



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:34 AM UTC

PDB ID : 3T05 / pdb_00003t05
Title : Crystal structure of S. aureus Pyruvate Kinase
Authors : Worrall, L.J.; Vuckovic, M.; Strynadka, N.C.J.
Deposited on : 2011-07-19
Resolution : 3.05 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

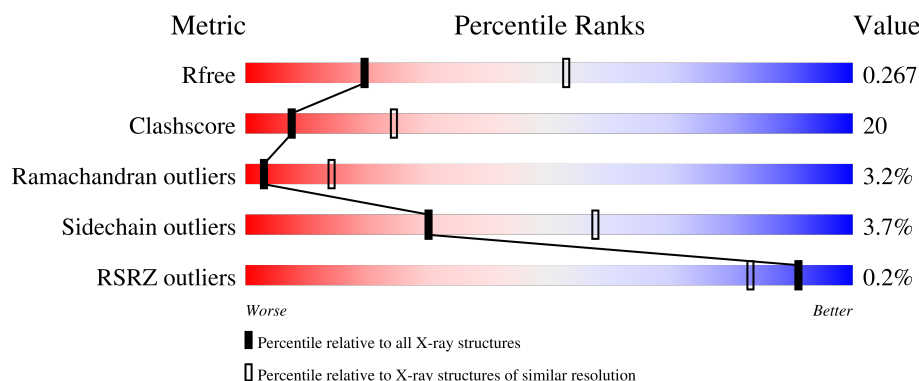
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	606	60% 32% 5% .
1	B	606	59% 33% . .
1	C	606	60% 32% . .
1	D	606	62% 30% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	B	586	-	-	X	-
2	PO4	C	586	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17648 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 Pyruvate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	583	Total	C	N	O	S	0	0	0
			4407	2745	764	880	18			
1	B	583	Total	C	N	O	S	0	0	0
			4407	2745	764	880	18			
1	C	583	Total	C	N	O	S	0	0	0
			4407	2745	764	880	18			
1	D	583	Total	C	N	O	S	0	0	0
			4407	2745	764	880	18			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q6GG09
A	-19	GLY	-	expression tag	UNP Q6GG09
A	-18	SER	-	expression tag	UNP Q6GG09
A	-17	SER	-	expression tag	UNP Q6GG09
A	-16	HIS	-	expression tag	UNP Q6GG09
A	-15	HIS	-	expression tag	UNP Q6GG09
A	-14	HIS	-	expression tag	UNP Q6GG09
A	-13	HIS	-	expression tag	UNP Q6GG09
A	-12	HIS	-	expression tag	UNP Q6GG09
A	-11	HIS	-	expression tag	UNP Q6GG09
A	-10	SER	-	expression tag	UNP Q6GG09
A	-9	SER	-	expression tag	UNP Q6GG09
A	-8	GLY	-	expression tag	UNP Q6GG09
A	-7	LEU	-	expression tag	UNP Q6GG09
A	-6	VAL	-	expression tag	UNP Q6GG09
A	-5	PRO	-	expression tag	UNP Q6GG09
A	-4	ARG	-	expression tag	UNP Q6GG09
A	-3	GLY	-	expression tag	UNP Q6GG09
A	-2	SER	-	expression tag	UNP Q6GG09
A	-1	HIS	-	expression tag	UNP Q6GG09
A	0	MET	-	expression tag	UNP Q6GG09

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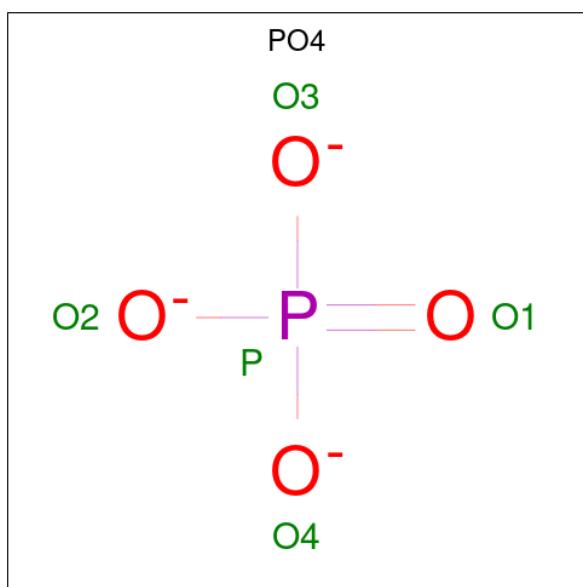
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	expression tag	UNP Q6GG09
B	-19	GLY	-	expression tag	UNP Q6GG09
B	-18	SER	-	expression tag	UNP Q6GG09
B	-17	SER	-	expression tag	UNP Q6GG09
B	-16	HIS	-	expression tag	UNP Q6GG09
B	-15	HIS	-	expression tag	UNP Q6GG09
B	-14	HIS	-	expression tag	UNP Q6GG09
B	-13	HIS	-	expression tag	UNP Q6GG09
B	-12	HIS	-	expression tag	UNP Q6GG09
B	-11	HIS	-	expression tag	UNP Q6GG09
B	-10	SER	-	expression tag	UNP Q6GG09
B	-9	SER	-	expression tag	UNP Q6GG09
B	-8	GLY	-	expression tag	UNP Q6GG09
B	-7	LEU	-	expression tag	UNP Q6GG09
B	-6	VAL	-	expression tag	UNP Q6GG09
B	-5	PRO	-	expression tag	UNP Q6GG09
B	-4	ARG	-	expression tag	UNP Q6GG09
B	-3	GLY	-	expression tag	UNP Q6GG09
B	-2	SER	-	expression tag	UNP Q6GG09
B	-1	HIS	-	expression tag	UNP Q6GG09
B	0	MET	-	expression tag	UNP Q6GG09
C	-20	MET	-	expression tag	UNP Q6GG09
C	-19	GLY	-	expression tag	UNP Q6GG09
C	-18	SER	-	expression tag	UNP Q6GG09
C	-17	SER	-	expression tag	UNP Q6GG09
C	-16	HIS	-	expression tag	UNP Q6GG09
C	-15	HIS	-	expression tag	UNP Q6GG09
C	-14	HIS	-	expression tag	UNP Q6GG09
C	-13	HIS	-	expression tag	UNP Q6GG09
C	-12	HIS	-	expression tag	UNP Q6GG09
C	-11	HIS	-	expression tag	UNP Q6GG09
C	-10	SER	-	expression tag	UNP Q6GG09
C	-9	SER	-	expression tag	UNP Q6GG09
C	-8	GLY	-	expression tag	UNP Q6GG09
C	-7	LEU	-	expression tag	UNP Q6GG09
C	-6	VAL	-	expression tag	UNP Q6GG09
C	-5	PRO	-	expression tag	UNP Q6GG09
C	-4	ARG	-	expression tag	UNP Q6GG09
C	-3	GLY	-	expression tag	UNP Q6GG09
C	-2	SER	-	expression tag	UNP Q6GG09
C	-1	HIS	-	expression tag	UNP Q6GG09
C	0	MET	-	expression tag	UNP Q6GG09

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	expression tag	UNP Q6GG09
D	-19	GLY	-	expression tag	UNP Q6GG09
D	-18	SER	-	expression tag	UNP Q6GG09
D	-17	SER	-	expression tag	UNP Q6GG09
D	-16	HIS	-	expression tag	UNP Q6GG09
D	-15	HIS	-	expression tag	UNP Q6GG09
D	-14	HIS	-	expression tag	UNP Q6GG09
D	-13	HIS	-	expression tag	UNP Q6GG09
D	-12	HIS	-	expression tag	UNP Q6GG09
D	-11	HIS	-	expression tag	UNP Q6GG09
D	-10	SER	-	expression tag	UNP Q6GG09
D	-9	SER	-	expression tag	UNP Q6GG09
D	-8	GLY	-	expression tag	UNP Q6GG09
D	-7	LEU	-	expression tag	UNP Q6GG09
D	-6	VAL	-	expression tag	UNP Q6GG09
D	-5	PRO	-	expression tag	UNP Q6GG09
D	-4	ARG	-	expression tag	UNP Q6GG09
D	-3	GLY	-	expression tag	UNP Q6GG09
D	-2	SER	-	expression tag	UNP Q6GG09
D	-1	HIS	-	expression tag	UNP Q6GG09
D	0	MET	-	expression tag	UNP Q6GG09

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		

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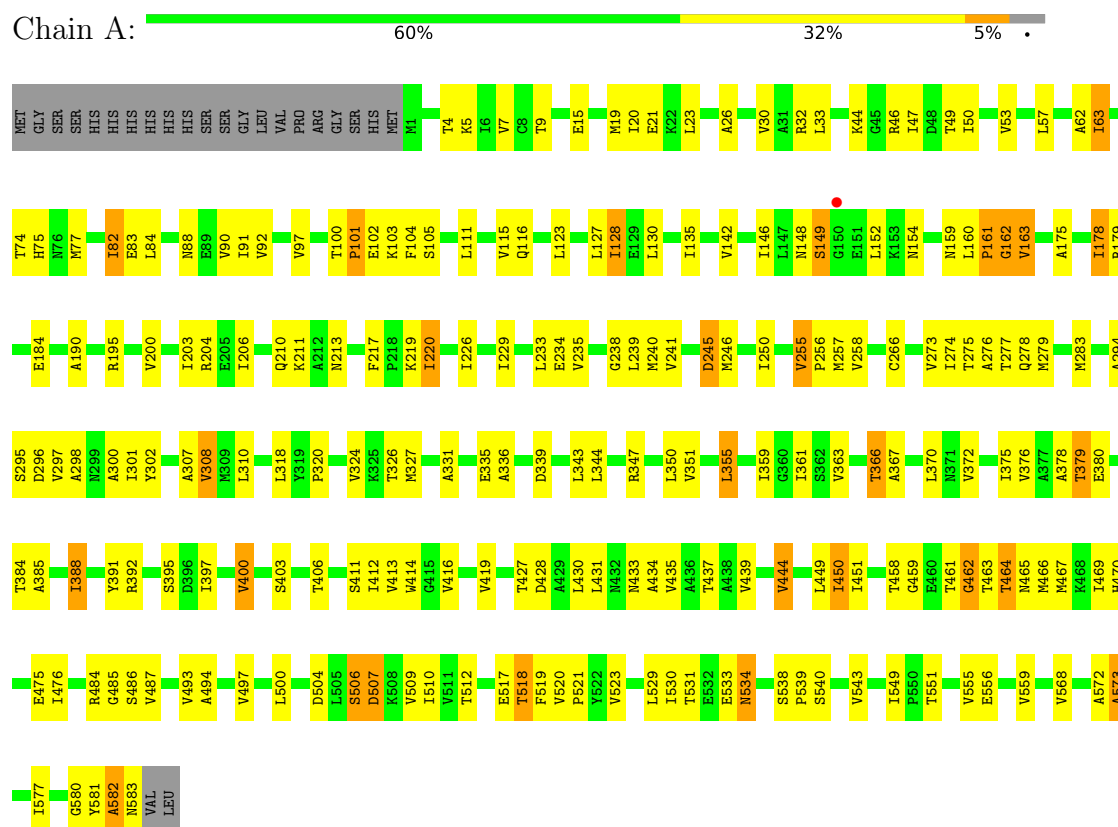
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

