.55
1:B:457:LEU:HD11	1:B:459:ILE:CD1	2.37	0.55
1:A:207:THR:OG1	1:A:209:GLU:HB2	2.07	0.55
1:B:145:VAL:HG21	1:B:161:ILE:HG21	1.88	0.54
1:A:206:LYS:HB3	4:A:832:HOH:O	2.06	0.54
1:A:56:VAL:CG1	1:A:80:VAL:HG22	2.38	0.54
1:A:50:VAL:HG13	1:A:54:THR:HB	1.89	0.54
1:B:343:ASP:OD1	1:B:343:ASP:N	2.34	0.54
1:A:42:VAL:N	1:A:43:PRO:CD	2.70	0.54
1:A:152:ARG:NH2	1:A:152:ARG:HG3	2.22	0.54
1:B:111:LEU:C	1:B:111:LEU:HD23	2.33	0.54
1:A:459:ILE:HB	1:A:498:ILE:CG2	2.37	0.54
1:A:523:LEU:CD1	1:A:523:LEU:C	2.81	0.54
1:B:201:SER:OG	1:B:203:HIS:CE1	2.60	0.54
1:B:25:VAL:CG1	1:B:26:GLU:N	2.70	0.53
1:B:487:LEU:HB3	1:B:498:ILE:HG13	1.90	0.53
1:A:313:VAL:HG13	1:A:382:VAL:HA	1.89	0.53
1:B:243:ALA:HB2	1:B:269:LEU:HD13	1.90	0.53
1:A:69:ILE:CD1	1:A:303:ALA:HB3	2.33	0.53
1:B:450:LEU:HD13	1:B:499:LEU:HD22	1.90	0.53
1:A:113:ALA:HA	1:A:118:ILE:HG13	1.89	0.53
1:A:442:GLN:HA	1:A:446:ARG:O	2.09	0.53
1:A:150:LEU:HD22	1:A:155:GLN:HG2	1.92	0.52
1:B:510:VAL:O	1:B:514:ILE:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:VAL:O	1:A:312:ALA:HB2	2.10	0.52
1:A:151:GLY:O	1:A:155:GLN:HG3	2.10	0.52
1:B:94:ASN:HD22	1:B:94:ASN:H	1.58	0.52
1:B:118:ILE:HB	1:B:119:PRO:CD	2.36	0.52
1:A:350:SER:HB3	1:A:416:ARG:HB2	1.91	0.52
1:B:334:LEU:HD22	1:B:427:VAL:HG12	1.92	0.52
1:B:203:HIS:HA	1:B:232:ALA:HB2	1.91	0.51
1:B:91:LEU:HD12	1:B:91:LEU:N	2.26	0.51
1:A:331:VAL:HG22	1:A:413:VAL:HG11	1.93	0.51
1:B:502:LEU:HD13	1:B:502:LEU:N	2.25	0.51
1:A:14:ALA:O	1:A:17:THR:HB	2.11	0.51
1:A:487:LEU:HA	1:A:497:THR:O	2.10	0.51
1:B:345:LEU:HD12	1:B:346:PRO:HD2	1.88	0.51
1:A:24:GLN:HA	1:A:24:GLN:NE2	2.25	0.50
1:A:222:THR:HB	4:A:818:HOH:O	2.10	0.50
1:A:312:ALA:O	1:A:384:PHE:CD1	2.63	0.50
1:A:152:ARG:HG3	1:A:152:ARG:HH21	1.74	0.50
1:A:82:VAL:HG21	1:A:381:ALA:HB1	1.94	0.50
1:B:23:ASP:CB	1:B:24:GLN:HE21	2.24	0.50
1:A:259:PHE:O	1:A:260:ALA:C	2.55	0.50
1:A:317:GLY:C	1:A:319:VAL:H	2.20	0.50
1:A:448:PHE:CD1	1:A:486:GLN:CD	2.90	0.50
1:A:467:ALA:HB1	1:A:518:VAL:HG12	1.93	0.49
1:A:487:LEU:HB3	1:A:498:ILE:HD12	1.94	0.49
1:B:262:GLU:HA	1:B:263:PRO:C	2.36	0.49
1:A:93:VAL:HG23	1:A:312:ALA:HA	1.95	0.49
