



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 3NZQ / pdb_00003nzq
Title : Crystal Structure of Biosynthetic arginine decarboxylase ADC (SpeA) from Escherichia coli, Northeast Structural Genomics Consortium Target ER600
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Deposited on : 2010-07-16
Resolution : 3.10 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

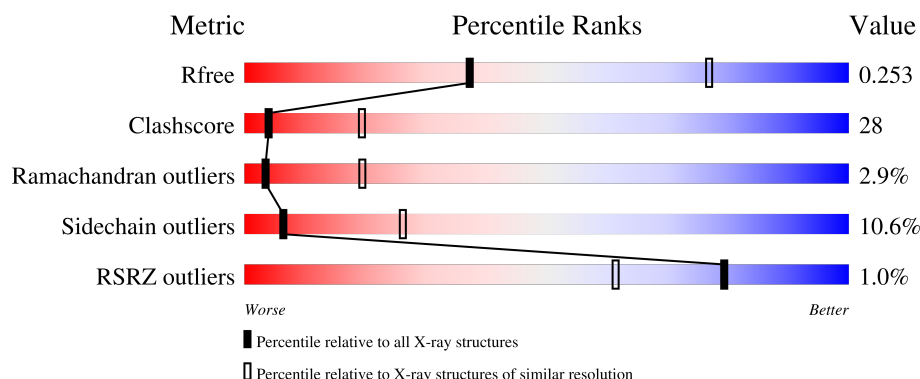
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	666	% 49% 38% 7% 6%
1	B	666	% 49% 39% 6% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10064 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 Biosynthetic arginine decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	628	Total	C	N	O	S	0	0	0
			4984	3142	862	953	27			
1	B	628	Total	C	N	O	S	0	0	0
			4984	3142	862	953	27			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	659	LEU	-	expression tag	UNP P21170
A	660	GLU	-	expression tag	UNP P21170
A	661	HIS	-	expression tag	UNP P21170
A	662	HIS	-	expression tag	UNP P21170
A	663	HIS	-	expression tag	UNP P21170
A	664	HIS	-	expression tag	UNP P21170
A	665	HIS	-	expression tag	UNP P21170
A	666	HIS	-	expression tag	UNP P21170
B	659	LEU	-	expression tag	UNP P21170
B	660	GLU	-	expression tag	UNP P21170
B	661	HIS	-	expression tag	UNP P21170
B	662	HIS	-	expression tag	UNP P21170
B	663	HIS	-	expression tag	UNP P21170
B	664	HIS	-	expression tag	UNP P21170
B	665	HIS	-	expression tag	UNP P21170
B	666	HIS	-	expression tag	UNP P21170

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

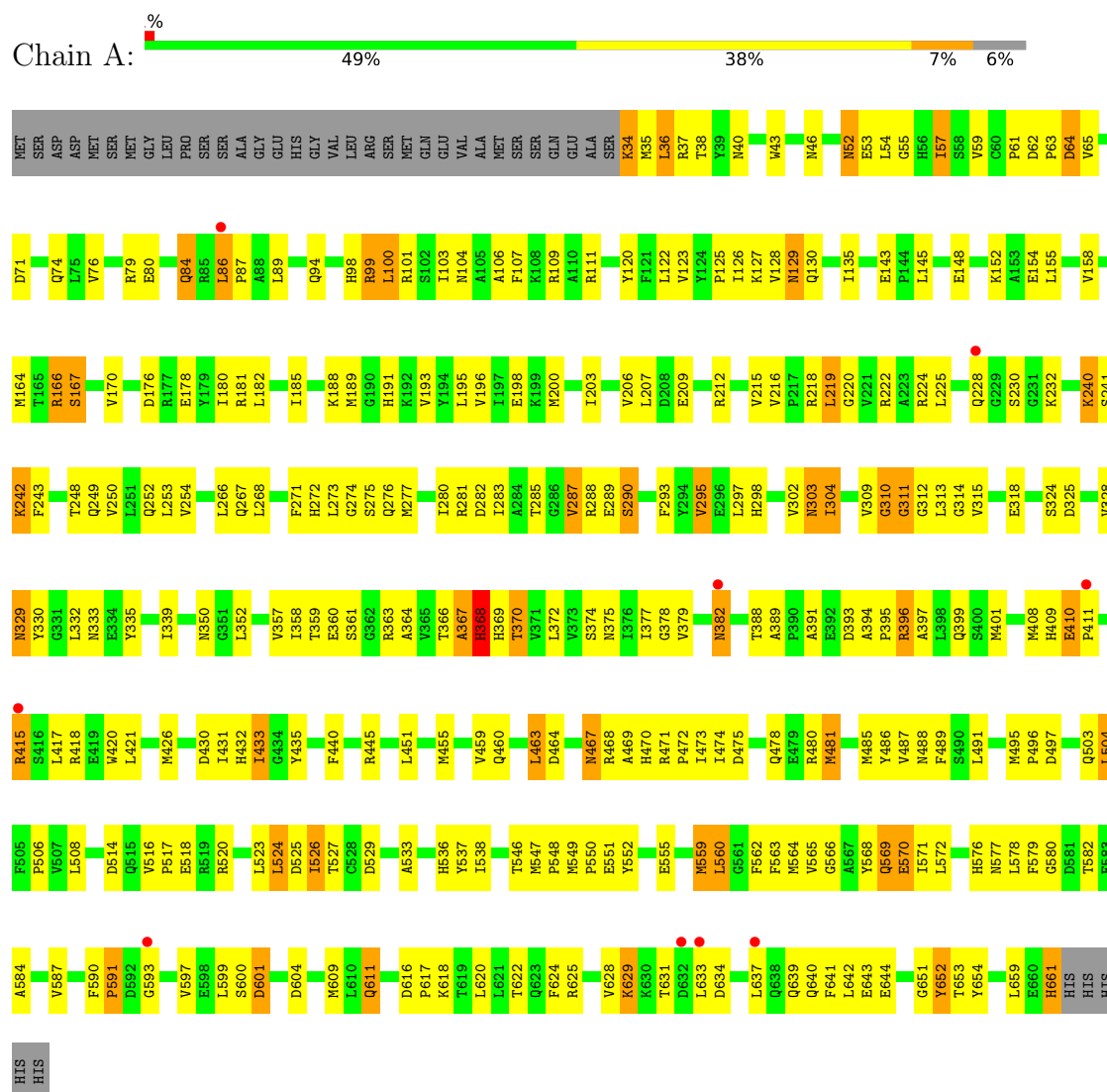
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	36	Total	O	0	0
			36	36		
3	B	40	Total	O	0	0
			40	40		

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: Biosynthetic arginine decarboxylase