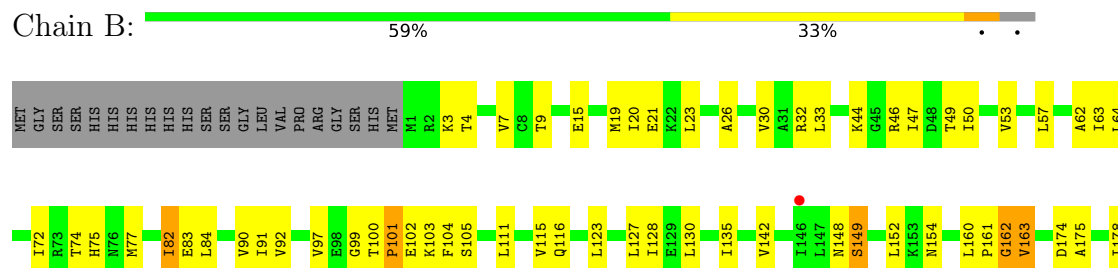
3 Residue-property plots

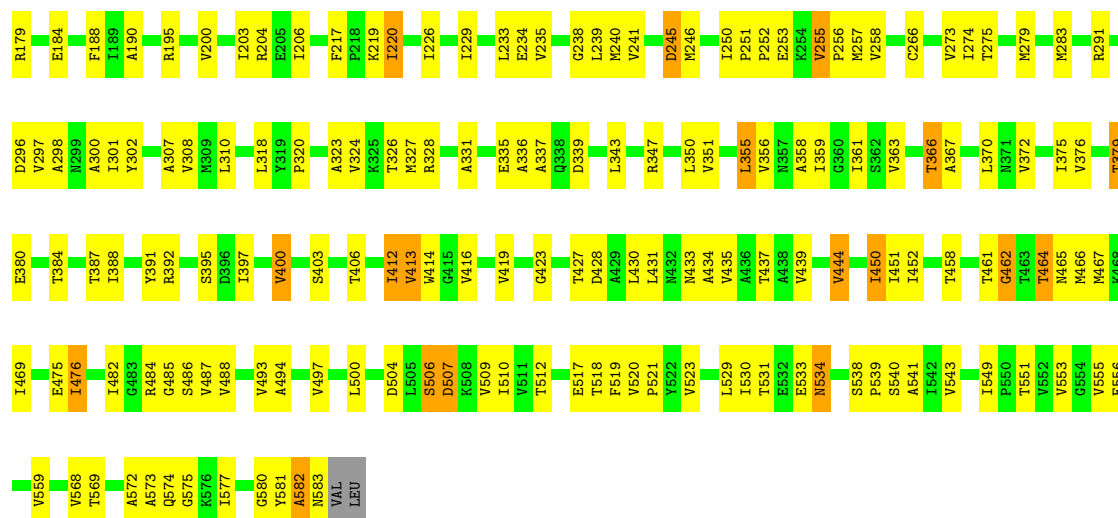
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Pyruvate kinase



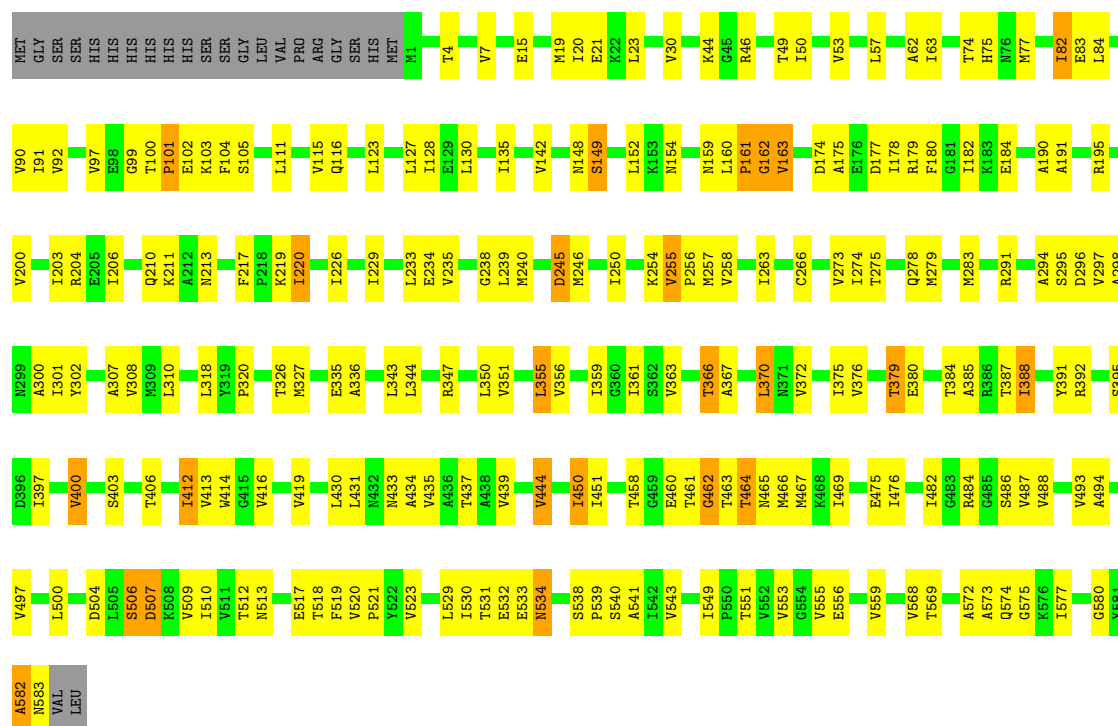
• Molecule 1: Pyruvate kinase





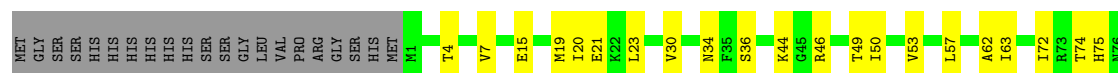
• Molecule 1: Pyruvate kinase

Chain C: 60% 32%



• Molecule 1: Pyruvate kinase

Chain D: 62% 30%



M77	I203	A307	V400	V497
I82	R204	V308	T401	L500
E83	E205	M309	P402	D504
L84	I206	L310	S403	L505
N88	Q210	L318	T406	S506
E89	K211	P319	T412	D507
V90	F217	P320	V413	R508
I91	P218	T326	V414	V509
V92	K219	M327	G415	I510
V97	I220	R328	V416	V511
T512	I226	A331	V419	T512
T100	I229	E335	V420	E517
P101	L233	A336	L430	T518
E102	E234	A337	N433	F519
K103	V235	Q338	A434	V520
F104	G238	D339	V435	P521
V115	L239	L343	A436	T522
Q116	W240	R347	T437	V523
L123	V241	L350	A438	I529
L127	D245	V351	V439	I530
I128	M246	L355	T441	T531
E129	I250	V356	V444	P532
L130	E253	I359	L449	E533
I135	V255	G360	T450	N534
V142	P256	I361	T451	S538
I146	M257	S362	A454	P539
L147	V258	V363	T458	S540
N148	C266	T366	T461	V543
S149	R152	A367	G462	I549
L152	N153	V372	T463	P550
K153	I274	I375	T464	T551
N154	T275	V376	I465	V555
L160	M279	A377	R466	E556
P161	M283	A378	R467	V559
G162	R291	T379	I469	V568
V163	A292	E380	H470	A573
D174	E293	T384	E475	A574
A175	A294	T387	I476	G575
I178	V297	Y391	I482	R576
R179	A298	R392	G483	I577
E184	N299	G396	R484	G580
A190	A300	S395	G485	Y581
A191	I301	D396	V493	A582
R195	Y302	I397	A494	N583
				VAL
				LEU

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	84.02Å 111.26Å 111.16Å 85.36° 80.15° 70.46°	Depositor
Resolution (Å)	19.90 – 3.05 19.90 – 3.05	Depositor EDS
% Data completeness (in resolution range)	97.6 (19.90-3.05) 97.5 (19.90-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 3.04Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.236 , 0.264 0.237 , 0.267	Depositor DCC
R_{free} test set	3539 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	95.4	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 79.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,-h+k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17648	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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: PO4

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	0.96	4/4452 (0.1%)	1.00	3/6022 (0.0%)
1	B	0.85	2/4452 (0.0%)	0.96	3/6022 (0.0%)
1	C	0.82	1/4452 (0.0%)	0.94	4/6022 (0.1%)
1	D	0.85	1/4452 (0.0%)	0.96	5/6022 (0.1%)
All	All	0.87	8/17808 (0.0%)	0.97	15/24088 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	388	ILE	CG1-CD1	7.75	1.81	1.51
1	C	388	ILE	CG1-CD1	7.59	1.81	1.51
1	B	413	VAL	CA-CB	-7.09	1.45	1.54
1	A	63	ILE	CA-CB	7.05	1.62	1.54
1	B	358	ALA	CA-CB	-5.63	1.44	1.53
1	D	273	VAL	CA-CB	-5.25	1.47	1.54
1	A	378	ALA	CA-CB	-5.01	1.46	1.53
1	A	178	ILE	CA-CB	5.01	1.60	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	255	VAL	CB-CA-C	-7.80	106.08	114.35
1	B	255	VAL	CB-CA-C	-7.62	106.27	114.35
1	A	255	VAL	CB-CA-C	-7.16	106.76	114.35
1	D	255	VAL	CB-CA-C	-6.84	107.10	114.35
1	D	307	ALA	N-CA-C	6.50	118.95	109.07
1	A	307	ALA	N-CA-C	5.73	117.78	109.07
1	B	307	ALA	N-CA-C	5.54	117.48	109.07
1	C	307	ALA	N-CA-C	5.50	117.43	109.07
1	B	72	ILE	CB-CA-C	-5.46	105.26	111.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	573	ALA	N-CA-C	-5.31	103.48	110.33
1	D	72	ILE	CB-CA-C	-5.25	105.50	111.59
1	A	573	ALA	N-CA-C	-5.24	103.96	110.41
1	D	239	LEU	N-CA-C	5.20	116.42	108.52
1	C	254	LYS	CA-C-N	5.15	123.49	120.24
1	C	254	LYS	C-N-CA	5.15	123.49	120.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4407	0	4533	195	0
1	B	4407	0	4533	194	1
1	C	4407	0	4533	193	1
1	D	4407	0	4533	183	0
2	A	5	0	0	1	0
2	B	5	0	0	2	0
2	C	5	0	0	2	0
2	D	5	0	0	1	0
All	All	17648	0	18132	721	1

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 20.