1:A:135:PHE:HB2	1:B:281:LEU:HD21	1.95	0.49
1:B:328:LEU:HD21	1:B:364:VAL:HG13	1.93	0.49
1:A:50:VAL:CG1	1:A:54:THR:HB	2.42	0.49
1:B:228:ILE:O	1:B:254:ALA:HA	2.13	0.49
1:B:267:SER:OG	1:B:269:LEU:HB2	2.13	0.49
1:B:487:LEU:C	1:B:487:LEU:HD22	2.37	0.49
1:B:285:THR:HG22	1:B:285:THR:O	2.11	0.48
1:A:275:VAL:HG12	1:A:277:VAL:HG13	1.94	0.48
1:A:367:LEU:HD13	1:A:384:PHE:CD2	2.48	0.48
1:B:362:VAL:CG2	1:B:402:LYS:HD3	2.42	0.48
1:B:321:ASN:HB3	1:B:324:VAL:HG23	1.95	0.48
1:A:354:ARG:NH2	1:A:414:ASP:OD1	2.47	0.48
1:A:492:GLU:OE2	1:A:492:GLU:HA	2.12	0.48
1:A:324:VAL:HG21	1:A:360:GLU:HB3	1.96	0.48
1:A:50:VAL:CG1	1:A:51:ARG:N	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:LYS:NZ	1:A:449:ASP:OD1	2.43	0.48
1:B:334:LEU:CB	1:B:415:VAL:HG21	2.43	0.48
1:B:336:VAL:CG1	1:B:526:VAL:HG21	2.44	0.47
1:B:11:ASP:OD1	1:B:54:THR:HG23	2.14	0.47
1:B:298:GLU:HA	1:B:298:GLU:OE2	2.14	0.47
1:B:456:ASN:ND2	1:B:528:LEU:HD23	2.29	0.47
1:B:94:ASN:O	1:B:96:PRO:HD3	2.14	0.47
1:B:463:ASP:C	1:B:463:ASP:OD2	2.57	0.47
1:B:487:LEU:HD22	1:B:488:SER:N	2.30	0.47
1:A:362:VAL:HB	1:A:365:LEU:HD12	1.97	0.47
1:A:461:TYR:CD1	1:A:461:TYR:N	2.80	0.47
1:A:510:VAL:O	1:A:511:ARG:C	2.57	0.47
1:B:275:VAL:HG12	1:B:277:VAL:HG13	1.97	0.47
1:B:421:ASP:OD1	1:B:421:ASP:N	2.47	0.47
1:B:207:THR:O	1:B:207:THR:HG22	2.14	0.47
1:B:377:VAL:HG12	1:B:378:ILE:HG13	1.97	0.47
1:A:384:PHE:O	1:A:385:VAL:HG13	2.15	0.46
1:A:273:ALA:C	1:A:275:VAL:H	2.23	0.46
1:A:487:LEU:C	1:A:487:LEU:HD12	2.39	0.46
1:B:523:LEU:O	1:B:524:GLU:HG2	2.15	0.46
1:A:345:LEU:HD22	1:A:346:PRO:HD2	1.97	0.46
1:A:38:LEU:O	1:A:42:VAL:HG13	2.14	0.46
1:B:304:LEU:C	1:B:306:GLY:H	2.23	0.46
1:B:363:GLU:CD	1:B:366:ARG:NH1	2.74	0.46
1:B:511:ARG:NH2	1:B:525:VAL:CB	2.69	0.46
1:B:226:VAL:HG11	4:B:803:HOH:O	2.15	0.46
1:B:527:ASP:OD2	1:B:527:ASP:C	2.58	0.46
1:A:192:ASP:O	1:A:196:ARG:HB2	2.15	0.46
1:A:262:GLU:HA	1:A:263:PRO:C	2.41	0.46
1:A:400:ILE:HG22	1:A:401:CYS:N	2.32	0.45
1:B:285:THR:O	1:B:286:ALA:C	2.59	0.45
1:A:366:ARG:HB2	1:A:400:ILE:HG12	1.97	0.45
1:B:155:GLN:HB3	1:B:183:LEU:HD13	1.98	0.45
1:A:354:ARG:HG2	1:A:403:ALA:HB3	1.98	0.45