• Molecule 1: Biosynthetic arginine decarboxylase



MET	Q74	M164	S241	V328	B415	V516	F588
SER	Q75	T165	K242	V329	S416	P517	V589
ASP	L76	R166	F243	Y330	R417	E518	F590
ASP	V76	S167	T248	G331	R418	D592	P591
MET	R79	V170	Q249	L332	W420	R520	G593
SER	E80	D176	V250	N333	L421	L523	E596
MET	Q84	R177	L251	Y334	M426	L524	V597
GLY	R85	E178	Q252	Y335	D430	D525	E598
PRO	L86	Y179	V254	I339	I431	I526	L599
SER	P87	I180	L266	N350	I433	T527	S600
ALA	A88	R181	Q267	G351	I433	C528	D601
GLY	L89	L182	L268	L352	L451	D529	D604
GLU	Q94	I185	F271	I358	M455	A533	M609
HIS	H98	K188	H272	T359	V459	H536	L610
GLY	R99	M189	L273	E360	Q460	Y537	Q611
VAL	L100	G190	G274	S361	I463	I538	Q611
ARG	R101	K191	S275	G362	D464	T546	D616
MET	S102	K192	Q276	R363	M467	M547	P617
GLN	I103	V193	M277	A364	R468	P548	K618
GLU	N104	Y194	I280	A367	H470	M549	T619
VAL	A105	V195	R281	H368	P472	P550	L620
ALA	A106	V196	D282	H369	L473	F551	L621
MET	F107	E198	L283	T370	D475	Y552	T622
SER	K108	E199	T285	V371	Q478	D553	Q623
SER	R109	K199	T286	L372	F479	P554	F624
GLN	A110	M200	G286	V373	R480	E555	R625
GLU	R111	L203	V287	G376	M481	N556	V628
ALA	Y120	V206	R288	V379	R481	P557	K629
SER	F121	L207	E289	N382	M485	P558	K630
M35	L122	D208	S290	T388	Y486	M559	T631
L36	V123	E209	F293	A389	V487	L560	D632
R37	Y124	R212	Y294	P390	M488	G561	L633
T38	P125	L213	V295	A391	F489	F562	D634
T39	I126	N214	E296	E392	S490	F563	Q639
N40	K127	V215	L297	D393	L491	M564	Q640
N46	N129	V216	H298	A394	M495	V565	F641
V51	Q130	P217	V302	P395	P496	G566	L642
N52	I135	R218	N303	R396	D497	A567	E643
E53	E143	L219	I304	A397	M498	Y568	E644
L54	P144	G220	V309	P399	F503	Q569	Y652
I57	L145	V221	G310	L396	L504	E570	T653
S58	E148	A223	G311	Q399	F505	L572	Y654
V59	S151	R224	L225	S400	P506	H576	D657
O60	K152	L225	L313	M401	F507	N577	E658
P61	Q228	G229	V315	M408	L509	F579	L659
D62	E153	S230	E318	H409	L509	G580	E660
P63	E154	G231	Q323	E410	L513	D581	H661
D64	L155	K232	S324	P411		T582	HIS
V65	V158	K240	D325			E583	HIS
V70						A584	HIS
D71						V587	HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	192.52Å 192.52Å 119.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 3.10 19.94 – 3.10	Depositor EDS
% Data completeness (in resolution range)	82.2 (19.94-3.10) 91.9 (19.94-3.10)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.58 (at 3.11Å)	Xtriage
Refinement program	REFMAC, CNS 1.2	Depositor
R, R_{free}	0.200 , 0.239 0.217 , 0.253	Depositor DCC
R_{free} test set	4133 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å ²)	65.3	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 57.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10064	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.57	1/5094 (0.0%)	0.91	7/6910 (0.1%)
1	B	0.55	1/5094 (0.0%)	0.91	5/6910 (0.1%)
All	All	0.56	2/10188 (0.0%)	0.91	12/13820 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	426	MET	SD-CE	6.11	1.94	1.79
1	A	426	MET	SD-CE	5.78	1.94	1.79

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	SER	CB-CA-C	-6.69	97.48	110.46
1	B	290	SER	CB-CA-C	-6.69	97.48	110.46
1	B	368	HIS	N-CA-C	6.58	118.46	109.11
1	A	368	HIS	N-CA-C	6.42	118.22	109.11
1	A	591	PRO	N-CA-C	-5.50	106.99	113.86
1	A	196	VAL	N-CA-C	5.43	116.01	108.84
1	A	64	ASP	N-CA-C	-5.39	106.20	112.89
1	B	593	GLY	N-CA-C	-5.23	108.26	114.48
1	B	196	VAL	N-CA-C	5.14	115.62	108.84
1	A	593	GLY	N-CA-C	-5.09	108.43	114.48
1	B	591	PRO	N-CA-C	-5.05	107.55	113.86
1	A	43	TRP	N-CA-C	5.04	117.55	111.40

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	4984	0	4830	280	0
1	B	4984	0	4830	270	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	36	0	0	3	0
3	B	40	0	0	1	0
All	All	10064	0	9660	550	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 28.