All (721) 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:A:388:ILE:CD1	1:A:388:ILE:CG1	1.82	1.53
1:C:388:ILE:CG1	1:C:388:ILE:CD1	1.81	1.51
1:B:257:MET:HE3	1:C:302:TYR:OH	1.30	1.22
1:B:379:THR:HG22	2:B:586:PO4:O4	1.40	1.18
1:A:302:TYR:OH	1:D:257:MET:HE3	1.45	1.15
1:A:467:MET:HE2	1:B:467:MET:HE2	1.43	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:467:MET:HE2	1:D:467:MET:HE2	1.47	0.95
1:D:379:THR:HG22	2:D:586:PO4:O2	1.66	0.95
1:D:4:THR:HG22	1:D:335:GLU:OE2	1.67	0.94
1:C:379:THR:HG22	2:C:586:PO4:O3	1.68	0.93
1:A:4:THR:HG22	1:A:335:GLU:OE2	1.67	0.93
1:A:275:THR:HG22	1:A:279:MET:HE1	1.50	0.91
1:D:275:THR:HG22	1:D:279:MET:HE1	1.50	0.91
1:A:363:VAL:HG22	1:A:451:ILE:HD11	1.53	0.91
1:B:257:MET:HE3	1:C:302:TYR:CZ	2.05	0.91
1:C:275:THR:HG22	1:C:279:MET:HE1	1.54	0.90
1:B:275:THR:HG22	1:B:279:MET:HE1	1.54	0.90
1:A:379:THR:HG22	2:A:586:PO4:O1	1.72	0.89
1:B:308:VAL:HG11	1:B:327:MET:SD	2.15	0.86
1:B:4:THR:HG22	1:B:335:GLU:OE2	1.75	0.86
1:A:302:TYR:CZ	1:D:257:MET:HE3	2.10	0.86
1:D:74:THR:HG22	1:D:75:HIS:O	1.75	0.86
1:C:363:VAL:HG22	1:C:451:ILE:HD11	1.57	0.86
1:A:74:THR:HG22	1:A:75:HIS:O	1.76	0.85
1:B:74:THR:HG22	1:B:75:HIS:O	1.75	0.85
1:C:74:THR:HG22	1:C:75:HIS:O	1.77	0.84
1:B:363:VAL:HG22	1:B:451:ILE:HD11	1.59	0.84
1:B:226:ILE:HD11	1:B:246:MET:HE3	1.60	0.83
1:A:123:LEU:HD11	1:A:130:LEU:HD11	1.59	0.83
1:B:531:THR:HG21	1:B:540:SER:HB3	1.61	0.82
1:D:226:ILE:HD11	1:D:246:MET:HE3	1.61	0.82
1:D:419:VAL:HG21	1:D:437:THR:HG21	1.60	0.82
1:A:92:VAL:HG23	1:A:142:VAL:HB	1.62	0.81
1:C:419:VAL:HG21	1:C:437:THR:HG21	1.60	0.81
1:A:419:VAL:HG21	1:A:437:THR:HG21	1.62	0.80
1:C:4:THR:HG22	1:C:335:GLU:OE2	1.81	0.80
1:C:531:THR:HG21	1:C:540:SER:HB3	1.62	0.79
1:B:419:VAL:HG21	1:B:437:THR:HG21	1.65	0.78
1:A:226:ILE:HD11	1:A:246:MET:HE3	1.65	0.78
1:A:531:THR:HG21	1:A:540:SER:HB3	1.67	0.77
1:B:92:VAL:HG23	1:B:142:VAL:HB	1.65	0.77
1:C:92:VAL:HG23	1:C:142:VAL:HB	1.65	0.77
1:D:510:ILE:HD11	1:D:523:VAL:HG22	1.66	0.77
1:D:92:VAL:HG23	1:D:142:VAL:HB	1.65	0.77
1:D:275:THR:HG22	1:D:279:MET:CE	2.14	0.77
1:D:363:VAL:HG22	1:D:451:ILE:HD11	1.67	0.77
1:C:308:VAL:HG11	1:C:327:MET:SD	2.25	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:LEU:HD11	1:B:130:LEU:HD11	1.68	0.76
1:D:123:LEU:HD11	1:D:130:LEU:HD11	1.68	0.76
1:D:308:VAL:HG11	1:D:327:MET:SD	2.25	0.76
1:D:379:THR:HG23	1:D:384:THR:HB	1.68	0.76
1:C:123:LEU:HD11	1:C:130:LEU:HD11	1.66	0.75
1:D:531:THR:HG21	1:D:540:SER:HB3	1.69	0.74
1:B:510:ILE:HD11	1:B:523:VAL:HG22	1.68	0.74
1:A:257:MET:HG2	1:D:337:ALA:HB1	1.67	0.74
1:C:226:ILE:HD11	1:C:246:MET:HE3	1.69	0.74
1:B:275:THR:HG22	1:B:279:MET:CE	2.18	0.74
1:C:510:ILE:HD11	1:C:523:VAL:HG22	1.68	0.74
1:A:19:MET:O	1:A:23:LEU:HD13	1.87	0.74
1:A:379:THR:HG23	1:A:384:THR:HB	1.68	0.73
1:B:379:THR:HG23	1:B:384:THR:HB	1.68	0.73
1:D:351:VAL:HG21	1:D:391:TYR:OH	1.89	0.72
1:A:510:ILE:HD11	1:A:523:VAL:HG22	1.72	0.71
1:A:275:THR:HG22	1:A:279:MET:CE	2.18	0.71
1:B:351:VAL:HG21	1:B:391:TYR:OH	1.91	0.71
1:A:367:ALA:HA	1:A:372:VAL:HG22	1.70	0.71
1:C:351:VAL:HG21	1:C:391:TYR:OH	1.91	0.70
1:A:308:VAL:HG11	1:A:327:MET:SD	2.33	0.69
1:D:84:LEU:HD23	1:D:90:VAL:HG21	1.74	0.69
1:D:274:ILE:HD11	1:D:412:ILE:HD11	1.74	0.69
1:C:84:LEU:HD23	1:C:90:VAL:HG21	1.74	0.69
1:C:419:VAL:HG21	1:C:437:THR:CG2	2.23	0.69
1:D:419:VAL:HG21	1:D:437:THR:CG2	2.22	0.69
1:B:257:MET:CE	1:C:302:TYR:OH	2.26	0.68
1:B:77:MET:HE2	1:B:152:LEU:HD23	1.73	0.68
1:A:430:LEU:C	1:A:430:LEU:HD23	2.19	0.68
1:D:19:MET:O	1:D:23:LEU:HD13	1.93	0.68
1:C:77:MET:HE2	1:C:152:LEU:HD23	1.76	0.68
1:B:84:LEU:HD23	1:B:90:VAL:HG21	1.76	0.68
1:A:308:VAL:CG1	1:A:327:MET:HE3	2.24	0.68
1:D:363:VAL:HG13	1:D:451:ILE:HD13	1.76	0.67
1:A:30:VAL:HG13	1:A:62:ALA:HB3	1.77	0.67
1:C:275:THR:HG22	1:C:279:MET:CE	2.25	0.67
1:B:257:MET:CE	1:C:302:TYR:CZ	2.77	0.66
1:B:275:THR:CG2	1:B:279:MET:HE1	2.25	0.66
1:C:219:LYS:O	1:C:220:ILE:C	2.39	0.66
1:D:275:THR:CG2	1:D:279:MET:HE1	2.22	0.66
1:A:363:VAL:HG13	1:A:451:ILE:HD13	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:MET:SD	1:C:326:THR:HG21	2.36	0.66
1:B:337:ALA:HB1	1:C:257:MET:HG2	1.79	0.65
1:A:77:MET:HE1	1:A:104:PHE:CD2	2.31	0.65
1:B:379:THR:CG2	2:B:586:PO4:O4	2.32	0.65
1:B:430:LEU:HD23	1:B:430:LEU:C	2.22	0.65
1:A:494:ALA:HB2	1:A:500:LEU:HD23	1.79	0.65
1:A:219:LYS:O	1:A:220:ILE:C	2.38	0.65
1:B:266:CYS:SG	1:B:273:VAL:CG2	2.85	0.64
1:C:7:VAL:HG22	1:C:30:VAL:HB	1.79	0.64
1:A:162:GLY:HA2	1:A:163:VAL:O	1.97	0.64
1:A:275:THR:CG2	1:A:279:MET:HE1	2.26	0.64
1:B:379:THR:CG2	1:B:384:THR:HB	2.27	0.64
1:D:83:GLU:C	1:D:84:LEU:HD12	2.23	0.64
1:A:419:VAL:HG21	1:A:437:THR:CG2	2.26	0.64
1:A:274:ILE:HD11	1:A:412:ILE:HD11	1.80	0.64
1:D:430:LEU:C	1:D:430:LEU:HD23	2.23	0.64
1:C:379:THR:HG23	1:C:384:THR:HB	1.78	0.64
1:B:363:VAL:HG13	1:B:451:ILE:HD13	1.80	0.64
1:C:530:ILE:HG23	1:C:555:VAL:HG21	1.79	0.64
1:A:379:THR:CG2	1:A:384:THR:HB	2.27	0.63
1:B:530:ILE:HG23	1:B:555:VAL:HG21	1.79	0.63
1:D:162:GLY:HA2	1:D:163:VAL:O	1.99	0.63
1:A:363:VAL:CG1	1:A:375:ILE:HD13	2.28	0.63
1:B:403:SER:OG	1:B:406:THR:HG23	1.97	0.63
1:B:419:VAL:HG21	1:B:437:THR:CG2	2.28	0.63
1:C:274:ILE:HD11	1:C:412:ILE:HD11	1.80	0.63
1:C:297:VAL:O	1:C:300:ALA:HB3	1.99	0.63
1:D:355:LEU:O	1:D:355:LEU:HD22	1.98	0.63
1:A:115:VAL:HG12	1:A:160:LEU:HD23	1.81	0.63
1:B:517:GLU:O	1:B:520:VAL:HG22	1.98	0.62
1:A:7:VAL:HG22	1:A:30:VAL:HB	1.80	0.62
1:A:582:ALA:O	1:A:583:ASN:ND2	2.31	0.62
1:B:253:GLU:HA	1:C:294:ALA:CB	2.29	0.62
1:A:77:MET:HE2	1:A:152:LEU:HD23	1.81	0.62
1:C:162:GLY:HA2	1:C:163:VAL:O	1.98	0.62
1:C:363:VAL:CG1	1:C:375:ILE:HD13	2.30	0.62
1:B:127:LEU:HD22	1:B:128:ILE:HG23	1.82	0.62
1:C:367:ALA:HA	1:C:372:VAL:HG22	1.81	0.62
1:D:509:VAL:HG23	1:D:509:VAL:O	2.00	0.62
1:A:297:VAL:O	1:A:300:ALA:HB3	2.00	0.62
1:D:379:THR:CG2	1:D:384:THR:HB	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:VAL:HG22	1:A:419:VAL:CG2	2.30	0.61
1:D:266:CYS:SG	1:D:273:VAL:CG2	2.88	0.61
1:D:30:VAL:HG13	1:D:62:ALA:HB3	1.82	0.61
1:D:274:ILE:CD1	1:D:412:ILE:HD11	2.31	0.61
1:B:19:MET:O	1:B:23:LEU:HD13	2.01	0.61
1:C:430:LEU:C	1:C:430:LEU:HD23	2.25	0.61
1:D:77:MET:HE2	1:D:152:LEU:HD23	1.82	0.61
1:A:413:VAL:HG12	1:A:416:VAL:HG23	1.83	0.61
1:C:115:VAL:HG12	1:C:160:LEU:HD23	1.83	0.61
1:D:297:VAL:O	1:D:300:ALA:HB3	2.01	0.61
1:D:77:MET:HE1	1:D:104:PHE:CD2	2.36	0.60
1:B:77:MET:HE1	1:B:104:PHE:CD2	2.37	0.60
1:C:19:MET:O	1:C:23:LEU:HD13	2.01	0.60
1:C:275:THR:CG2	1:C:279:MET:HE1	2.29	0.60
1:A:84:LEU:HD23	1:A:90:VAL:HG21	1.82	0.60
1:A:283:MET:SD	1:A:326:THR:HG21	2.42	0.60
1:D:7:VAL:HG22	1:D:30:VAL:HB	1.84	0.60
1:A:530:ILE:HG23	1:A:555:VAL:HG21	1.84	0.60
1:C:77:MET:HE1	1:C:104:PHE:CD2	2.36	0.60
1:C:266:CYS:SG	1:C:273:VAL:CG2	2.90	0.60
1:D:283:MET:SD	1:D:326:THR:HG21	2.42	0.60
1:B:494:ALA:HB2	1:B:500:LEU:HD23	1.83	0.60
1:D:539:PRO:O	1:D:543:VAL:HG13	2.01	0.60
1:A:294:ALA:CB	1:D:253:GLU:HA	2.32	0.59
1:C:517:GLU:O	1:C:520:VAL:HG22	2.01	0.59
1:D:494:ALA:HB2	1:D:500:LEU:HD23	1.84	0.59
1:A:278:GLN:HB3	1:D:291:ARG:NH2	2.17	0.59
1:D:530:ILE:HG23	1:D:555:VAL:HG21	1.84	0.59
1:A:403:SER:OG	1:A:406:THR:HG23	2.03	0.59
1:A:302:TYR:CZ	1:D:257:MET:CE	2.84	0.59
1:B:20:ILE:HG22	1:B:53:VAL:HG11	1.85	0.59
1:C:400:VAL:HG22	1:C:419:VAL:CG2	2.33	0.59
1:B:539:PRO:O	1:B:543:VAL:HG13	2.03	0.58
1:A:433:ASN:O	1:A:434:ALA:C	2.45	0.58
1:A:444:VAL:HG21	1:A:450:ILE:HD11	1.85	0.58
1:C:379:THR:CG2	1:C:384:THR:HB	2.33	0.58
1:A:83:GLU:C	1:A:84:LEU:HD12	2.28	0.58
1:B:283:MET:SD	1:B:326:THR:HG21	2.43	0.58
1:B:367:ALA:HA	1:B:372:VAL:HG22	1.86	0.58
1:C:376:VAL:HG11	1:C:434:ALA:HB1	1.84	0.58
1:D:178:ILE:HD11	1:D:206:ILE:CD1	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:THR:OG1	1:A:464:THR:HB	2.03	0.58
1:B:162:GLY:HA2	1:B:163:VAL:O	2.02	0.58
1:B:115:VAL:HG12	1:B:160:LEU:HD23	1.85	0.58
1:B:363:VAL:CG1	1:B:375:ILE:HD13	2.34	0.58
1:C:380:GLU:O	1:C:406:THR:HG21	2.04	0.58
1:B:82:ILE:HG22	1:B:152:LEU:HB3	1.86	0.58
1:C:384:THR:OG1	1:C:464:THR:HB	2.04	0.58
1:D:497:VAL:HG11	1:D:518:THR:OG1	2.04	0.58
1:A:539:PRO:O	1:A:543:VAL:HG13	2.03	0.58
1:A:549:ILE:O	1:A:551:THR:HG23	2.03	0.58
1:D:367:ALA:HA	1:D:372:VAL:HG22	1.86	0.58
1:C:355:LEU:HD22	1:C:355:LEU:O	2.04	0.58
1:D:403:SER:OG	1:D:406:THR:HG23	2.03	0.57
1:B:178:ILE:HD11	1:B:206:ILE:CD1	2.35	0.57
1:B:310:LEU:HD21	1:B:327:MET:HE2	1.86	0.57
1:C:494:ALA:HB2	1:C:500:LEU:HD23	1.86	0.57
1:C:549:ILE:O	1:C:551:THR:HG23	2.03	0.57
1:D:115:VAL:HG12	1:D:160:LEU:HD23	1.85	0.57
1:C:539:PRO:O	1:C:543:VAL:HG13	2.04	0.57
1:B:226:ILE:CD1	1:B:246:MET:HE3	2.34	0.57
1:A:509:VAL:HG23	1:A:509:VAL:O	2.04	0.57
1:D:517:GLU:O	1:D:520:VAL:HG22	2.04	0.57
1:C:435:VAL:O	1:C:439:VAL:HG23	2.05	0.57
1:A:376:VAL:HG11	1:A:434:ALA:HB1	1.86	0.57
1:C:127:LEU:HD22	1:C:128:ILE:HG23	1.86	0.57
1:D:219:LYS:O	1:D:220:ILE:C	2.47	0.57
1:A:308:VAL:HG12	1:A:327:MET:HE3	1.86	0.56
1:A:351:VAL:HG21	1:A:391:TYR:OH	2.05	0.56
1:B:83:GLU:C	1:B:84:LEU:HD12	2.31	0.56
1:B:235:VAL:HG12	1:B:235:VAL:O	2.05	0.56
1:C:82:ILE:HG22	1:C:152:LEU:HB3	1.88	0.56
1:A:461:THR:HG23	1:A:462:GLY:H	1.70	0.56
1:B:274:ILE:CD1	1:B:412:ILE:HD11	2.36	0.56
1:B:274:ILE:HD11	1:B:412:ILE:HD11	1.86	0.56
1:B:308:VAL:CG1	1:B:327:MET:SD	2.93	0.56
1:D:20:ILE:HG22	1:D:53:VAL:HG11	1.88	0.56
1:D:226:ILE:CD1	1:D:246:MET:HE3	2.33	0.56
1:D:582:ALA:O	1:D:583:ASN:ND2	2.38	0.56
1:A:204:ARG:NH1	1:A:235:VAL:O	2.39	0.56
1:D:116:GLN:HA	1:D:135:ILE:HD11	1.88	0.56
1:D:310:LEU:HD21	1:D:327:MET:HE2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:461:THR:HG23	1:D:462:GLY:H	1.70	0.56
1:A:127:LEU:HD22	1:A:128:ILE:HG23	1.87	0.56
1:C:204:ARG:NH1	1:C:235:VAL:O	2.39	0.56
1:D:444:VAL:HG21	1:D:450:ILE:HD11	1.86	0.56
1:C:461:THR:HG23	1:C:462:GLY:H	1.72	0.55
1:B:380:GLU:O	1:B:406:THR:HG21	2.05	0.55
1:B:484:ARG:C	1:B:572:ALA:HB3	2.31	0.55
1:A:178:ILE:HD11	1:A:206:ILE:CD1	2.36	0.55
1:C:363:VAL:HG13	1:C:451:ILE:HD13	1.86	0.55
1:A:82:ILE:HG22	1:A:152:LEU:HB3	1.88	0.55
1:A:529:LEU:HB3	1:A:551:THR:HG22	1.89	0.55
1:A:278:GLN:OE1	1:D:291:ARG:NE	2.40	0.54
1:D:549:ILE:O	1:D:551:THR:HG23	2.08	0.54
1:A:111:LEU:HD23	1:A:111:LEU:C	2.32	0.54
1:B:30:VAL:HG13	1:B:62:ALA:HB3	1.89	0.54
1:C:497:VAL:HG11	1:C:518:THR:OG1	2.07	0.54
1:D:82:ILE:HG22	1:D:152:LEU:HB3	1.89	0.54
1:D:484:ARG:C	1:D:572:ALA:HB3	2.32	0.54
1:D:494:ALA:HB3	1:D:512:THR:HG22	1.89	0.54
1:B:461:THR:HG23	1:B:462:GLY:H	1.72	0.54
1:B:529:LEU:HB3	1:B:551:THR:HG22	1.89	0.54
1:B:444:VAL:HG21	1:B:450:ILE:HD11	1.90	0.54
1:D:351:VAL:HG21	1:D:391:TYR:CZ	2.42	0.54
1:A:486:SER:O	1:A:487:VAL:HG13	2.07	0.54
1:B:20:ILE:CG2	1:B:53:VAL:HG11	2.38	0.54
1:B:97:VAL:HG11	1:B:103:LYS:HE3	1.88	0.54