1:B:330:LEU:HD23	1:B:438:GLN:HB3	1.99	0.45
1:B:445:GLY:O	1:B:446:ARG:HD2	2.17	0.45
1:B:32:GLY:HA3	1:B:54:THR:CG2	2.47	0.45
1:A:230:ASN:HD22	1:A:232:ALA:H	1.65	0.45
1:A:318:GLY:C	1:A:320:VAL:H	2.23	0.45
1:B:459:ILE:HB	1:B:498:ILE:HG22	1.99	0.45
1:B:460:HIS:O	1:B:521:TYR:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:HIS:HD2	1:A:497:THR:CG2	2.28	0.45
1:B:483:GLN:OE1	1:B:501:ARG:HG2	2.17	0.45
1:A:446:ARG:HH21	1:A:491:ALA:H	1.64	0.45
1:A:32:GLY:HA3	1:A:54:THR:OG1	2.17	0.45
1:A:156:LEU:O	1:A:160:ARG:HD2	2.17	0.45
1:A:210:THR:O	1:A:211:ALA:C	2.60	0.45
1:B:209:GLU:OE2	1:B:209:GLU:CA	2.64	0.45
1:B:266:ASP:O	1:B:267:SER:C	2.57	0.45
1:A:122:ASP:OD1	1:A:126:ARG:NH2	2.50	0.44
1:A:246:ILE:CD1	1:A:251:VAL:CG2	2.89	0.44
1:B:8:LEU:C	1:B:8:LEU:HD22	2.42	0.44
1:A:322:GLU:O	1:A:326:PRO:HD3	2.17	0.44
1:B:487:LEU:CB	1:B:498:ILE:HG13	2.47	0.44
1:B:334:LEU:HB3	1:B:415:VAL:HG23	1.99	0.44
1:A:312:ALA:O	1:A:384:PHE:HD1	2.00	0.44
1:B:108:LEU:HD11	1:B:161:ILE:HG12	1.98	0.44
1:B:326:PRO:HB2	1:B:431:LEU:CD1	2.47	0.44
1:B:339:GLY:C	1:B:341:LEU:N	2.75	0.44
1:B:353:VAL:HG21	1:B:362:VAL:HG21	1.99	0.44
1:B:269:LEU:HD12	1:B:269:LEU:HA	1.84	0.44
1:B:475:LEU:HD13	1:B:475:LEU:HA	1.74	0.44
1:A:254:ALA:HB3	1:A:275:VAL:HG22	2.00	0.44
1:A:290:ASP:O	1:A:294:THR:HG23	2.17	0.44
1:B:330:LEU:HD11	1:B:429:GLY:HA3	1.99	0.44
1:B:337:LEU:HB3	1:B:427:VAL:HG21	1.99	0.44
1:B:467:ALA:HA	1:B:518:VAL:HG12	1.99	0.44
1:A:461:TYR:CB	1:A:518:VAL:HB	2.48	0.44
1:B:57:ASP:OD2	1:B:60:VAL:HG23	2.18	0.44
1:B:235:GLY:C	1:B:237:VAL:N	2.74	0.44
1:A:214:ILE:CB	1:A:237:VAL:HG22	2.47	0.43
1:A:450:LEU:HD12	1:A:499:LEU:HD22	2.00	0.43
1:A:459:ILE:HB	1:A:498:ILE:HG22	1.99	0.43
1:B:523:LEU:C	1:B:524:GLU:HG2	2.43	0.43
1:A:315:VAL:HG11	1:A:320:VAL:HG11	2.00	0.43
1:B:11:ASP:OD1	1:B:53:ALA:HB3	2.18	0.43
1:B:255:GLY:HA2	1:B:276:VAL:O	2.17	0.43
1:A:145:VAL:HG21	1:A:161:ILE:HG12	1.99	0.43
1:B:440:ILE:HG13	1:B:452:ALA:HB2	2.00	0.43
1:B:161:ILE:HG21	1:B:161:ILE:HD13	1.65	0.43
1:B:463:ASP:H	1:B:495:GLY:HA2	1.83	0.43
1:A:275:VAL:HG12	1:A:275:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:LEU:HD23	1:B:4:LEU:HA	1.82	0.43