All (550) 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:212:ARG:NH2	1:B:212:ARG:HB3	1.86	0.90
1:B:126:ILE:HG22	1:B:130:GLN:HG3	1.53	0.90
1:A:212:ARG:HB3	1:A:212:ARG:NH2	1.86	0.90
1:B:297:LEU:O	1:B:302:VAL:HG12	1.73	0.89
1:A:631:THR:HG23	1:A:633:LEU:H	1.37	0.88
1:B:631:THR:HG23	1:B:633:LEU:H	1.37	0.88
1:A:126:ILE:HG22	1:A:130:GLN:HG3	1.55	0.87
1:B:396:ARG:H	1:B:396:ARG:HE	1.23	0.86
1:B:527:THR:HG22	1:B:529:ASP:H	1.40	0.86
1:B:266:LEU:HD22	1:B:302:VAL:HG21	1.58	0.86
1:A:297:LEU:O	1:A:302:VAL:HG12	1.74	0.86
1:A:266:LEU:HD22	1:A:302:VAL:HG21	1.57	0.85
1:A:396:ARG:H	1:A:396:ARG:HE	1.22	0.84
1:A:527:THR:HG22	1:A:529:ASP:H	1.41	0.84
1:B:122:LEU:HD12	1:B:359:THR:HG23	1.60	0.84
1:B:212:ARG:HB3	1:B:212:ARG:HH21	1.40	0.84
1:A:212:ARG:HB3	1:A:212:ARG:HH21	1.41	0.83
1:A:122:LEU:HD12	1:A:359:THR:HG23	1.62	0.82
1:B:375:ASN:HB3	1:B:559:MET:HE2	1.61	0.81
1:A:375:ASN:HB3	1:A:559:MET:HE2	1.62	0.81
1:A:485:MET:SD	1:A:549:MET:HE2	2.22	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:ASP:H	1:A:569:GLN:HE22	1.30	0.79
1:B:485:MET:SD	1:B:549:MET:HE2	2.22	0.79
1:B:418:ARG:HG2	3:B:670:HOH:O	1.82	0.79
1:B:297:LEU:HG	1:B:302:VAL:HG11	1.67	0.77
1:B:565:VAL:HG23	1:B:569:GLN:HG2	1.67	0.77
1:A:297:LEU:HG	1:A:302:VAL:HG11	1.66	0.77
1:B:571:ILE:O	1:B:571:ILE:HG12	1.82	0.77
1:A:571:ILE:HG12	1:A:571:ILE:O	1.83	0.76
1:B:280:ILE:H	1:B:329:ASN:HD21	1.34	0.76
1:B:497:ASP:H	1:B:569:GLN:HE22	1.33	0.75
1:A:280:ILE:H	1:A:329:ASN:HD21	1.34	0.74
1:A:379:VAL:HG12	1:A:485:MET:HB3	1.71	0.73
1:A:372:LEU:HB3	1:A:562:PHE:HB2	1.71	0.73
1:A:524:LEU:HB3	1:A:533:ALA:HB2	1.72	0.72
1:A:565:VAL:HG23	1:A:569:GLN:HG2	1.70	0.72
1:B:79:ARG:HB3	1:B:84:GLN:HG3	1.72	0.71
1:B:379:VAL:HG12	1:B:485:MET:HB3	1.73	0.71
1:B:86:LEU:HD22	1:B:86:LEU:H	1.56	0.70
1:B:628:VAL:HG21	1:B:642:LEU:HD11	1.74	0.70
1:A:276:GLN:HE22	1:A:315:VAL:H	1.40	0.69
1:A:79:ARG:HB3	1:A:84:GLN:HG3	1.74	0.69
1:A:467:ASN:HD22	1:A:468:ARG:N	1.90	0.69
1:B:200:MET:O	1:B:203:ILE:HG22	1.93	0.69
1:B:276:GLN:HE22	1:B:315:VAL:H	1.41	0.69
1:A:628:VAL:HG21	1:A:642:LEU:HD11	1.73	0.68
1:B:293:PHE:O	1:B:297:LEU:HB2	1.93	0.68
1:A:497:ASP:H	1:A:569:GLN:NE2	1.91	0.68
1:A:293:PHE:O	1:A:297:LEU:HB2	1.94	0.68
1:B:372:LEU:HB3	1:B:562:PHE:HB2	1.75	0.68
1:B:467:ASN:HD22	1:B:468:ARG:N	1.92	0.68
1:A:86:LEU:H	1:A:86:LEU:HD22	1.58	0.67
1:B:57:ILE:HD13	1:B:57:ILE:C	2.19	0.67
1:A:200:MET:O	1:A:203:ILE:HG22	1.95	0.67
1:A:497:ASP:HB2	1:A:569:GLN:HE22	1.59	0.67
1:B:524:LEU:HB3	1:B:533:ALA:HB2	1.77	0.67
1:B:497:ASP:HB2	1:B:569:GLN:HE22	1.60	0.67
1:B:86:LEU:HD12	1:B:375:ASN:HD21	1.60	0.66
1:A:368:HIS:H	1:A:368:HIS:CD2	2.12	0.66
1:A:489:PHE:O	1:A:525:ASP:HB2	1.96	0.66
1:B:63:PRO:HG2	1:B:98:HIS:NE2	2.10	0.66
1:A:86:LEU:HB2	1:A:87:PRO:CD	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:GLN:OE1	1:A:232:LYS:HG3	1.96	0.66
1:A:152:LYS:NZ	1:A:178:GLU:HG2	2.11	0.65
1:B:471:ARG:O	1:B:474:ILE:HG22	1.95	0.65
1:A:467:ASN:HD22	1:A:467:ASN:C	2.05	0.65
1:B:103:ILE:CD1	1:B:122:LEU:HD13	2.26	0.65
1:B:584:ALA:HB3	1:B:601:ASP:HB2	1.79	0.65
1:B:228:GLN:OE1	1:B:232:LYS:HG3	1.97	0.65
1:B:368:HIS:CD2	1:B:368:HIS:H	2.14	0.65
1:B:497:ASP:H	1:B:569:GLN:NE2	1.94	0.64
1:B:86:LEU:HB2	1:B:87:PRO:CD	2.27	0.64
1:B:273:LEU:HB2	1:B:277:MET:HE3	1.78	0.64
1:B:580:GLY:H	1:B:653:THR:HG21	1.62	0.64
1:B:467:ASN:HD22	1:B:467:ASN:C	2.06	0.64
1:A:63:PRO:HG2	1:A:98:HIS:NE2	2.12	0.64
1:B:489:PHE:O	1:B:525:ASP:HB2	1.97	0.64
1:A:57:ILE:C	1:A:57:ILE:HD13	2.23	0.63
1:A:71:ASP:HB3	1:A:74:GLN:HB2	1.80	0.63
1:B:471:ARG:N	1:B:472:PRO:HD2	2.13	0.63
1:B:274:GLY:O	1:B:312:GLY:HA2	1.99	0.63
1:A:471:ARG:O	1:A:474:ILE:HG22	1.99	0.63
1:B:52:ASN:HD22	1:B:52:ASN:C	2.06	0.63
1:A:188:LYS:HE3	3:A:688:HOH:O	1.97	0.63
1:B:495:MET:HA	1:B:569:GLN:HE21	1.61	0.63
1:A:276:GLN:NE2	1:A:315:VAL:H	1.96	0.62
1:A:471:ARG:HA	1:A:474:ILE:HG22	1.81	0.62
1:A:471:ARG:N	1:A:472:PRO:HD2	2.14	0.62
1:A:584:ALA:HB3	1:A:601:ASP:HB2	1.81	0.62
1:A:86:LEU:HD12	1:A:375:ASN:HD21	1.64	0.62
1:B:276:GLN:NE2	1:B:315:VAL:H	1.97	0.62
1:A:280:ILE:HB	1:A:330:TYR:HB3	1.81	0.62
1:A:491:LEU:HD12	1:A:495:MET:HE3	1.81	0.62
1:B:152:LYS:NZ	1:B:178:GLU:HG2	2.15	0.62
1:B:280:ILE:HB	1:B:330:TYR:HB3	1.81	0.62
1:B:394:ALA:HB1	1:B:395:PRO:HD2	1.82	0.62
1:A:52:ASN:C	1:A:52:ASN:HD22	2.06	0.62
1:A:127:LYS:HG3	1:A:128:VAL:N	2.14	0.62
1:A:273:LEU:HB2	1:A:277:MET:HE3	1.81	0.61
1:B:120:TYR:HE1	1:B:359:THR:HG22	1.65	0.61
1:B:127:LYS:HG3	1:B:128:VAL:N	2.15	0.61
1:B:471:ARG:HA	1:B:474:ILE:HG22	1.81	0.61
1:B:35:MET:SD	1:B:550:PRO:HG3	2.41	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:ILE:HD13	1:B:433:ILE:O	2.01	0.61
1:B:71:ASP:HB3	1:B:74:GLN:HB2	1.83	0.60
1:A:274:GLY:O	1:A:312:GLY:HA2	2.01	0.60
1:B:87:PRO:HD3	1:B:488:ASN:ND2	2.16	0.60
1:B:524:LEU:HD22	1:B:524:LEU:H	1.65	0.60
1:A:394:ALA:HB1	1:A:395:PRO:HD2	1.81	0.60
1:A:408:MET:HG2	1:A:420:TRP:CE3	2.36	0.60
1:A:120:TYR:HE1	1:A:359:THR:HG22	1.66	0.60
1:A:271:PHE:CE1	1:A:309:VAL:HA	2.36	0.60
1:A:565:VAL:HG22	1:A:565:VAL:O	2.01	0.60
1:A:103:ILE:CD1	1:A:122:LEU:HD13	2.32	0.60
1:A:433:ILE:HD13	1:A:433:ILE:O	2.02	0.60
1:A:87:PRO:HD3	1:A:488:ASN:ND2	2.16	0.59
1:A:620:LEU:HD23	1:A:620:LEU:O	2.02	0.59
1:B:297:LEU:HD23	1:B:304:ILE:CD1	2.32	0.59
1:B:314:GLY:HA3	1:B:328:VAL:HG11	1.82	0.59
1:B:639:GLN:O	1:B:643:GLU:HG2	2.02	0.59
1:A:495:MET:HA	1:A:569:GLN:HE21	1.66	0.59
1:B:620:LEU:O	1:B:620:LEU:HD23	2.02	0.59
1:A:297:LEU:HD23	1:A:304:ILE:CD1	2.32	0.59
1:A:311:GLY:H	1:A:360:GLU:H	1.50	0.59
1:A:524:LEU:HD22	1:A:524:LEU:H	1.67	0.59
1:A:639:GLN:O	1:A:643:GLU:HG2	2.02	0.59
1:A:280:ILE:N	1:A:329:ASN:HD21	1.99	0.59
1:B:565:VAL:HG22	1:B:565:VAL:O	2.01	0.59
1:A:491:LEU:CD1	1:A:495:MET:HE3	2.32	0.59
1:A:123:VAL:HG23	1:A:358:ILE:HG23	1.84	0.58
1:B:280:ILE:N	1:B:329:ASN:HD21	2.00	0.58
1:A:248:THR:HG22	1:A:252:GLN:HE21	1.68	0.58
1:B:271:PHE:CE1	1:B:309:VAL:HA	2.38	0.58
1:A:188:LYS:HD3	1:A:215:VAL:HG22	1.86	0.58
1:B:123:VAL:HG23	1:B:358:ILE:HG23	1.85	0.58
1:B:408:MET:HG2	1:B:420:TRP:CE3	2.38	0.58
1:B:590:PHE:HB3	1:B:591:PRO:HD2	1.84	0.58
1:A:275:SER:HB3	1:A:363:ARG:HH11	1.69	0.58