1:B:235:VAL:O	1:B:235:VAL:CG1	2.55	0.54
1:D:127:LEU:HD22	1:D:128:ILE:HG23	1.90	0.54
1:D:582:ALA:O	1:D:583:ASN:CG	2.51	0.54
1:A:92:VAL:CG2	1:A:142:VAL:HB	2.37	0.54
1:B:174:ASP:O	1:B:178:ILE:HG23	2.07	0.54
1:C:444:VAL:HG21	1:C:450:ILE:HD11	1.90	0.54
1:C:494:ALA:HB3	1:C:512:THR:HG22	1.90	0.54
1:D:274:ILE:HD11	1:D:412:ILE:CD1	2.37	0.54
1:B:219:LYS:O	1:B:220:ILE:C	2.51	0.53
1:B:361:ILE:HG13	1:B:391:TYR:CZ	2.42	0.53
1:A:274:ILE:CD1	1:A:412:ILE:HD11	2.37	0.53
1:B:274:ILE:HD11	1:B:412:ILE:CD1	2.39	0.53
1:C:44:LYS:HE2	1:C:184:GLU:OE2	2.08	0.53
1:A:159:ASN:O	1:A:161:PRO:HD3	2.09	0.53
1:D:435:VAL:O	1:D:439:VAL:HG23	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:GLU:O	1:A:520:VAL:HG22	2.08	0.53
1:D:355:LEU:HD22	1:D:355:LEU:C	2.34	0.53
1:B:175:ALA:O	1:B:179:ARG:HG3	2.09	0.53
1:D:400:VAL:HG22	1:D:419:VAL:CG2	2.38	0.53
1:C:245:ASP:N	1:C:245:ASP:OD1	2.42	0.53
1:C:509:VAL:HG23	1:C:509:VAL:O	2.08	0.53
1:D:384:THR:OG1	1:D:464:THR:HB	2.08	0.53
1:B:226:ILE:HD12	1:B:258:VAL:CG1	2.39	0.53
1:D:245:ASP:OD1	1:D:245:ASP:N	2.42	0.53
1:A:308:VAL:CG1	1:A:327:MET:CE	2.86	0.53
1:A:367:ALA:CA	1:A:372:VAL:HG22	2.38	0.53
1:B:256:PRO:CG	1:C:295:SER:HB2	2.39	0.53
1:B:359:ILE:CD1	1:B:465:ASN:C	2.82	0.53
1:B:384:THR:OG1	1:B:464:THR:HB	2.09	0.53
1:D:178:ILE:HD11	1:D:206:ILE:HD13	1.91	0.53
1:A:428:ASP:OD2	1:B:427:THR:N	2.41	0.52
1:D:239:LEU:CD2	1:D:241:VAL:HG23	2.40	0.52
1:D:529:LEU:HB3	1:D:551:THR:HG22	1.92	0.52
1:A:380:GLU:O	1:A:406:THR:HG21	2.09	0.52
1:B:494:ALA:HB3	1:B:512:THR:HG22	1.90	0.52
1:A:469:ILE:HG21	1:B:355:LEU:HD23	1.91	0.52
1:D:174:ASP:O	1:D:178:ILE:HG23	2.09	0.52
1:A:278:GLN:OE1	1:D:291:ARG:CZ	2.57	0.52
1:C:83:GLU:C	1:C:84:LEU:HD12	2.34	0.52
1:A:494:ALA:HB3	1:A:512:THR:HG22	1.91	0.52
1:A:44:LYS:HE2	1:A:184:GLU:OE2	2.09	0.52
1:C:226:ILE:HD12	1:C:258:VAL:CG1	2.39	0.52
1:A:392:ARG:HA	1:A:414:TRP:CZ3	2.44	0.52
1:A:463:THR:HG23	1:B:574:GLN:OE1	2.10	0.52
1:B:127:LEU:CD2	1:B:128:ILE:HG23	2.39	0.52
1:C:20:ILE:HG22	1:C:53:VAL:HG11	1.91	0.52
1:C:30:VAL:HG13	1:C:62:ALA:HB3	1.92	0.52
1:C:178:ILE:HD11	1:C:206:ILE:CD1	2.39	0.52
1:A:506:SER:OG	1:A:507:ASP:N	2.43	0.52
1:C:20:ILE:HD12	1:C:49:THR:CG2	2.40	0.52
1:D:380:GLU:O	1:D:406:THR:HG21	2.10	0.52
1:B:92:VAL:CG2	1:B:142:VAL:HB	2.38	0.51
1:A:20:ILE:HG22	1:A:53:VAL:HG11	1.92	0.51
1:A:397:ILE:HB	1:A:416:VAL:HA	1.92	0.51
1:C:310:LEU:HD21	1:C:327:MET:HE2	1.91	0.51
1:A:359:ILE:HD12	1:A:465:ASN:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:ILE:HD12	1:B:49:THR:CG2	2.40	0.51
1:A:116:GLN:HA	1:A:135:ILE:HD11	1.92	0.51
1:A:226:ILE:CD1	1:A:246:MET:HE3	2.37	0.51
1:A:359:ILE:CD1	1:A:465:ASN:HA	2.40	0.51
1:B:297:VAL:O	1:B:300:ALA:HB3	2.10	0.51
1:B:509:VAL:O	1:B:509:VAL:HG23	2.10	0.51
1:C:15:GLU:HG2	1:C:46:ARG:HE	1.75	0.51
1:D:359:ILE:HD12	1:D:465:ASN:HA	1.93	0.51
1:A:295:SER:HB2	1:D:256:PRO:HG3	1.91	0.51
1:A:582:ALA:O	1:A:583:ASN:CG	2.54	0.51
1:B:433:ASN:O	1:B:434:ALA:C	2.54	0.51
1:D:92:VAL:CG2	1:D:142:VAL:HB	2.39	0.51
1:D:204:ARG:NH1	1:D:235:VAL:O	2.43	0.51
1:D:359:ILE:CD1	1:D:465:ASN:C	2.84	0.51
1:A:310:LEU:HD21	1:A:327:MET:HE2	1.93	0.51
1:B:253:GLU:HA	1:C:294:ALA:HB2	1.93	0.51
1:C:77:MET:SD	1:C:99:GLY:HA3	2.51	0.51
1:C:392:ARG:HA	1:C:414:TRP:CZ3	2.46	0.51
1:C:484:ARG:C	1:C:572:ALA:HB3	2.36	0.51
1:A:497:VAL:HG11	1:A:518:THR:OG1	2.11	0.50
1:B:359:ILE:HD12	1:B:465:ASN:HA	1.93	0.50
1:C:361:ILE:HG13	1:C:391:TYR:CZ	2.46	0.50
1:C:397:ILE:HB	1:C:416:VAL:HA	1.93	0.50
1:B:44:LYS:HE2	1:B:184:GLU:OE2	2.11	0.50
1:D:20:ILE:CG2	1:D:53:VAL:HG11	2.41	0.50
1:D:376:VAL:HG11	1:D:434:ALA:HB1	1.94	0.50
1:D:493:VAL:CG1	1:D:559:VAL:HG13	2.42	0.50
1:A:175:ALA:O	1:A:179:ARG:HG3	2.11	0.50
1:A:400:VAL:HG22	1:A:419:VAL:HG23	1.93	0.50
1:B:351:VAL:HG21	1:B:391:TYR:CZ	2.46	0.50
1:C:50:ILE:HG21	1:C:63:ILE:HD11	1.94	0.50
1:C:351:VAL:HG21	1:C:391:TYR:CZ	2.46	0.50
1:C:403:SER:OG	1:C:406:THR:HG23	2.12	0.50
1:D:239:LEU:HD21	1:D:241:VAL:HG23	1.94	0.50
1:A:310:LEU:CD2	1:A:327:MET:HE2	2.42	0.49
1:A:344:LEU:O	1:A:344:LEU:HD12	2.11	0.49
1:C:229:ILE:HD11	1:C:239:LEU:CD1	2.42	0.49
1:D:400:VAL:HG12	1:D:400:VAL:O	2.11	0.49
1:A:367:ALA:HA	1:A:372:VAL:CG2	2.40	0.49
1:A:484:ARG:C	1:A:572:ALA:HB3	2.38	0.49
1:B:484:ARG:HG3	1:B:573:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:ILE:CD1	1:C:246:MET:HE3	2.41	0.49
1:C:175:ALA:O	1:C:179:ARG:HG3	2.13	0.49
1:D:298:ALA:HB1	1:D:302:TYR:CE2	2.47	0.49
1:D:363:VAL:CG1	1:D:375:ILE:HD13	2.42	0.49
1:C:127:LEU:CD2	1:C:128:ILE:HG23	2.42	0.49
1:A:100:THR:HG23	1:A:101:PRO:HD2	1.94	0.49
1:B:291:ARG:CZ	1:C:278:GLN:OE1	2.60	0.49
1:A:92:VAL:HG22	1:A:142:VAL:O	2.12	0.49
1:B:435:VAL:O	1:B:439:VAL:HG23	2.12	0.49
1:C:363:VAL:HG22	1:C:451:ILE:CD1	2.38	0.49
1:D:226:ILE:HD12	1:D:258:VAL:CG1	2.43	0.49
1:D:538:SER:HB2	1:D:539:PRO:HD2	1.94	0.49
1:A:359:ILE:CD1	1:A:465:ASN:C	2.85	0.49
1:B:256:PRO:HG3	1:C:295:SER:HB2	1.93	0.49
1:C:359:ILE:CD1	1:C:465:ASN:HA	2.42	0.49
1:C:384:THR:O	1:C:385:ALA:C	2.55	0.49
1:C:529:LEU:HB3	1:C:551:THR:HG22	1.94	0.49
1:D:44:LYS:HE2	1:D:184:GLU:OE2	2.12	0.49
1:D:175:ALA:O	1:D:179:ARG:HG3	2.13	0.49
1:D:359:ILE:CD1	1:D:465:ASN:HA	2.42	0.49
1:D:392:ARG:HA	1:D:414:TRP:CZ3	2.48	0.49
1:B:7:VAL:HG22	1:B:30:VAL:HB	1.95	0.49
1:B:178:ILE:HD11	1:B:206:ILE:HD13	1.94	0.49
1:B:549:ILE:O	1:B:551:THR:HG23	2.13	0.49
1:C:274:ILE:CD1	1:C:412:ILE:HD11	2.42	0.49
1:A:301:ILE:CD1	1:A:331:ALA:HA	2.43	0.48
1:C:400:VAL:HG22	1:C:419:VAL:HG23	1.94	0.48
1:D:97:VAL:HG11	1:D:103:LYS:HE3	1.95	0.48
1:D:100:THR:HG23	1:D:101:PRO:HD2	1.95	0.48
1:D:15:GLU:HG2	1:D:46:ARG:HE	1.77	0.48
1:A:15:GLU:HG2	1:A:46:ARG:HE	1.78	0.48
1:A:335:GLU:O	1:A:336:ALA:C	2.56	0.48
1:C:20:ILE:CG2	1:C:53:VAL:HG11	2.43	0.48
1:C:116:GLN:HA	1:C:135:ILE:HD11	1.95	0.48
1:D:433:ASN:O	1:D:434:ALA:C	2.55	0.48
1:A:97:VAL:HG11	1:A:103:LYS:HE3	1.96	0.48
1:A:276:ALA:C	1:A:277:THR:HG23	2.39	0.48
1:C:582:ALA:O	1:C:583:ASN:ND2	2.47	0.48
1:A:190:ALA:HA	1:A:217:PHE:O	2.13	0.48
1:D:128:ILE:HG22	1:D:148:ASN:O	2.14	0.48
1:A:178:ILE:HD12	1:A:203:ILE:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:VAL:HG22	1:B:419:VAL:CG2	2.42	0.48
1:C:433:ASN:O	1:C:434:ALA:C	2.57	0.48
1:D:400:VAL:CG2	1:D:437:THR:HG21	2.44	0.48
1:A:298:ALA:O	1:A:301:ILE:N	2.44	0.48
1:A:493:VAL:CG1	1:A:559:VAL:HG13	2.44	0.48
1:B:355:LEU:O	1:B:355:LEU:HD22	2.14	0.48
1:C:97:VAL:HG11	1:C:103:LYS:HE3	1.95	0.48
1:C:484:ARG:HG3	1:C:573:ALA:HB2	1.96	0.48
1:A:127:LEU:CD2	1:A:128:ILE:HG23	2.44	0.48
1:B:366:THR:HG22	1:B:367:ALA:N	2.29	0.48
1:B:493:VAL:CG1	1:B:559:VAL:HG13	2.43	0.48
1:C:178:ILE:HD12	1:C:203:ILE:HG23	1.96	0.48
1:A:20:ILE:HD12	1:A:49:THR:CG2	2.44	0.48
1:C:275:THR:O	1:C:279:MET:HE3	2.13	0.48
1:D:573:ALA:O	1:D:575:GLY:N	2.42	0.48
1:C:375:ILE:HG23	1:C:451:ILE:HG23	1.95	0.48
1:C:367:ALA:CA	1:C:372:VAL:HG22	2.44	0.47
1:A:339:ASP:C	1:A:339:ASP:OD1	2.57	0.47
1:B:497:VAL:HG11	1:B:518:THR:OG1	2.14	0.47
1:C:359:ILE:CD1	1:C:465:ASN:C	2.87	0.47
1:A:484:ARG:HG3	1:A:573:ALA:HB2	1.95	0.47
1:B:200:VAL:O	1:B:203:ILE:N	2.48	0.47
1:D:91:ILE:HD13	1:D:102:GLU:HG3	1.96	0.47
1:A:75:HIS:HB2	1:A:105:SER:OG	2.14	0.47
1:A:366:THR:HG22	1:A:367:ALA:N	2.29	0.47
1:B:275:THR:O	1:B:279:MET:HE3	2.14	0.47
1:A:255:VAL:N	1:A:256:PRO:CD	2.77	0.47
1:A:274:ILE:HD11	1:A:412:ILE:CD1	2.43	0.47
1:A:295:SER:HB2	1:D:256:PRO:CG	2.44	0.47
1:A:361:ILE:HG13	1:A:391:TYR:CZ	2.49	0.47
1:B:15:GLU:HG2	1:B:46:ARG:HE	1.78	0.47
1:C:355:LEU:HD22	1:C:355:LEU:C	2.39	0.47
1:C:488:VAL:HG12	1:C:569:THR:OG1	2.14	0.47
1:D:266:CYS:SG	1:D:273:VAL:HG22	2.55	0.47
1:D:375:ILE:HG23	1:D:451:ILE:HG23	1.96	0.47
1:A:351:VAL:HG21	1:A:391:TYR:CZ	2.50	0.47
1:A:435:VAL:O	1:A:439:VAL:HG23	2.14	0.47
1:B:582:ALA:O	1:B:583:ASN:CG	2.58	0.47
1:C:530:ILE:HG12	1:C:577:ILE:HD13	1.97	0.47
1:A:50:ILE:HG21	1:A:63:ILE:HD11	1.96	0.47
1:A:494:ALA:CB	1:A:500:LEU:HD23	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:GLU:HG3	1:B:57:LEU:HD11	1.96	0.47
1:B:91:ILE:HD13	1:B:102:GLU:HG3	1.97	0.47
1:C:298:ALA:O	1:C:301:ILE:N	2.46	0.47
1:C:400:VAL:CG2	1:C:437:THR:HG21	2.44	0.47
1:D:229:ILE:HD11	1:D:239:LEU:CD1	2.45	0.47
1:D:298:ALA:O	1:D:301:ILE:N	2.45	0.47
1:D:506:SER:OG	1:D:507:ASP:N	2.43	0.47
1:D:509:VAL:O	1:D:509:VAL:CG2	2.62	0.47
1:A:226:ILE:HD12	1:A:258:VAL:CG1	2.44	0.47
1:C:100:THR:HG23	1:C:101:PRO:HD2	1.96	0.47
1:C:210:GLN:O	1:C:211:LYS:C	2.57	0.47
1:C:356:VAL:HG12	1:C:387:THR:HG21	1.96	0.47
1:A:88:ASN:C	1:A:146:ILE:HG22	2.40	0.47
1:A:239:LEU:CD2	1:A:241:VAL:HG23	2.45	0.47
1:C:91:ILE:HD13	1:C:102:GLU:HG3	1.97	0.47
1:C:217:PHE:CE1	1:C:238:GLY:HA3	2.50	0.47
1:C:379:THR:CG2	2:C:586:PO4:O3	2.52	0.47
1:D:485:GLY:N	1:D:572:ALA:HB3	2.30	0.47
1:A:266:CYS:SG	1:A:273:VAL:CG2	3.03	0.47
1:A:520:VAL:HG12	1:A:543:VAL:HG11	1.97	0.47
1:B:239:LEU:CD2	1:B:241:VAL:HG23	2.45	0.47
1:A:21:GLU:HG3	1:A:57:LEU:HD11	1.97	0.46
1:A:302:TYR:OH	1:D:257:MET:CE	2.38	0.46
1:B:116:GLN:HA	1:B:135:ILE:HD11	1.97	0.46
1:C:235:VAL:O	1:C:235:VAL:CG1	2.62	0.46
1:A:200:VAL:O	1:A:203:ILE:N	2.48	0.46
1:B:100:THR:HG23	1:B:101:PRO:HD2	1.96	0.46
1:B:266:CYS:SG	1:B:273:VAL:HG22	2.55	0.46
1:B:582:ALA:O	1:B:583:ASN:ND2	2.48	0.46
1:C:520:VAL:HG12	1:C:543:VAL:HG11	1.97	0.46
1:B:226:ILE:HD12	1:B:258:VAL:HG11	1.97	0.46
1:D:497:VAL:HG11	1:D:518:THR:CB	2.45	0.46
1:A:91:ILE:HD13	1:A:102:GLU:HG3	1.98	0.46
1:A:240:MET:CE	1:A:274:ILE:HD12	2.45	0.46
1:D:226:ILE:HD12	1:D:258:VAL:HG11	1.96	0.46
1:A:427:THR:N	1:B:428:ASP:OD2	2.48	0.46
1:B:204:ARG:NH1	1:B:235:VAL:O	2.48	0.46
1:B:239:LEU:HD21	1:B:241:VAL:HG23	1.97	0.46
1:C:92:VAL:CG2	1:C:142:VAL:HB	2.39	0.46
1:C:486:SER:O	1:C:487:VAL:HG13	2.15	0.46
1:D:233:LEU:O	1:D:234:GLU:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:MET:CE	1:C:274:ILE:HD12	2.46	0.46
1:D:160:LEU:O	1:D:162:GLY:N	2.49	0.46
1:A:520:VAL:N	1:A:521:PRO:CD	2.79	0.46
1:C:308:VAL:HG12	1:C:327:MET:HE3	1.98	0.46
1:A:257:MET:HG2	1:D:337:ALA:CB	2.41	0.46
1:B:229:ILE:HD11	1:B:239:LEU:CD1	2.46	0.46
1:B:356:VAL:HG12	1:B:387:THR:HG21	1.98	0.46
1:C:308:VAL:CG1	1:C:327:MET:HE3	2.45	0.46
1:D:20:ILE:HD12	1:D:49:THR:CG2	2.45	0.46
1:A:372:VAL:HG23	1:A:395:SER:OG	2.15	0.46
1:A:384:THR:O	1:A:385:ALA:C	2.59	0.46
1:B:392:ARG:HA	1:B:414:TRP:CZ3	2.51	0.46
1:D:266:CYS:CB	1:D:273:VAL:CG2	2.94	0.46
1:D:438:ALA:O	1:D:441:THR:OG1	2.34	0.46
1:A:430:LEU:C	1:A:430:LEU:CD2	2.89	0.46
1:C:308:VAL:CG1	1:C:327:MET:SD	3.00	0.46
1:D:301:ILE:CD1	1:D:331:ALA:HA	2.46	0.46
1:D:366:THR:HG22	1:D:367:ALA:N	2.31	0.46
1:A:20:ILE:CG2	1:A:53:VAL:HG11	2.46	0.45
1:A:178:ILE:HD11	1:A:206:ILE:HD13	1.97	0.45
1:B:323:ALA:O	1:B:326:THR:HG22	2.16	0.45
1:B:359:ILE:HD13	1:B:466:MET:N	2.30	0.45
1:B:376:VAL:HG11	1:B:434:ALA:HB1	1.96	0.45