1:B:463:ASP:HB2	1:B:496:ALA:HB2	2.01	0.43
1:A:127:GLU:O	1:A:128:HIS:HB2	2.19	0.43
1:A:82:VAL:O	1:A:83:ASP:C	2.59	0.43
1:B:511:ARG:HH22	1:B:525:VAL:HB	1.74	0.43
1:A:500:LEU:HD12	1:A:500:LEU:N	2.34	0.42
1:A:11:ASP:OD1	1:A:50:VAL:HG13	2.19	0.42
1:A:122:ASP:OD1	1:A:122:ASP:C	2.63	0.42
1:A:174:TYR:O	1:A:394:ARG:HD3	2.19	0.42
1:A:309:VAL:O	1:A:312:ALA:CB	2.67	0.42
1:A:471:ILE:HD11	1:A:518:VAL:HG11	2.00	0.42
1:A:480:VAL:HG22	1:A:504:GLN:CD	2.44	0.42
1:B:430:THR:CG2	1:B:431:LEU:H	2.28	0.42
1:B:483:GLN:OE1	1:B:501:ARG:NE	2.52	0.42
1:B:345:LEU:CD1	1:B:346:PRO:CD	2.87	0.42
1:B:523:LEU:HD23	1:B:524:GLU:N	2.33	0.42
1:A:119:PRO:HB3	1:B:119:PRO:HA	2.01	0.42
1:A:317:GLY:O	1:A:319:VAL:N	2.53	0.42
1:A:328:LEU:HD12	1:A:365:LEU:HD23	2.02	0.42
1:B:285:THR:HG22	1:B:287:GLU:N	2.35	0.42
1:A:183:LEU:HB3	1:A:185:ILE:HD12	2.01	0.42
1:B:32:GLY:HA3	1:B:54:THR:HG22	2.01	0.42
1:B:32:GLY:N	1:B:33:PRO:HD2	2.35	0.42
1:B:457:LEU:HD11	1:B:459:ILE:HG12	2.01	0.42
1:A:126:ARG:NH1	1:B:275:VAL:O	2.43	0.42
1:A:127:GLU:O	1:A:128:HIS:CB	2.68	0.42
1:A:382:VAL:HG12	1:A:384:PHE:O	2.20	0.42
1:A:121:ALA:HB1	1:B:279:PRO:HD3	2.02	0.41
1:B:72:ARG:HD2	1:B:76:GLY:O	2.20	0.41
1:B:523:LEU:O	1:B:524:GLU:CG	2.67	0.41
1:A:67:LEU:HA	1:A:67:LEU:HD23	1.84	0.41
1:A:230:ASN:ND2	1:A:230:ASN:C	2.76	0.41
1:A:515:ALA:O	1:A:520:ALA:N	2.50	0.41
1:B:261:THR:O	1:B:264:CYS:HB2	2.20	0.41
1:B:285:THR:HG23	1:B:287:GLU:OE1	2.20	0.41
1:A:486:GLN:O	1:A:498:ILE:HA	2.20	0.41
1:B:292:ALA:O	1:B:296:VAL:HG22	2.20	0.41
1:A:281:LEU:O	1:A:282:GLY:C	2.64	0.41
1:B:28:ARG:NH1	1:B:44:GLU:OE2	2.53	0.41
1:B:313:VAL:O	1:B:313:VAL:CG1	2.68	0.41
1:A:214:ILE:CG1	1:A:237:VAL:HG22	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:LEU:HA	1:B:67:LEU:HD12	1.89	0.41
1:A:125:LEU:HD12	1:B:277:VAL:CG2	2.50	0.41
1:A:390:LEU:HA	1:A:390:LEU:HD12	1.87	0.41
1:A:462:VAL:HG13	1:A:521:TYR:OH	2.21	0.41
1:B:25:VAL:HG12	1:B:26:GLU:N	2.35	0.41
1:A:206:LYS:HA	1:A:210:THR:HG21	2.02	0.41
1:A:355:GLY:HA3	1:A:410:ARG:O	2.20	0.41
1:B:378:ILE:HD11	1:B:394:ARG:HD3	2.02	0.41
1:A:49:LEU:N	1:A:49:LEU:HD23	2.35	0.41