1:A:314:GLY:HA3	1:A:328:VAL:HG11	1.85	0.58
1:A:35:MET:SD	1:A:550:PRO:HG3	2.44	0.57
1:B:220:GLY:HA3	1:B:268:LEU:HB3	1.86	0.57
1:B:248:THR:HG22	1:B:252:GLN:HE21	1.69	0.57
1:A:87:PRO:HD2	1:A:652:TYR:HE2	1.68	0.57
1:A:152:LYS:HZ1	1:A:178:GLU:HG2	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:LEU:HD23	1:A:182:LEU:HD23	1.85	0.57
1:A:401:MET:HB3	1:A:451:LEU:HD22	1.85	0.57
1:B:128:VAL:O	1:B:129:ASN:HB2	2.04	0.57
1:A:401:MET:HE2	1:A:451:LEU:HD22	1.86	0.57
1:A:128:VAL:O	1:A:129:ASN:HB2	2.05	0.57
1:A:640:GLN:HA	1:A:643:GLU:HG3	1.86	0.57
1:A:369:HIS:CE1	1:A:370:THR:HG22	2.40	0.57
1:B:433:ILE:HD13	1:B:433:ILE:C	2.30	0.57
1:A:504:LEU:HD21	1:A:536:HIS:HB2	1.86	0.57
1:B:401:MET:HE2	1:B:451:LEU:HD22	1.86	0.57
1:B:218:ARG:HH21	1:B:267:GLN:HE22	1.52	0.56
1:A:62:ASP:OD1	1:A:64:ASP:HB2	2.04	0.56
1:B:76:VAL:HG11	1:B:559:MET:HG2	1.87	0.56
1:B:640:GLN:HA	1:B:643:GLU:HG3	1.87	0.56
1:A:198:GLU:HB3	1:A:243:PHE:HB3	1.88	0.56
1:B:311:GLY:H	1:B:360:GLU:H	1.53	0.56
1:B:401:MET:HB3	1:B:451:LEU:HD22	1.87	0.56
1:A:220:GLY:HA3	1:A:268:LEU:HB3	1.88	0.56
1:B:188:LYS:HD3	1:B:215:VAL:HG22	1.88	0.56
1:B:491:LEU:HD12	1:B:495:MET:HE3	1.86	0.56
1:B:463:LEU:HD23	1:B:474:ILE:CD1	2.36	0.56
1:B:504:LEU:HD21	1:B:536:HIS:HB2	1.87	0.56
1:B:604:ASP:HB3	1:B:609:MET:HE3	1.88	0.56
1:A:433:ILE:HD13	1:A:433:ILE:C	2.31	0.55
1:A:89:LEU:HD13	1:A:372:LEU:HD23	1.88	0.55
1:A:520:ARG:HH11	1:A:546:THR:HG23	1.70	0.55
1:A:524:LEU:HB3	1:A:533:ALA:CB	2.36	0.55
1:A:418:ARG:HD2	1:A:473:ILE:HD11	1.89	0.55
1:A:382:ASN:N	1:A:382:ASN:HD22	2.05	0.55
1:B:62:ASP:OD1	1:B:64:ASP:HB2	2.07	0.55
1:B:491:LEU:CD1	1:B:495:MET:HE3	2.36	0.55
1:B:275:SER:HB3	1:B:363:ARG:HH11	1.71	0.55
1:A:480:ARG:O	1:A:481:MET:HE3	2.07	0.54
1:B:155:LEU:HD23	1:B:182:LEU:HD23	1.90	0.54
1:A:604:ASP:HB3	1:A:609:MET:HE3	1.88	0.54
1:A:282:ASP:O	1:A:285:THR:HG22	2.07	0.54
1:A:297:LEU:HD23	1:A:304:ILE:HD11	1.90	0.54
1:B:520:ARG:HH11	1:B:546:THR:HG23	1.72	0.54
1:A:463:LEU:HD23	1:A:474:ILE:CD1	2.38	0.54
1:A:653:THR:HG23	1:A:654:TYR:CD1	2.43	0.54
1:B:382:ASN:N	1:B:382:ASN:HD22	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ILE:HG13	1:B:104:ASN:N	2.23	0.54
1:B:198:GLU:HB3	1:B:243:PHE:HB3	1.89	0.54
1:A:640:GLN:O	1:A:644:GLU:HG2	2.08	0.53
1:B:212:ARG:HH21	1:B:212:ARG:CB	2.16	0.53
1:B:266:LEU:C	1:B:266:LEU:HD23	2.33	0.53
1:A:65:VAL:HG23	1:A:65:VAL:O	2.09	0.53
1:A:313:LEU:C	1:A:313:LEU:HD23	2.33	0.53
1:B:176:ASP:O	1:B:180:ILE:HG12	2.08	0.53
1:B:218:ARG:NH2	1:B:267:GLN:HE22	2.06	0.53
1:B:417:LEU:HD23	1:B:418:ARG:H	1.74	0.53
1:A:76:VAL:HG11	1:A:559:MET:HG2	1.91	0.53
1:B:65:VAL:O	1:B:65:VAL:HG23	2.09	0.53
1:B:369:HIS:CE1	1:B:370:THR:HG22	2.44	0.53
1:A:409:HIS:O	1:A:410:GLU:HB2	2.09	0.53
1:A:625:ARG:HH22	1:A:629:LYS:HD3	1.73	0.53
1:B:495:MET:CA	1:B:569:GLN:HE21	2.22	0.53
1:A:103:ILE:HG13	1:A:104:ASN:N	2.22	0.53
1:A:417:LEU:HD23	1:A:418:ARG:H	1.74	0.53
1:A:218:ARG:HH21	1:A:267:GLN:HE22	1.56	0.53
1:A:361:SER:HB3	1:A:364:ALA:HB3	1.90	0.53
1:A:497:ASP:N	1:A:569:GLN:HE22	2.04	0.53
1:B:520:ARG:HB3	1:B:546:THR:OG1	2.09	0.53
1:B:625:ARG:HH22	1:B:629:LYS:HD3	1.73	0.53
1:B:87:PRO:HD2	1:B:652:TYR:HE2	1.75	0.52
1:A:176:ASP:O	1:A:180:ILE:HG12	2.09	0.52
1:A:537:TYR:CD2	1:A:547:MET:HB2	2.45	0.52
1:B:418:ARG:HD2	1:B:473:ILE:HD11	1.90	0.52
1:B:87:PRO:HG3	1:B:654:TYR:CG	2.44	0.52
1:B:480:ARG:O	1:B:481:MET:HE3	2.08	0.52
1:B:368:HIS:HB3	1:B:564:MET:SD	2.50	0.52
1:B:409:HIS:O	1:B:410:GLU:HB2	2.09	0.52
1:A:485:MET:HE2	1:A:552:TYR:OH	2.09	0.52
1:B:297:LEU:HD23	1:B:304:ILE:HD11	1.91	0.52
1:A:418:ARG:HD2	1:A:473:ILE:CD1	2.39	0.52
1:B:658:GLU:HG3	1:B:659:LEU:H	1.75	0.52
1:B:180:ILE:HG23	1:B:206:VAL:HG12	1.92	0.51
1:B:640:GLN:O	1:B:644:GLU:HG2	2.09	0.51
1:B:485:MET:HE2	1:B:552:TYR:OH	2.10	0.51
1:B:40:ASN:HD22	1:B:538:ILE:CG2	2.23	0.51
1:B:537:TYR:CD2	1:B:547:MET:HB2	2.45	0.51
1:A:212:ARG:HH21	1:A:212:ARG:CB	2.17	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ASN:HD22	1:A:538:ILE:CG2	2.23	0.51
1:A:266:LEU:HD23	1:A:266:LEU:C	2.36	0.51
1:B:361:SER:HB3	1:B:364:ALA:HB3	1.92	0.51
1:B:250:VAL:O	1:B:254:VAL:HG23	2.09	0.51
1:B:455:MET:O	1:B:459:VAL:HG23	2.11	0.51
1:B:624:PHE:O	1:B:628:VAL:HG22	2.11	0.51
1:B:232:LYS:O	1:B:232:LYS:HD3	2.11	0.51
1:A:180:ILE:HG23	1:A:206:VAL:HG12	1.93	0.50
1:B:126:ILE:HD12	1:B:135:ILE:HD12	1.92	0.50
1:B:185:ILE:O	1:B:189:MET:HE2	2.10	0.50
1:B:418:ARG:HD2	1:B:473:ILE:CD1	2.40	0.50
1:A:79:ARG:O	1:A:84:GLN:HB2	2.12	0.50
1:A:100:LEU:HD22	1:A:104:ASN:HD22	1.77	0.50
1:B:222:ARG:NH1	1:B:272:HIS:HB3	2.25	0.50
1:A:460:GLN:HE22	1:A:481:MET:HG2	1.77	0.50
1:B:87:PRO:HG3	1:B:654:TYR:CD2	2.45	0.50
1:B:181:ARG:HD3	1:B:209:GLU:OE1	2.12	0.50
1:B:520:ARG:NH2	1:B:548:PRO:HB3	2.26	0.50
1:A:86:LEU:CB	1:A:87:PRO:CD	2.89	0.50
1:A:109:ARG:NH1	1:A:333:ASN:HD21	2.10	0.50
1:B:34:LYS:O	1:B:38:THR:HG23	2.12	0.50
1:B:86:LEU:CB	1:B:87:PRO:CD	2.90	0.50
1:B:485:MET:CE	1:B:552:TYR:OH	2.59	0.50
1:A:232:LYS:O	1:A:232:LYS:HD3	2.11	0.50
1:A:653:THR:HG23	1:A:654:TYR:CE1	2.46	0.50
1:B:120:TYR:CE1	1:B:359:THR:HG22	2.47	0.50
1:A:181:ARG:HD3	1:A:209:GLU:OE1	2.11	0.50
1:A:295:VAL:HG21	1:A:350:ASN:ND2	2.26	0.50
1:A:375:ASN:CB	1:A:559:MET:HE2	2.36	0.50
1:B:375:ASN:CB	1:B:559:MET:HE2	2.37	0.50
1:A:86:LEU:HB2	1:A:87:PRO:HD2	1.94	0.50
1:A:107:PHE:O	1:A:111:ARG:HG3	2.12	0.50
1:A:218:ARG:NH2	1:A:267:GLN:HE22	2.09	0.50
1:A:401:MET:HE2	1:A:451:LEU:CD2	2.42	0.50
1:A:590:PHE:HB3	1:A:591:PRO:HD2	1.92	0.50
1:B:86:LEU:HB3	1:B:488:ASN:HD22	1.77	0.50
1:B:107:PHE:O	1:B:111:ARG:HG3	2.12	0.50
1:B:313:LEU:HD23	1:B:313:LEU:C	2.37	0.50
1:B:100:LEU:HD22	1:B:104:ASN:HD22	1.76	0.49
1:A:222:ARG:NH1	1:A:272:HIS:HB3	2.27	0.49
1:A:417:LEU:HD21	1:A:470:HIS:NE2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:PRO:HG2	1:A:563:PHE:HB2	1.95	0.49
1:B:368:HIS:CD2	1:B:368:HIS:N	2.79	0.49
1:A:101:ARG:HG2	1:A:143:GLU:CG	2.42	0.49
1:A:520:ARG:HB3	1:A:546:THR:OG1	2.12	0.49
1:B:218:ARG:HH21	1:B:267:GLN:NE2	2.10	0.49
1:B:295:VAL:HG21	1:B:350:ASN:ND2	2.26	0.49
1:A:86:LEU:HB3	1:A:488:ASN:HD22	1.77	0.49
1:A:282:ASP:C	1:A:285:THR:HG22	2.37	0.49