1:C:235:VAL:O	1:C:235:VAL:HG12	2.15	0.45
1:C:574:GLN:OE1	1:D:463:THR:HG23	2.16	0.45
1:B:128:ILE:HG22	1:B:148:ASN:O	2.16	0.45
1:A:245:ASP:OD1	1:A:245:ASP:N	2.48	0.45
1:B:245:ASP:OD1	1:B:245:ASP:N	2.50	0.45
1:C:370:LEU:HD21	1:D:355:LEU:HA	1.98	0.45
1:C:497:VAL:HG11	1:C:518:THR:CB	2.47	0.45
1:B:77:MET:SD	1:B:99:GLY:HA3	2.57	0.45
1:C:92:VAL:HG22	1:C:142:VAL:O	2.17	0.45
1:C:359:ILE:HD12	1:C:465:ASN:HA	1.97	0.45
1:C:21:GLU:HG3	1:C:57:LEU:HD11	1.98	0.45
1:A:343:LEU:O	1:A:347:ARG:HG2	2.17	0.45
1:A:497:VAL:HG11	1:A:518:THR:CB	2.47	0.45
1:B:397:ILE:HB	1:B:416:VAL:HA	1.99	0.45
1:B:431:LEU:HD21	1:B:466:MET:HE1	1.99	0.45
1:B:530:ILE:HG12	1:B:577:ILE:HD13	1.99	0.45
1:D:435:VAL:HG21	1:D:470:HIS:CE1	2.51	0.45
1:D:191:ALA:HB2	1:D:203:ILE:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:484:ARG:HG3	1:D:573:ALA:HB2	1.99	0.45
1:B:64:LEU:HD12	1:B:188:PHE:CB	2.47	0.44
1:B:255:VAL:HB	1:C:291:ARG:HG2	1.99	0.44
1:C:148:ASN:O	1:C:149:SER:C	2.60	0.44
1:C:226:ILE:HD12	1:C:258:VAL:HG11	1.98	0.44
1:D:520:VAL:HG12	1:D:543:VAL:HG11	1.99	0.44
1:A:217:PHE:CE1	1:A:238:GLY:HA3	2.52	0.44
1:A:375:ILE:HG23	1:A:451:ILE:HG23	1.99	0.44
1:A:509:VAL:O	1:A:509:VAL:CG2	2.65	0.44
1:C:274:ILE:HD11	1:C:412:ILE:CD1	2.48	0.44
1:D:127:LEU:CD2	1:D:128:ILE:HG23	2.46	0.44
1:D:339:ASP:C	1:D:339:ASP:OD1	2.59	0.44
1:D:397:ILE:HB	1:D:416:VAL:HA	1.98	0.44
1:B:538:SER:HB2	1:B:539:PRO:HD2	1.99	0.44
1:B:573:ALA:O	1:B:575:GLY:N	2.46	0.44
1:C:363:VAL:HG11	1:C:388:ILE:HD12	1.97	0.44
1:C:413:VAL:HG12	1:C:416:VAL:HG23	1.99	0.44
1:D:372:VAL:HG23	1:D:395:SER:OG	2.17	0.44
1:A:33:LEU:HD11	1:A:47:ILE:HG13	1.99	0.44
1:B:533:GLU:O	1:B:534:ASN:HB2	2.18	0.44
1:D:77:MET:HE1	1:D:104:PHE:HD2	1.82	0.44
1:D:367:ALA:CA	1:D:372:VAL:HG22	2.46	0.44
1:B:291:ARG:NH2	1:C:278:GLN:HB3	2.32	0.44
1:D:92:VAL:HG12	1:D:104:PHE:CD1	2.53	0.44
1:D:328:ARG:O	1:D:331:ALA:HB3	2.18	0.44
1:A:435:VAL:HG21	1:A:470:HIS:CE1	2.53	0.44
1:D:217:PHE:CE1	1:D:238:GLY:HA3	2.53	0.44
1:D:361:ILE:HG13	1:D:391:TYR:CZ	2.52	0.44
1:A:5:LYS:HG3	1:A:411:SER:O	2.17	0.44
1:B:148:ASN:O	1:B:149:SER:C	2.61	0.44
1:B:361:ILE:HG13	1:B:391:TYR:CE1	2.53	0.44
1:C:200:VAL:O	1:C:203:ILE:N	2.50	0.44
1:D:376:VAL:HG13	1:D:376:VAL:O	2.17	0.44
1:B:240:MET:CE	1:B:274:ILE:HD12	2.47	0.44
1:C:111:LEU:HG	1:C:160:LEU:HD21	2.00	0.44
1:C:493:VAL:CG1	1:C:559:VAL:HG13	2.48	0.44
1:D:88:ASN:C	1:D:146:ILE:HG22	2.43	0.44
1:A:266:CYS:CB	1:A:273:VAL:CG2	2.96	0.43
1:B:9:THR:OG1	1:B:32:ARG:NH1	2.45	0.43
1:B:33:LEU:HD11	1:B:47:ILE:HG13	2.00	0.43
1:B:255:VAL:HB	1:C:291:ARG:CG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:482:ILE:HG13	1:C:541:ALA:HB1	1.99	0.43
1:B:266:CYS:CB	1:B:273:VAL:CG2	2.96	0.43
1:C:372:VAL:HG23	1:C:395:SER:OG	2.18	0.43
1:A:355:LEU:HD22	1:A:355:LEU:O	2.18	0.43
1:A:400:VAL:CG2	1:A:437:THR:HG21	2.47	0.43
1:B:97:VAL:HG21	1:B:103:LYS:HG2	2.01	0.43
1:B:485:GLY:N	1:B:572:ALA:HB3	2.33	0.43
1:C:263:ILE:HG12	1:C:273:VAL:HG11	2.00	0.43
1:C:308:VAL:CG1	1:C:327:MET:CE	2.96	0.43
1:C:310:LEU:CD2	1:C:327:MET:HE2	2.48	0.43
1:D:50:ILE:HG21	1:D:63:ILE:HD11	2.01	0.43
1:A:485:GLY:N	1:A:572:ALA:HB3	2.33	0.43
1:B:20:ILE:HD12	1:B:49:THR:HG22	2.00	0.43
1:B:512:THR:HG21	1:B:519:PHE:CE2	2.54	0.43
1:C:266:CYS:CB	1:C:273:VAL:CG2	2.96	0.43
1:C:469:ILE:HG21	1:D:355:LEU:HD23	1.98	0.43
1:D:378:ALA:HB3	1:D:454:ALA:HB2	1.99	0.43
1:D:533:GLU:O	1:D:534:ASN:CB	2.67	0.43
1:A:7:VAL:HG21	1:A:274:ILE:HD13	2.00	0.43
1:B:372:VAL:HG23	1:B:395:SER:OG	2.19	0.43
1:D:190:ALA:HA	1:D:217:PHE:O	2.19	0.43
1:D:413:VAL:HG12	1:D:416:VAL:HG23	2.00	0.43
1:A:235:VAL:O	1:A:235:VAL:CG1	2.67	0.43
1:A:400:VAL:CG2	1:A:419:VAL:CG2	2.97	0.43
1:B:257:MET:HA	1:B:257:MET:HE2	2.01	0.43
1:B:497:VAL:HG11	1:B:518:THR:CB	2.48	0.43
1:B:533:GLU:O	1:B:534:ASN:CB	2.67	0.43
1:C:255:VAL:N	1:C:256:PRO:CD	2.82	0.43
1:C:335:GLU:O	1:C:336:ALA:C	2.61	0.43
1:A:210:GLN:O	1:A:211:LYS:C	2.62	0.43
1:B:75:HIS:HB2	1:B:105:SER:OG	2.19	0.43
1:B:190:ALA:HA	1:B:217:PHE:O	2.19	0.43
1:C:541:ALA:HB2	1:C:553:VAL:HG11	2.00	0.43
1:D:298:ALA:O	1:D:299:ASN:C	2.60	0.43
1:D:449:LEU:HD23	1:D:449:LEU:HA	1.84	0.43
1:D:482:ILE:HD13	1:D:482:ILE:HA	1.92	0.43
1:D:533:GLU:O	1:D:534:ASN:ND2	2.51	0.43
1:B:217:PHE:CE1	1:B:238:GLY:HA3	2.53	0.43
1:B:328:ARG:O	1:B:331:ALA:HB3	2.19	0.43
1:B:497:VAL:HG11	1:B:518:THR:HB	2.01	0.43
1:C:160:LEU:O	1:C:162:GLY:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:ASP:O	1:C:178:ILE:HG23	2.19	0.43
1:C:355:LEU:HD13	1:C:356:VAL:N	2.34	0.43
1:A:160:LEU:O	1:A:162:GLY:N	2.52	0.43
1:C:512:THR:HG21	1:C:519:PHE:CE2	2.54	0.43
1:A:275:THR:O	1:A:279:MET:HE3	2.19	0.42
1:C:178:ILE:HD11	1:C:206:ILE:HD13	2.01	0.42
1:C:573:ALA:O	1:C:575:GLY:N	2.46	0.42
1:D:160:LEU:HD12	1:D:160:LEU:N	2.34	0.42
1:A:533:GLU:O	1:A:534:ASN:CB	2.67	0.42
1:B:7:VAL:HG21	1:B:274:ILE:HD13	2.00	0.42
1:B:326:THR:HG23	1:B:327:MET:N	2.34	0.42
1:B:376:VAL:O	1:B:376:VAL:HG13	2.19	0.42
1:C:431:LEU:HD21	1:C:466:MET:HE1	1.99	0.42
1:D:504:ASP:OD2	1:D:504:ASP:N	2.52	0.42
1:B:92:VAL:HG22	1:B:142:VAL:O	2.19	0.42
1:B:291:ARG:NE	1:C:278:GLN:OE1	2.52	0.42
1:B:520:VAL:HG12	1:B:543:VAL:HG11	2.01	0.42
1:D:356:VAL:HG13	1:D:464:THR:HG23	2.02	0.42
1:D:497:VAL:HG11	1:D:518:THR:HB	2.02	0.42
1:B:233:LEU:O	1:B:234:GLU:C	2.62	0.42
1:D:530:ILE:HG12	1:D:577:ILE:HD13	2.01	0.42
1:A:9:THR:OG1	1:A:32:ARG:NH1	2.46	0.42
1:A:229:ILE:HD11	1:A:239:LEU:CD1	2.50	0.42
1:A:486:SER:C	1:A:487:VAL:HG13	2.45	0.42
1:B:367:ALA:CA	1:B:372:VAL:HG22	2.48	0.42
1:C:355:LEU:HD23	1:D:469:ILE:HG21	2.00	0.42
1:C:363:VAL:CG1	1:C:388:ILE:HD12	2.50	0.42
1:D:301:ILE:HD11	1:D:331:ALA:HA	2.01	0.42
1:A:533:GLU:O	1:A:534:ASN:HB2	2.20	0.42
1:D:520:VAL:N	1:D:521:PRO:CD	2.83	0.42
1:B:494:ALA:CB	1:B:500:LEU:HD23	2.50	0.42
1:C:178:ILE:O	1:C:182:ILE:HG13	2.20	0.42
1:C:190:ALA:HA	1:C:217:PHE:O	2.19	0.42
1:A:148:ASN:O	1:A:149:SER:C	2.63	0.42
1:A:449:LEU:HD23	1:A:449:LEU:HA	1.91	0.42
1:C:533:GLU:O	1:C:534:ASN:HB2	2.20	0.42
1:D:533:GLU:O	1:D:534:ASN:HB2	2.19	0.42
1:A:294:ALA:HB1	1:D:253:GLU:HA	2.02	0.42
1:A:363:VAL:HG11	1:A:388:ILE:HD12	2.01	0.42
1:B:255:VAL:N	1:B:256:PRO:CD	2.83	0.42
1:B:482:ILE:HG13	1:B:541:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:VAL:O	1:D:235:VAL:CG1	2.67	0.42
1:A:295:SER:CA	1:D:256:PRO:HG2	2.50	0.42
1:B:363:VAL:HG11	1:B:388:ILE:HD12	2.01	0.42
1:B:520:VAL:N	1:B:521:PRO:CD	2.83	0.42
1:C:75:HIS:HB2	1:C:105:SER:OG	2.20	0.42
1:D:21:GLU:HG3	1:D:57:LEU:HD11	2.01	0.42
1:A:26:ALA:O	1:A:324:VAL:HG12	2.20	0.41
1:A:463:THR:CG2	1:B:574:GLN:OE1	2.68	0.41
1:A:504:ASP:OD2	1:A:504:ASP:N	2.53	0.41
1:B:256:PRO:HG2	1:C:295:SER:CA	2.50	0.41
1:B:359:ILE:CD1	1:B:465:ASN:HA	2.50	0.41
1:C:266:CYS:SG	1:C:273:VAL:HG22	2.60	0.41
1:D:178:ILE:HD11	1:D:206:ILE:HD12	2.02	0.41
1:B:486:SER:O	1:B:487:VAL:HG13	2.21	0.41
1:A:128:ILE:HG22	1:A:148:ASN:O	2.19	0.41
1:A:239:LEU:HD21	1:A:241:VAL:HG23	2.01	0.41
1:A:400:VAL:O	1:A:400:VAL:HG12	2.20	0.41
1:A:538:SER:HB2	1:A:539:PRO:HD2	2.01	0.41
1:B:26:ALA:O	1:B:324:VAL:HG12	2.21	0.41
1:B:343:LEU:O	1:B:347:ARG:HG2	2.21	0.41
1:C:191:ALA:HB2	1:C:203:ILE:CD1	2.50	0.41
1:B:160:LEU:O	1:B:162:GLY:N	2.54	0.41
1:B:488:VAL:HG12	1:B:569:THR:OG1	2.20	0.41
1:D:34:ASN:ND2	1:D:36:SER:HB2	2.36	0.41
1:A:486:SER:O	1:A:487:VAL:CG1	2.69	0.41
1:C:513:ASN:HA	1:C:532:GLU:CG	2.51	0.41
1:C:530:ILE:HG12	1:C:577:ILE:CD1	2.51	0.41
1:A:355:LEU:HD23	1:B:469:ILE:HG21	2.02	0.41
1:A:530:ILE:HG12	1:A:577:ILE:HD13	2.02	0.41
1:B:298:ALA:O	1:B:301:ILE:N	2.53	0.41
1:B:355:LEU:HD22	1:B:355:LEU:C	2.45	0.41
1:C:463:THR:HG23	1:D:574:GLN:OE1	2.21	0.41
1:D:210:GLN:O	1:D:211:LYS:C	2.63	0.41
1:D:476:ILE:HD13	1:D:476:ILE:HA	1.90	0.41
1:A:97:VAL:HG22	1:A:105:SER:HB3	2.03	0.41
1:B:111:LEU:HG	1:B:160:LEU:HD21	2.02	0.41
1:B:482:ILE:HD13	1:B:482:ILE:HA	1.95	0.41
1:C:97:VAL:HG22	1:C:105:SER:HB3	2.02	0.41
1:C:233:LEU:O	1:C:234:GLU:C	2.63	0.41
1:A:533:GLU:O	1:A:534:ASN:ND2	2.51	0.41
1:B:339:ASP:OD1	1:B:339:ASP:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:LEU:C	1:B:430:LEU:CD2	2.91	0.41
1:B:476:ILE:HD13	1:B:476:ILE:HA	1.91	0.41
1:B:541:ALA:HB2	1:B:553:VAL:HG11	2.02	0.41
1:C:177:ASP:O	1:C:180:PHE:HB3	2.20	0.41
1:A:4:THR:CG2	1:A:331:ALA:HB1	2.50	0.41
1:A:111:LEU:HG	1:A:160:LEU:HD21	2.03	0.41
1:A:370:LEU:HD21	1:B:355:LEU:HA	2.02	0.41
1:B:3:LYS:HD2	1:B:414:TRP:CZ2	2.56	0.41
1:B:77:MET:CE	1:B:82:ILE:HG21	2.51	0.41
1:B:266:CYS:SG	1:B:273:VAL:HG21	2.59	0.41
1:B:376:VAL:CG1	1:B:452:ILE:HG12	2.51	0.41
1:B:504:ASP:OD2	1:B:504:ASP:N	2.53	0.41
1:C:20:ILE:HD12	1:C:49:THR:HG22	2.03	0.41
1:C:343:LEU:O	1:C:347:ARG:HG2	2.21	0.41
1:C:356:VAL:HG13	1:C:464:THR:HG23	2.02	0.41
1:C:582:ALA:O	1:C:583:ASN:CG	2.64	0.41
1:D:355:LEU:HD13	1:D:356:VAL:N	2.35	0.41
1:D:401:THR:O	1:D:420:VAL:HA	2.21	0.41
1:D:494:ALA:CB	1:D:500:LEU:HD23	2.49	0.41
1:D:512:THR:HG21	1:D:519:PHE:CE2	2.56	0.41
1:A:233:LEU:O	1:A:234:GLU:C	2.63	0.41
1:A:497:VAL:HG11	1:A:518:THR:HB	2.02	0.41
1:A:512:THR:HG21	1:A:519:PHE:CE2	2.55	0.41
1:B:50:ILE:HG21	1:B:63:ILE:HD11	2.02	0.41
1:D:235:VAL:O	1:D:235:VAL:HG12	2.21	0.41
1:D:400:VAL:HG22	1:D:419:VAL:HG23	2.02	0.41
1:A:363:VAL:CG1	1:A:388:ILE:HD12	2.51	0.40
1:B:413:VAL:HG12	1:B:416:VAL:HG23	2.03	0.40
1:C:344:LEU:O	1:C:344:LEU:HD12	2.22	0.40
1:C:400:VAL:CG2	1:C:419:VAL:CG2	2.99	0.40
1:C:509:VAL:O	1:C:509:VAL:CG2	2.68	0.40
1:D:343:LEU:O	1:D:347:ARG:HG2	2.20	0.40
1:D:356:VAL:HG12	1:D:387:THR:HG21	2.03	0.40
1:D:530:ILE:HG12	1:D:577:ILE:CD1	2.52	0.40
1:A:162:GLY:HA2	1:A:163:VAL:C	2.44	0.40
1:A:431:LEU:HD21	1:A:466:MET:HE1	2.03	0.40
1:B:251:PRO:O	1:B:252:PRO:C	2.65	0.40
1:C:111:LEU:HD23	1:C:111:LEU:C	2.46	0.40
1:C:159:ASN:O	1:C:161:PRO:HD3	2.21	0.40
1:C:366:THR:HG22	1:C:367:ALA:N	2.37	0.40
1:C:538:SER:HB2	1:C:539:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:ALA:HB1	1:B:302:TYR:CE2	2.57	0.40
1:C:504:ASP:N	1:C:504:ASP:OD2	2.54	0.40
1:C:506:SER:OG	1:C:507:ASP:N	2.49	0.40
1:C:520:VAL:N	1:C:521:PRO:CD	2.84	0.40
1:C:533:GLU:O	1:C:534:ASN:CB	2.69	0.40
1:C:574:GLN:CD	1:D:463:THR:HG23	2.47	0.40
1:A:235:VAL:O	1:A:235:VAL:HG12	2.20	0.40
1:A:392:ARG:HD2	1:A:414:TRP:CE2	2.56	0.40
1:B:335:GLU:O	1:B:336:ALA:C	2.64	0.40
1:C:361:ILE:HG13	1:C:391:TYR:CE1	2.56	0.40
1:C:583:ASN:HD22	1:C:583:ASN:HA	1.73	0.40
1:D:92:VAL:HG12	1:D:104:PHE:CE1	2.56	0.40
1:D:178:ILE:HD12	1:D:203:ILE:HG23	2.02	0.40
1:A:431:LEU:HA	1:A:431:LEU:HD23	1.86	0.40
1:B:91:ILE:HD12	1:B:91:ILE:N	2.36	0.40
1:B:506:SER:OG	1:B:507:ASP:N	2.52	0.40
1:C:497:VAL:HG11	1:C:518:THR:HB	2.03	0.40
1:D:20:ILE:HD12	1:D:49:THR:HG22	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:GLY:O	1:C:460:GLU:OE1[1_455]	2.15	0.05