1:A:115:SER:O	1:A:137:GLY:HA2	2.21	0.41
1:B:239:GLU:OE1	1:B:259:PHE:HA	2.21	0.41
1:B:450:LEU:CD1	1:B:499:LEU:HD22	2.51	0.41
1:A:152:ARG:HH21	1:A:152:ARG:CG	2.31	0.41
1:B:93:VAL:HG22	1:B:311:ASP:C	2.46	0.41
1:B:246:ILE:HG22	1:B:247:THR:N	2.34	0.41
1:B:328:LEU:HA	1:B:328:LEU:HD23	1.74	0.41
1:A:366:ARG:HD2	1:A:398:ALA:O	2.20	0.40
1:B:49:LEU:HD22	1:B:71:ALA:HB3	2.03	0.40
1:B:334:LEU:CD2	1:B:427:VAL:HG12	2.51	0.40
1:B:464:ARG:HH22	1:B:519:ASP:CG	2.29	0.40
1:A:318:GLY:C	1:A:320:VAL:N	2.79	0.40
1:B:387:ALA:HB3	1:B:388:PRO:HD3	2.04	0.40
1:A:174:TYR:O	1:A:394:ARG:CD	2.69	0.40
1:B:157:VAL:O	1:B:158:ALA:C	2.63	0.40
1:A:207:THR:O	1:A:208:PRO:C	2.64	0.40
1:A:462:VAL:HG23	1:A:518:VAL:O	2.22	0.40
1:B:224:PRO:HG3	1:B:250:HIS:CE1	2.56	0.40
1:B:351:VAL:O	1:B:400:ILE:HA	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	524/529 (99%)	471 (90%)	47 (9%)	6 (1%)	11	29
1	B	519/529 (98%)	466 (90%)	50 (10%)	3 (1%)	21	44
All	All	1043/1058 (99%)	937 (90%)	97 (9%)	9 (1%)	14	35

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	GLU
1	A	491	ALA
1	A	12	LYS
1	A	22	GLY
1	A	128	HIS
1	B	234	GLY
1	B	316	GLY
1	B	452	ALA
1	A	318	GLY

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	396/399 (99%)	339 (86%)	57 (14%)	3	8
1	B	394/399 (99%)	341 (86%)	53 (14%)	4	9
All	All	790/798 (99%)	680 (86%)	110 (14%)	3	9

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	12	LYS
1	A	13	LEU
1	A	21	LEU
1	A	24	GLN
1	A	28	ARG
1	A	39	LEU

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Mol	Chain	Res	Type
1	A	49	LEU
1	A	56	VAL
1	A	57	ASP
1	A	67	LEU
1	A	69	ILE
1	A	72	ARG
1	A	90	VAL
1	A	93	VAL
1	A	102	SER
1	A	108	LEU
1	A	110	LEU
1	A	118	ILE
1	A	133	SER
1	A	150	LEU
1	A	194	LEU
1	A	202	VAL
1	A	210	THR
1	A	213	LEU
1	A	216	LYS
1	A	219	LEU
1	A	226	VAL
1	A	242	LEU
1	A	246	ILE
1	A	251	VAL
1	A	261	THR
1	A	269	LEU
1	A	285	THR
1	A	296	VAL
1	A	328	LEU
1	A	333	LYS
1	A	337	LEU
1	A	347	VAL
1	A	384	PHE
1	A	385	VAL
1	A	418	VAL
1	A	430	THR
1	A	436	LEU
1	A	437	SER
1	A	442	GLN
1	A	462	VAL
1	A	475	LEU
1	A	489	GLU

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Mol	Chain	Res	Type