1:A:467:ASN:ND2	1:A:469:ALA:H	2.10	0.49
1:B:53:GLU:CD	1:B:53:GLU:H	2.20	0.49
1:B:86:LEU:H	1:B:86:LEU:CD2	2.25	0.49
1:B:106:ALA:HA	1:B:109:ARG:NH1	2.27	0.49
1:A:520:ARG:NH2	1:A:548:PRO:HB3	2.27	0.49
1:A:485:MET:CE	1:A:552:TYR:OH	2.60	0.49
1:A:106:ALA:HA	1:A:109:ARG:NH1	2.28	0.49
1:A:250:VAL:O	1:A:254:VAL:HG23	2.12	0.49
1:B:100:LEU:CD2	1:B:104:ASN:ND2	2.75	0.49
1:B:467:ASN:ND2	1:B:469:ALA:H	2.10	0.49
1:B:370:THR:HG23	1:B:566:GLY:HA2	1.95	0.49
1:A:52:ASN:C	1:A:52:ASN:ND2	2.71	0.48
1:A:368:HIS:CD2	1:A:368:HIS:N	2.78	0.48
1:B:377:ILE:HD11	1:B:488:ASN:HB2	1.94	0.48
1:B:471:ARG:HH11	1:B:471:ARG:HG2	1.78	0.48
1:B:495:MET:C	1:B:569:GLN:HE21	2.20	0.48
1:B:415:ARG:HG3	1:B:415:ARG:HH11	1.78	0.48
1:A:36:LEU:HD13	1:A:37:ARG:N	2.28	0.48
1:B:460:GLN:HE22	1:B:481:MET:HG2	1.78	0.48
1:B:478:GLN:HB3	1:B:520:ARG:HG3	1.96	0.48
1:A:100:LEU:CD2	1:A:104:ASN:ND2	2.76	0.48
1:B:86:LEU:HB2	1:B:87:PRO:HD2	1.94	0.48
1:B:587:VAL:HG13	1:B:597:VAL:HG22	1.95	0.48
1:B:79:ARG:O	1:B:84:GLN:HB2	2.14	0.48
1:A:126:ILE:HD12	1:A:135:ILE:HD12	1.96	0.48
1:A:370:THR:CG2	1:A:566:GLY:HA2	2.44	0.48
1:A:377:ILE:HD11	1:A:488:ASN:HB2	1.95	0.48
1:B:52:ASN:C	1:B:52:ASN:ND2	2.70	0.48
1:B:100:LEU:HD22	1:B:104:ASN:ND2	2.29	0.48
1:B:639:GLN:C	1:B:641:PHE:H	2.21	0.48
1:B:417:LEU:HD21	1:B:470:HIS:NE2	2.29	0.48
1:A:310:GLY:O	1:A:311:GLY:C	2.57	0.48
1:A:455:MET:O	1:A:459:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ILE:HG22	1:B:189:MET:CE	2.44	0.48
1:A:180:ILE:HG21	1:A:206:VAL:HA	1.96	0.48
1:A:587:VAL:HG13	1:A:597:VAL:HG22	1.96	0.48
1:B:89:LEU:HD13	1:B:372:LEU:HD23	1.95	0.48
1:A:53:GLU:H	1:A:53:GLU:CD	2.22	0.47
1:A:523:LEU:HD23	1:A:547:MET:CE	2.43	0.47
1:B:109:ARG:NH1	1:B:333:ASN:HD21	2.11	0.47
1:A:34:LYS:O	1:A:38:THR:HG23	2.14	0.47
1:A:368:HIS:HB3	1:A:564:MET:SD	2.54	0.47
1:B:103:ILE:HD11	1:B:122:LEU:HD13	1.96	0.47
1:A:478:GLN:HB3	1:A:520:ARG:HG3	1.96	0.47
1:A:128:VAL:HG12	1:A:568:TYR:CZ	2.49	0.47
1:B:471:ARG:HA	1:B:474:ILE:CG2	2.44	0.47
1:A:370:THR:HG23	1:A:566:GLY:HA2	1.96	0.47
1:A:495:MET:CA	1:A:569:GLN:HE21	2.27	0.47
1:B:523:LEU:HD23	1:B:547:MET:CE	2.44	0.47
1:B:524:LEU:HB3	1:B:533:ALA:CB	2.42	0.47
1:A:369:HIS:ND1	1:A:370:THR:HG22	2.30	0.47
1:A:464:ASP:H	1:A:470:HIS:CD2	2.32	0.47
1:A:464:ASP:H	1:A:470:HIS:HD2	1.63	0.47
1:B:401:MET:HE2	1:B:451:LEU:CD2	2.43	0.47
1:A:87:PRO:HG3	1:A:654:TYR:CG	2.49	0.47
1:A:100:LEU:HD22	1:A:104:ASN:ND2	2.30	0.47
1:A:185:ILE:HG22	1:A:189:MET:CE	2.45	0.47
1:A:200:MET:HG2	1:A:249:GLN:HB3	1.97	0.47
1:A:218:ARG:HH21	1:A:267:GLN:NE2	2.13	0.47
1:A:518:GLU:HG3	1:A:551:GLU:HB2	1.95	0.47
1:A:624:PHE:O	1:A:628:VAL:HG22	2.15	0.47
1:B:167:SER:H	1:B:191:HIS:CD2	2.33	0.47
1:B:195:LEU:O	1:B:219:LEU:HB2	2.15	0.47
1:B:335:TYR:O	1:B:339:ILE:HG12	2.15	0.47
1:B:370:THR:CG2	1:B:566:GLY:HA2	2.45	0.47
1:B:497:ASP:N	1:B:569:GLN:HE22	2.06	0.47
1:A:120:TYR:CE1	1:A:359:THR:HG22	2.48	0.47
1:B:152:LYS:HZ1	1:B:178:GLU:HG2	1.80	0.47
1:B:518:GLU:HG3	1:B:551:GLU:HB2	1.97	0.47
1:B:180:ILE:HG21	1:B:206:VAL:HA	1.96	0.47
1:B:232:LYS:HE2	1:B:241:SER:HB3	1.97	0.47
1:A:185:ILE:O	1:A:189:MET:HE2	2.15	0.46
1:A:495:MET:C	1:A:569:GLN:HE21	2.23	0.46
1:B:282:ASP:O	1:B:285:THR:HG22	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:ASN:OD1	1:B:481:MET:HE2	2.15	0.46
1:B:242:LYS:HB3	1:B:243:PHE:CD1	2.50	0.46
1:B:313:LEU:HD23	1:B:314:GLY:O	2.16	0.46
1:A:195:LEU:O	1:A:219:LEU:HB2	2.16	0.46
1:B:282:ASP:C	1:B:285:THR:HG22	2.40	0.46
1:A:496:PRO:HD2	1:A:569:GLN:NE2	2.31	0.46
1:A:109:ARG:NH1	1:A:333:ASN:ND2	2.64	0.46
1:B:565:VAL:CG2	1:B:569:GLN:HG2	2.43	0.46
1:B:571:ILE:O	1:B:571:ILE:CG1	2.56	0.46
1:A:154:GLU:O	1:A:158:VAL:HG23	2.16	0.46
1:B:309:VAL:HG11	1:B:339:ILE:HG23	1.98	0.46
1:A:167:SER:H	1:A:191:HIS:CD2	2.34	0.46
1:A:303:ASN:O	1:A:304:ILE:HB	2.15	0.46
1:A:661:HIS:CD2	1:A:661:HIS:N	2.83	0.46
1:B:126:ILE:HG12	1:B:148:GLU:O	2.17	0.46
1:A:35:MET:HE3	1:A:517:PRO:HB3	1.98	0.45
1:A:417:LEU:HD21	1:A:470:HIS:CE1	2.51	0.45
1:B:101:ARG:HG2	1:B:143:GLU:CG	2.46	0.45
1:B:200:MET:HG2	1:B:249:GLN:HB3	1.97	0.45
1:B:303:ASN:O	1:B:304:ILE:HB	2.16	0.45
1:B:377:ILE:CG1	1:B:488:ASN:HB2	2.46	0.45
1:B:417:LEU:HD21	1:B:470:HIS:CE1	2.51	0.45
1:A:335:TYR:O	1:A:339:ILE:HG12	2.17	0.45
1:A:361:SER:HB3	1:A:364:ALA:CB	2.46	0.45
1:A:568:TYR:C	1:A:572:LEU:HD12	2.41	0.45
1:B:464:ASP:H	1:B:470:HIS:CD2	2.33	0.45
1:A:661:HIS:CD2	1:A:661:HIS:H	2.35	0.45
1:A:471:ARG:HA	1:A:474:ILE:CG2	2.45	0.45
1:A:471:ARG:N	1:A:472:PRO:CD	2.79	0.45
1:A:639:GLN:C	1:A:641:PHE:H	2.23	0.45
1:B:489:PHE:CE2	1:B:495:MET:HE2	2.51	0.45
1:A:418:ARG:NH2	3:A:670:HOH:O	2.50	0.45
1:B:489:PHE:HE2	1:B:495:MET:HE2	1.82	0.45
1:B:506:PRO:HG2	1:B:563:PHE:HB2	1.98	0.45
1:A:471:ARG:HG2	1:A:471:ARG:HH11	1.81	0.45
1:A:415:ARG:HG3	1:A:415:ARG:HH11	1.80	0.45
1:A:86:LEU:H	1:A:86:LEU:CD2	2.27	0.45
1:A:126:ILE:HG12	1:A:148:GLU:O	2.17	0.45
1:A:180:ILE:HD12	1:A:206:VAL:HG12	1.99	0.45
1:A:496:PRO:HD2	1:A:569:GLN:HE21	1.82	0.45
1:B:52:ASN:C	1:B:54:LEU:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:LEU:HD22	1:B:86:LEU:N	2.28	0.45
1:B:361:SER:HB3	1:B:364:ALA:CB	2.47	0.45
1:B:471:ARG:N	1:B:472:PRO:CD	2.78	0.45
1:B:524:LEU:HD22	1:B:524:LEU:N	2.31	0.45
1:A:489:PHE:HE2	1:A:495:MET:HE2	1.82	0.45
1:B:224:ARG:HH22	1:B:241:SER:CB	2.29	0.45
1:B:464:ASP:H	1:B:470:HIS:HD2	1.64	0.45
1:A:388:THR:O	1:A:389:ALA:C	2.60	0.44
1:A:463:LEU:HD23	1:A:474:ILE:HD13	1.99	0.44
1:A:523:LEU:HD22	1:A:560:LEU:HD21	1.99	0.44
1:B:396:ARG:HG2	1:B:397:ALA:N	2.32	0.44
1:B:653:THR:HG23	1:B:654:TYR:CD1	2.53	0.44
1:A:225:LEU:HB3	1:A:289:GLU:OE1	2.18	0.44
1:A:526:ILE:HD13	1:A:579:PHE:CZ	2.52	0.44
1:A:309:VAL:HG11	1:A:339:ILE:HG23	1.98	0.44
1:B:310:GLY:O	1:B:311:GLY:C	2.59	0.44
1:B:415:ARG:C	1:B:417:LEU:H	2.25	0.44
1:A:86:LEU:HB3	1:A:488:ASN:ND2	2.33	0.44
1:A:242:LYS:HB3	1:A:243:PHE:CD1	2.53	0.44
1:A:489:PHE:CE2	1:A:495:MET:HE2	2.52	0.44
1:A:313:LEU:HD22	1:A:364:ALA:HB2	2.00	0.44
1:A:318:GLU:O	1:A:538:ILE:HD12	2.18	0.44
1:A:516:VAL:HG23	1:A:517:PRO:HD2	2.00	0.44
1:B:109:ARG:NH1	1:B:333:ASN:ND2	2.66	0.44