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	581/606 (96%)	513 (88%)	48 (8%)	20 (3%)	3	13
1	B	581/606 (96%)	514 (88%)	49 (8%)	18 (3%)	3	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	581/606 (96%)	516 (89%)	47 (8%)	18 (3%)	3	14
1	D	581/606 (96%)	516 (89%)	47 (8%)	18 (3%)	3	14
All	All	2324/2424 (96%)	2059 (89%)	191 (8%)	74 (3%)	3	14

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	ASN
1	A	220	ILE
1	A	320	PRO
1	A	475	GLU
1	A	556	GLU
1	B	154	ASN
1	B	220	ILE
1	B	320	PRO
1	B	475	GLU
1	B	556	GLU
1	C	154	ASN
1	C	220	ILE
1	C	320	PRO
1	C	475	GLU
1	C	556	GLU
1	D	154	ASN
1	D	220	ILE
1	D	320	PRO
1	D	475	GLU
1	D	556	GLU
1	A	149	SER
1	A	162	GLY
1	A	462	GLY
1	A	506	SER
1	A	507	ASP
1	B	149	SER
1	B	162	GLY
1	B	462	GLY
1	B	506	SER
1	B	507	ASP
1	C	149	SER
1	C	162	GLY
1	C	462	GLY
1	C	506	SER