1	A	497	THR
1	A	499	LEU
1	A	508	ASP
1	A	514	ILE
1	A	518	VAL
1	A	523	LEU
1	A	524	GLU
1	A	529	SER
1	B	4	LEU
1	B	8	LEU
1	B	18	VAL
1	B	21	LEU
1	B	25	VAL
1	B	39	LEU
1	B	48	LEU
1	B	54	THR
1	B	61	LEU
1	B	88	ARG
1	B	94	ASN
1	B	99	ASN
1	B	125	LEU
1	B	129	THR
1	B	134	SER
1	B	160	ARG
1	B	188	LEU
1	B	194	LEU
1	B	209	GLU
1	B	210	THR
1	B	213	LEU
1	B	219	LEU
1	B	226	VAL
1	B	233	ARG
1	B	269	LEU
1	B	274	GLN
1	B	285	THR
1	B	299	SER
1	B	315	VAL
1	B	322	GLU
1	B	330	LEU
1	B	337	LEU
1	B	343	ASP
1	B	354	ARG

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Mol	Chain	Res	Type
1	B	363	GLU
1	B	370	LEU
1	B	371	ARG
1	B	373	LEU
1	B	383	THR
1	B	384	PHE
1	B	386	ASN
1	B	410	ARG
1	B	442	GLN
1	B	443	ILE
1	B	453	GLN
1	B	457	LEU
1	B	475	LEU
1	B	477	THR
1	B	487	LEU
1	B	499	LEU
1	B	502	LEU
1	B	509	ASP
1	B	528	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	230	ASN
1	A	409	HIS
1	A	435	GLN
1	A	504	GLN
1	B	24	GLN
1	B	94	ASN
1	B	99	ASN
1	B	128	HIS
1	B	203	HIS
1	B	274	GLN
1	B	321	ASN
1	B	352	GLN
1	B	456	ASN

5.3.3 RNA

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TLA	B	700	-	9,9,9	0.83	0	12,12,12	1.35	3 (25%)
2	SER	A	600	-	4,6,6	1.03	0	2,7,7	2.23	1 (50%)
2	SER	B	600	-	4,6,6	1.05	0	2,7,7	2.47	1 (50%)
3	TLA	A	700	-	9,9,9	0.83	0	12,12,12	1.56	3 (25%)
3	TLA	B	701	-	9,9,9	0.74	0	12,12,12	1.17	1 (8%)

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
3	TLA	B	700	-	-	0/12/12/12	-
2	SER	A	600	-	-	1/6/6/6	-
2	SER	B	600	-	-	0/6/6/6	-
3	TLA	A	700	-	-	4/12/12/12	-
3	TLA	B	701	-	-	7/12/12/12	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	SER	OXT-C-O	-3.33	116.52	124.08
2	A	600	SER	OXT-C-O	-3.12	117.00	124.08
3	A	700	TLA	O41-C4-C3	3.10	121.92	113.31
3	A	700	TLA	O41-C4-O4	-2.40	118.62	124.08
3	A	700	TLA	O11-C1-C2	2.34	119.80	113.31
3	B	700	TLA	O41-C4-O4	-2.31	118.85	124.08
3	B	700	TLA	O2-C2-C1	-2.19	106.00	110.69
3	B	701	TLA	O41-C4-C3	2.18	119.38	113.31
3	B	700	TLA	O41-C4-C3	2.10	119.16	113.31

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	700	TLA	C2-C3-C4-O41
3	B	701	TLA	C2-C3-C4-O4
3	B	701	TLA	C2-C3-C4-O41