1:B:185:ILE:HG22	1:B:189:MET:HE2	1.99	0.44
1:B:193:VAL:HG13	1:B:193:VAL:O	2.18	0.44
1:B:391:ALA:HB3	1:B:394:ALA:HB2	2.00	0.44
1:B:463:LEU:HD23	1:B:474:ILE:HD13	1.99	0.44
1:B:154:GLU:O	1:B:158:VAL:HG23	2.18	0.44
1:A:185:ILE:HG22	1:A:189:MET:HE2	1.99	0.44
1:A:224:ARG:HH22	1:A:241:SER:CB	2.30	0.44
1:A:287:VAL:O	1:A:288:ARG:C	2.60	0.44
1:A:313:LEU:HD23	1:A:314:GLY:O	2.18	0.44
1:A:377:ILE:CG1	1:A:488:ASN:HB2	2.47	0.44
1:A:382:ASN:HD22	1:A:382:ASN:H	1.65	0.44
1:B:222:ARG:HH21	1:B:222:ARG:HG3	1.83	0.44
1:B:382:ASN:HD22	1:B:382:ASN:H	1.65	0.44
1:A:382:ASN:OD1	1:A:481:MET:HE2	2.18	0.43
1:B:125:PRO:HB3	1:B:148:GLU:OE1	2.18	0.43
1:A:193:VAL:HG13	1:A:193:VAL:O	2.18	0.43
1:B:283:ILE:O	1:B:287:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:VAL:HG23	1:B:517:PRO:HD2	2.00	0.43
1:B:554:PRO:O	1:B:661:HIS:HB3	2.18	0.43
1:A:232:LYS:HE2	1:A:241:SER:HB3	2.00	0.43
1:A:580:GLY:HA3	1:A:604:ASP:HB2	2.00	0.43
1:B:128:VAL:HG12	1:B:568:TYR:CZ	2.53	0.43
1:B:329:ASN:HD22	1:B:329:ASN:H	1.67	0.43
1:B:496:PRO:HD2	1:B:569:GLN:NE2	2.33	0.43
1:A:103:ILE:HD11	1:A:122:LEU:HD13	2.00	0.43
1:A:617:PRO:HG2	1:A:618:LYS:HE2	1.99	0.43
1:B:590:PHE:HE1	1:B:596:GLU:HG3	1.83	0.43
1:B:46:ASN:ND2	1:B:99:ARG:HH12	2.16	0.43
1:B:611:GLN:HE21	1:B:611:GLN:HB3	1.50	0.43
1:A:86:LEU:HD22	1:A:86:LEU:N	2.30	0.43
1:A:99:ARG:HH21	1:A:99:ARG:HG2	1.84	0.43
1:A:222:ARG:HH21	1:A:222:ARG:HG3	1.84	0.43
1:A:486:TYR:CD2	1:A:524:LEU:HD23	2.54	0.43
1:A:523:LEU:HD23	1:A:547:MET:HE1	2.01	0.43
1:B:372:LEU:HD12	1:B:562:PHE:CD2	2.53	0.43
1:B:377:ILE:HG22	1:B:377:ILE:O	2.19	0.43
1:A:313:LEU:HD12	1:A:335:TYR:CD1	2.54	0.43
1:A:569:GLN:O	1:A:570:GLU:C	2.62	0.43
1:A:378:GLY:HA2	1:A:661:HIS:HA	2.00	0.43
1:A:206:VAL:HG23	1:A:207:LEU:N	2.34	0.42
1:A:549:MET:HA	1:A:550:PRO:HD3	1.91	0.42
1:B:79:ARG:HB3	1:B:84:GLN:CG	2.45	0.42
1:A:35:MET:CE	1:A:517:PRO:HB3	2.49	0.42
1:A:166:ARG:HA	1:A:191:HIS:HD2	1.85	0.42
1:A:577:ASN:O	1:A:578:LEU:HB2	2.19	0.42
1:B:86:LEU:HB3	1:B:488:ASN:ND2	2.34	0.42
1:B:206:VAL:HG23	1:B:207:LEU:N	2.34	0.42
1:B:287:VAL:O	1:B:288:ARG:C	2.62	0.42
1:A:86:LEU:HD12	1:A:375:ASN:ND2	2.32	0.42
1:A:125:PRO:HB3	1:A:148:GLU:OE1	2.19	0.42
1:A:415:ARG:C	1:A:417:LEU:H	2.26	0.42
1:A:435:TYR:HA	1:A:440:PHE:HB2	2.02	0.42
1:B:76:VAL:O	1:B:80:GLU:HB2	2.20	0.42
1:B:213:LEU:O	1:B:215:VAL:HG23	2.19	0.42
1:B:568:TYR:C	1:B:572:LEU:HD12	2.43	0.42
1:A:240:LYS:NZ	1:A:240:LYS:HB2	2.35	0.42
1:A:547:MET:HE3	1:A:549:MET:SD	2.59	0.42
1:B:35:MET:HE3	1:B:517:PRO:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:617:PRO:HG2	1:B:618:LYS:HE2	2.02	0.42
1:A:487:VAL:HB	1:A:489:PHE:CE1	2.54	0.42
1:A:520:ARG:HE	1:A:546:THR:HG23	1.84	0.42
1:A:329:ASN:H	1:A:329:ASN:HD22	1.65	0.42
1:A:368:HIS:H	1:A:368:HIS:HD2	1.64	0.42
1:A:396:ARG:HG2	1:A:397:ALA:N	2.35	0.42
1:B:604:ASP:CB	1:B:609:MET:HE3	2.50	0.42
1:A:524:LEU:HD22	1:A:524:LEU:N	2.34	0.42
1:B:36:LEU:HD13	1:B:37:ARG:N	2.35	0.42
1:B:314:GLY:HA3	1:B:328:VAL:CG1	2.47	0.42
1:A:52:ASN:C	1:A:54:LEU:H	2.28	0.42
1:A:74:GLN:HA	1:A:74:GLN:OE1	2.20	0.42
1:B:51:VAL:HG22	1:B:513:LEU:HD13	2.02	0.42
1:B:415:ARG:HH11	1:B:470:HIS:CE1	2.38	0.42
1:B:224:ARG:HH22	1:B:241:SER:HB3	1.85	0.41
1:B:388:THR:O	1:B:389:ALA:C	2.60	0.41
1:B:526:ILE:HD13	1:B:579:PHE:CZ	2.55	0.41
1:A:283:ILE:O	1:A:287:VAL:HG22	2.20	0.41
1:A:350:ASN:HB2	1:A:352:LEU:HD13	2.01	0.41
1:A:524:LEU:HA	1:A:533:ALA:HA	2.02	0.41
1:A:611:GLN:HE21	1:A:611:GLN:HB3	1.53	0.41
1:B:266:LEU:HD22	1:B:302:VAL:CG2	2.39	0.41
1:B:487:VAL:HB	1:B:489:PHE:CE1	2.55	0.41
1:B:639:GLN:C	1:B:641:PHE:N	2.78	0.41
1:A:46:ASN:ND2	1:A:99:ARG:HH12	2.18	0.41
1:B:166:ARG:HA	1:B:191:HIS:HD2	1.85	0.41
1:B:569:GLN:O	1:B:570:GLU:C	2.63	0.41
1:B:599:LEU:HD22	1:B:600:SER:H	1.85	0.41
1:A:55:GLY:HA3	1:A:514:ASP:OD2	2.19	0.41
1:A:61:PRO:HB2	1:A:94:GLN:HB2	2.02	0.41
1:A:224:ARG:HH22	1:A:241:SER:HB3	1.86	0.41
1:B:297:LEU:HD12	1:B:297:LEU:HA	1.95	0.41
1:B:496:PRO:HD2	1:B:569:GLN:HE21	1.86	0.41
1:A:366:THR:O	1:A:367:ALA:C	2.64	0.41
1:A:415:ARG:HA	1:A:415:ARG:NH1	2.34	0.41
1:B:318:GLU:O	1:B:538:ILE:HD12	2.21	0.41
1:A:76:VAL:O	1:A:80:GLU:HB2	2.21	0.41
1:A:104:ASN:HA	1:A:120:TYR:HE2	1.85	0.41
1:B:125:PRO:HA	1:B:148:GLU:HB3	2.03	0.41
1:B:222:ARG:HG3	1:B:222:ARG:NH2	2.35	0.41
1:B:225:LEU:HB3	1:B:289:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:GLN:HG2	1:B:323:GLN:O	2.21	0.41
1:B:520:ARG:HE	1:B:546:THR:HG23	1.86	0.41
1:B:577:ASN:O	1:B:578:LEU:HB2	2.21	0.41
1:A:125:PRO:HA	1:A:148:GLU:HB3	2.02	0.41
1:A:372:LEU:HD12	1:A:562:PHE:CD2	2.56	0.41
1:A:391:ALA:HB3	1:A:394:ALA:HB2	2.03	0.41
1:B:350:ASN:HB2	1:B:352:LEU:HD13	2.02	0.41
1:B:471:ARG:C	1:B:474:ILE:HG22	2.46	0.41
1:A:431:ILE:HD13	1:A:445:ARG:HA	2.03	0.41
1:A:599:LEU:HD13	1:A:599:LEU:C	2.46	0.41
1:B:240:LYS:HB2	1:B:240:LYS:NZ	2.36	0.41
1:B:329:ASN:HD22	1:B:329:ASN:N	2.19	0.41
1:A:358:ILE:HG22	1:A:359:THR:N	2.36	0.41
1:A:604:ASP:CB	1:A:609:MET:HE3	2.49	0.41
1:B:70:VAL:HG21	1:B:589:VAL:HG22	2.03	0.41
1:B:104:ASN:HA	1:B:120:TYR:HE2	1.86	0.41
1:B:313:LEU:HD22	1:B:364:ALA:HB2	2.02	0.41
1:A:408:MET:HG2	1:A:420:TRP:CZ3	2.56	0.40
1:A:637:LEU:HA	1:A:640:GLN:HG2	2.02	0.40
1:B:151:SER:OG	1:B:154:GLU:HG3	2.21	0.40
1:A:120:TYR:HD1	1:A:357:VAL:O	2.04	0.40
1:A:565:VAL:CG2	1:A:569:GLN:HG2	2.46	0.40
1:A:463:LEU:HD21	1:A:473:ILE:HG22	2.03	0.40
1:B:362:GLY:O	1:B:363:ARG:C	2.64	0.40
1:B:486:TYR:CD2	1:B:524:LEU:HD23	2.57	0.40
1:B:599:LEU:HD13	1:B:599:LEU:C	2.45	0.40
1:A:152:LYS:HD3	3:A:684:HOH:O	2.21	0.40
1:A:222:ARG:HG3	1:A:222:ARG:NH2	2.35	0.40
1:A:314:GLY:HA3	1:A:328:VAL:CG1	2.50	0.40
1:B:61:PRO:HB2	1:B:94:GLN:HB2	2.03	0.40
1:B:195:LEU:HD12	1:B:195:LEU:HA	1.88	0.40
1:A:329:ASN:HD22	1:A:329:ASN:N	2.18	0.40
1:A:431:ILE:HD12	1:A:431:ILE:C	2.46	0.40
1:A:599:LEU:HD22	1:A:600:SER:H	1.87	0.40
1:A:651:GLY:O	1:A:652:TYR:C	2.64	0.40
1:B:376:ILE:HB	1:B:557:PRO:HG3	2.04	0.40
1:B:547:MET:HE3	1:B:549:MET:SD	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	626/666 (94%)	552 (88%)	56 (9%)	18 (3%)	3	19
1	B	626/666 (94%)	549 (88%)	59 (9%)	18 (3%)	3	19
All	All	1252/1332 (94%)	1101 (88%)	115 (9%)	36 (3%)	3	19