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Mol	Chain	Res	Type
1	C	507	ASP
1	D	149	SER
1	D	162	GLY
1	D	462	GLY
1	D	506	SER
1	D	507	ASP
1	A	534	ASN
1	B	195	ARG
1	B	534	ASN
1	C	534	ASN
1	D	534	ASN
1	A	195	ARG
1	C	195	ARG
1	C	213	ASN
1	D	195	ARG
1	A	161	PRO
1	A	163	VAL
1	A	213	ASN
1	C	161	PRO
1	C	582	ALA
1	D	582	ALA
1	A	581	TYR
1	A	582	ALA
1	B	161	PRO
1	B	163	VAL
1	B	581	TYR
1	B	582	ALA
1	C	163	VAL
1	D	101	PRO
1	D	161	PRO
1	D	163	VAL
1	D	581	TYR
1	A	101	PRO
1	A	459	GLY
1	A	580	GLY
1	B	101	PRO
1	B	580	GLY
1	C	580	GLY
1	C	101	PRO
1	D	580	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	490/510 (96%)	471 (96%)	19 (4%)	28	56
1	B	490/510 (96%)	472 (96%)	18 (4%)	30	57
1	C	490/510 (96%)	472 (96%)	18 (4%)	30	57
1	D	490/510 (96%)	472 (96%)	18 (4%)	30	57
All	All	1960/2040 (96%)	1887 (96%)	73 (4%)	30	57