3	B	701	TLA	O3-C3-C4-O4
3	B	701	TLA	O3-C3-C4-O41
3	A	700	TLA	C2-C3-C4-O4
3	A	700	TLA	O3-C3-C4-O4
3	B	701	TLA	O1-C1-C2-C3
3	A	700	TLA	O3-C3-C4-O41
3	B	701	TLA	O11-C1-C2-C3
3	B	701	TLA	O1-C1-C2-O2
2	A	600	SER	OXT-C-CA-N

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	526/529 (99%)	0.39	24 (4%) 37 34	46, 65, 83, 101	8 (1%)
1	B	523/529 (98%)	0.63	44 (8%) 17 14	16, 67, 81, 99	18 (3%)
All	All	1049/1058 (99%)	0.51	68 (6%) 25 22	16, 66, 82, 101	26 (2%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	395	GLY	10.8
1	B	396	VAL	8.2
1	B	394	ARG	7.9
1	B	385	VAL	5.6
1	B	384	PHE	5.0
1	B	383	THR	4.9
1	A	125	LEU	4.2
1	B	482	ILE	3.8
1	B	436	LEU	3.5
1	B	374	PHE	3.5
1	B	526	VAL	3.4
1	A	123	ALA	3.3
1	A	308	PHE	3.3
1	A	263	PRO	3.3
1	B	379	GLU	3.3
1	A	162	ALA	3.3
1	B	435	GLN	3.3
1	B	458	ILE	3.3
1	B	388	PRO	3.0
1	B	319	VAL	3.0
1	B	90	VAL	3.0
1	B	370	LEU	2.9
1	B	391	ALA	2.9
1	B	481	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	62	ALA	2.8
1	B	212	GLY	2.7
1	B	377	VAL	2.6
1	B	452	ALA	2.6
1	A	104	ALA	2.6
1	B	58	ALA	2.6
1	B	210	THR	2.6
1	B	308	PHE	2.5
1	B	338	ALA	2.5
1	B	459	ILE	2.5
1	A	290	ASP	2.5
1	A	319	VAL	2.5
1	B	307	GLU	2.4
1	A	318	GLY	2.4
1	B	213	LEU	2.4
1	A	124	SER	2.4
1	B	21	LEU	2.4
1	B	240	ALA	2.4
1	A	183	LEU	2.3
1	A	182	GLN	2.3
1	A	129	THR	2.3
1	A	175	VAL	2.3
1	A	240	ALA	2.3
1	A	192	ASP	2.3
1	A	170	ALA	2.2
1	B	163	ALA	2.2
1	A	492	GLU	2.2
1	B	326	PRO	2.2
1	A	491	ALA	2.2
1	A	514	ILE	2.2
1	B	100	ILE	2.2
1	B	389	ALA	2.2
1	A	268	PRO	2.2
1	A	510	VAL	2.2
1	B	94	ASN	2.2
1	B	525	VAL	2.2
1	A	270	PHE	2.2
1	B	41	ALA	2.2
1	B	34	ASP	2.2
1	B	63	ALA	2.1
1	B	209	GLU	2.1
1	A	409	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	19	ALA	2.0
1	B	16	SER	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 oligosaccharides 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	TLA	B	701	10/10	0.78	0.18	63,79,81,81	10
3	TLA	A	700	10/10	0.79	0.11	82,94,101,102	0
3	TLA	B	700	10/10	0.79	0.14	81,93,100,100	0
2	SER	A	600	7/7	0.79	0.25	80,80,84,85	0
2	SER	B	600	7/7	0.90	0.19	72,82,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.