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	LEU
1	A	230	SER
1	A	576	HIS
1	B	86	LEU
1	B	230	SER
1	B	576	HIS
1	A	129	ASN
1	A	310	GLY
1	A	324	SER
1	A	367	ALA
1	A	634	ASP
1	A	652	TYR
1	B	129	ASN
1	B	310	GLY
1	B	324	SER
1	B	367	ALA
1	A	166	ARG
1	A	242	LYS
1	A	311	GLY
1	A	411	PRO
1	B	166	ARG
1	B	242	LYS
1	B	634	ASP
1	A	570	GLU
1	A	616	ASP

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Mol	Chain	Res	Type
1	B	311	GLY
1	B	411	PRO
1	B	570	GLU
1	B	616	ASP
1	A	304	ILE
1	B	304	ILE
1	B	657	ASP
1	A	410	GLU
1	B	526	ILE
1	A	526	ILE
1	B	410	GLU

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	534/566 (94%)	478 (90%)	56 (10%)	6	26
1	B	534/566 (94%)	477 (89%)	57 (11%)	6	25
All	All	1068/1132 (94%)	955 (89%)	113 (11%)	6	26

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	36	LEU
1	A	52	ASN
1	A	57	ILE
1	A	59	VAL
1	A	84	GLN
1	A	99	ARG
1	A	100	LEU
1	A	145	LEU
1	A	164	MET
1	A	167	SER
1	A	170	VAL