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ILE
1	A	128	ILE
1	A	245	ASP
1	A	250	ILE
1	A	296	ASP
1	A	308	VAL
1	A	318	LEU
1	A	350	LEU
1	A	355	LEU
1	A	366	THR
1	A	379	THR
1	A	400	VAL
1	A	444	VAL
1	A	450	ILE
1	A	458	THR
1	A	464	THR
1	A	476	ILE
1	A	518	THR
1	A	568	VAL
1	B	82	ILE
1	B	245	ASP
1	B	250	ILE
1	B	296	ASP
1	B	318	LEU

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Mol	Chain	Res	Type
1	B	350	LEU
1	B	355	LEU
1	B	366	THR
1	B	370	LEU
1	B	379	THR
1	B	400	VAL
1	B	412	ILE
1	B	444	VAL
1	B	450	ILE
1	B	458	THR
1	B	464	THR
1	B	476	ILE
1	B	568	VAL
1	C	82	ILE
1	C	245	ASP
1	C	250	ILE
1	C	296	ASP
1	C	318	LEU
1	C	350	LEU
1	C	355	LEU
1	C	366	THR
1	C	370	LEU
1	C	379	THR
1	C	400	VAL
1	C	412	ILE
1	C	444	VAL
1	C	450	ILE
1	C	458	THR
1	C	464	THR
1	C	476	ILE
1	C	568	VAL
1	D	77	MET
1	D	82	ILE
1	D	128	ILE
1	D	245	ASP
1	D	250	ILE
1	D	318	LEU
1	D	350	LEU
1	D	355	LEU
1	D	366	THR
1	D	379	THR
1	D	400	VAL

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Mol	Chain	Res	Type
1	D	412	ILE
1	D	444	VAL
1	D	450	ILE
1	D	458	THR
1	D	464	THR
1	D	476	ILE
1	D	568	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	110	ASN
1	A	131	GLN
1	A	228	ASN
1	A	265	GLN
1	A	394	HIS
1	A	470	HIS
1	A	583	ASN
1	B	34	ASN
1	B	228	ASN
1	B	299	ASN
1	B	357	ASN
1	B	394	HIS
1	B	583	ASN
1	C	34	ASN
1	C	75	HIS
1	C	148	ASN
1	C	228	ASN
1	C	299	ASN
1	C	357	ASN
1	C	394	HIS
1	C	583	ASN
1	D	34	ASN
1	D	75	HIS
1	D	110	ASN
1	D	228	ASN
1	D	265	GLN
1	D	299	ASN
1	D	394	HIS
1	D	470	HIS
1	D	583	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	B	586	-	4,4,4	0.89	0	6,6,6	0.89	0
2	PO4	A	586	-	4,4,4	0.83	0	6,6,6	0.74	0
2	PO4	C	586	-	4,4,4	0.84	0	6,6,6	0.68	0
2	PO4	D	586	-	4,4,4	0.87	0	6,6,6	0.58	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.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	586	PO4	2	0
2	A	586	PO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	586	PO4	2	0
2	D	586	PO4	1	0

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	583/606 (96%)	-0.34	1 (0%) 91 83	59, 108, 154, 195	0
1	B	583/606 (96%)	-0.28	1 (0%) 91 83	63, 123, 196, 226	0
1	C	583/606 (96%)	-0.33	0 100 100	66, 126, 196, 226	0
1	D	583/606 (96%)	-0.33	2 (0%) 90 80	74, 116, 155, 218	0
All	All	2332/2424 (96%)	-0.32	4 (0%) 91 83	59, 117, 184, 226	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	150	GLY	3.0
1	D	294	ALA	2.1
1	D	292	ALA	2.1
1	B	146	ILE	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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($\text{\AA}^2$)	Q<0.9
2	PO4	D	586	5/5	0.82	0.10	121,125,147,148	0
2	PO4	C	586	5/5	0.84	0.07	111,127,142,143	0
2	PO4	A	586	5/5	0.92	0.06	93,107,128,132	0
2	PO4	B	586	5/5	0.92	0.09	90,117,140,141	0

6.5 Other polymers [i](#)

There are no such residues in this entry.