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Mol	Chain	Res	Type
1	A	216	VAL
1	A	219	LEU
1	A	240	LYS
1	A	253	LEU
1	A	281	ARG
1	A	287	VAL
1	A	290	SER
1	A	295	VAL
1	A	298	HIS
1	A	303	ASN
1	A	325	ASP
1	A	329	ASN
1	A	332	LEU
1	A	368	HIS
1	A	370	THR
1	A	374	SER
1	A	382	ASN
1	A	393	ASP
1	A	396	ARG
1	A	399	GLN
1	A	415	ARG
1	A	421	LEU
1	A	430	ASP
1	A	432	HIS
1	A	433	ILE
1	A	463	LEU
1	A	467	ASN
1	A	475	ASP
1	A	481	MET
1	A	503	GLN
1	A	504	LEU
1	A	508	LEU
1	A	524	LEU
1	A	555	GLU
1	A	559	MET
1	A	560	LEU
1	A	569	GLN
1	A	582	THR
1	A	601	ASP
1	A	611	GLN
1	A	622	THR
1	A	629	LYS

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Mol	Chain	Res	Type
1	A	659	LEU
1	A	661	HIS
1	B	34	LYS
1	B	36	LEU
1	B	52	ASN
1	B	57	ILE
1	B	59	VAL
1	B	84	GLN
1	B	99	ARG
1	B	100	LEU
1	B	145	LEU
1	B	164	MET
1	B	167	SER
1	B	170	VAL
1	B	216	VAL
1	B	219	LEU
1	B	240	LYS
1	B	253	LEU
1	B	281	ARG
1	B	287	VAL
1	B	290	SER
1	B	295	VAL
1	B	298	HIS
1	B	325	ASP
1	B	329	ASN
1	B	332	LEU
1	B	368	HIS
1	B	370	THR
1	B	374	SER
1	B	382	ASN
1	B	393	ASP
1	B	396	ARG
1	B	399	GLN
1	B	415	ARG
1	B	421	LEU
1	B	430	ASP
1	B	432	HIS
1	B	433	ILE
1	B	463	LEU
1	B	467	ASN
1	B	475	ASP
1	B	481	MET

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Mol	Chain	Res	Type
1	B	497	ASP
1	B	503	GLN
1	B	504	LEU
1	B	508	LEU
1	B	524	LEU
1	B	555	GLU
1	B	559	MET
1	B	560	LEU
1	B	569	GLN
1	B	582	THR
1	B	601	ASP
1	B	611	GLN
1	B	618	LYS
1	B	622	THR
1	B	629	LYS
1	B	632	ASP
1	B	659	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	46	ASN
1	A	52	ASN
1	A	84	GLN
1	A	97	GLN
1	A	104	ASN
1	A	172	ASN
1	A	191	HIS
1	A	252	GLN
1	A	267	GLN
1	A	270	HIS
1	A	276	GLN
1	A	303	ASN
1	A	305	GLN
1	A	329	ASN
1	A	333	ASN
1	A	338	ASN
1	A	350	ASN
1	A	368	HIS
1	A	382	ASN
1	A	406	GLN

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Mol	Chain	Res	Type
1	A	460	GLN
1	A	466	GLN
1	A	467	ASN
1	A	470	HIS
1	A	488	ASN
1	A	503	GLN
1	A	515	GLN
1	A	556	ASN
1	A	569	GLN
1	A	574	ASN
1	A	611	GLN
1	A	638	GLN
1	A	639	GLN
1	B	40	ASN
1	B	46	ASN
1	B	52	ASN
1	B	84	GLN
1	B	97	GLN
1	B	104	ASN
1	B	172	ASN
1	B	191	HIS
1	B	252	GLN
1	B	267	GLN
1	B	270	HIS
1	B	276	GLN
1	B	303	ASN
1	B	305	GLN
1	B	329	ASN
1	B	333	ASN
1	B	338	ASN
1	B	350	ASN
1	B	368	HIS
1	B	382	ASN
1	B	406	GLN
1	B	429	HIS
1	B	460	GLN
1	B	467	ASN
1	B	470	HIS
1	B	488	ASN
1	B	503	GLN
1	B	515	GLN
1	B	556	ASN

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Mol	Chain	Res	Type
1	B	569	GLN
1	B	574	ASN
1	B	611	GLN
1	B	639	GLN
1	B	661	HIS

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	SO4	B	702	-	4,4,4	0.33	0	6,6,6	0.08	0
2	SO4	A	701	-	4,4,4	0.37	0	6,6,6	0.08	0
2	SO4	A	702	-	4,4,4	0.33	0	6,6,6	0.07	0
2	SO4	B	701	-	4,4,4	0.41	0	6,6,6	0.10	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	628/666 (94%)	-0.01	9 (1%) 73 53	45, 70, 111, 144	0
1	B	628/666 (94%)	-0.12	4 (0%) 85 70	40, 71, 109, 139	0
All	All	1256/1332 (94%)	-0.06	13 (1%) 79 61	40, 71, 110, 144	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	415	ARG	3.5
1	A	228	GLN	3.0
1	A	382	ASN	2.8
1	A	593	GLY	2.8
1	B	415	ARG	2.4
1	A	86	LEU	2.4
1	A	633	LEU	2.3
1	A	637	LEU	2.2
1	B	228	GLN	2.1
1	B	631	THR	2.1
1	A	411	PRO	2.1
1	B	518	GLU	2.1
1	A	632	ASP	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($\text{\AA}^2$)	Q<0.9
2	SO4	A	702	5/5	0.83	0.25	60,62,66,72	5
2	SO4	B	702	5/5	0.84	0.29	55,56,59,64	5
2	SO4	B	701	5/5	0.95	0.09	65,68,76,76	0
2	SO4	A	701	5/5	0.98	0.08	60,62,65,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.