



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2016 – 11:18 AM GMT

PDB ID : 4ZIC  
Title : Crystal Structure of Aspartate Semialdehyde Dehydrogenase with NADP from  
Trichophyton rubrum  
Authors : Li, Q.; Cui, S.  
Deposited on : 2015-04-28  
Resolution : 2.55 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

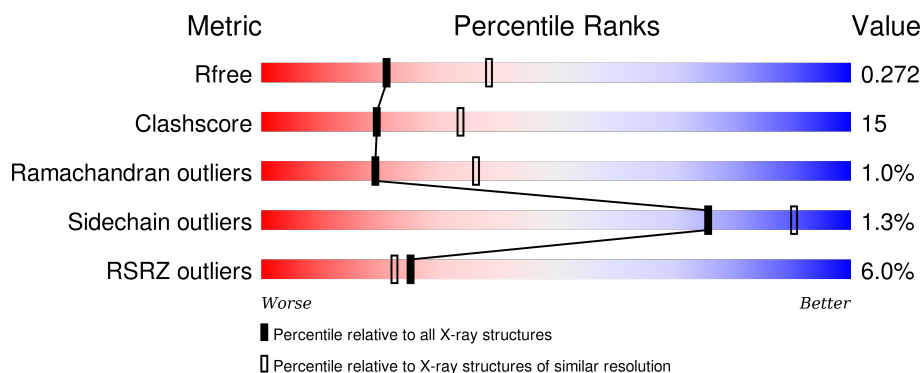
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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))
$R_{free}$	91344	3324 (2.60-2.52)
Clashscore	102246	3729 (2.60-2.52)
Ramachandran outliers	100387	3673 (2.60-2.52)
Sidechain outliers	100360	3673 (2.60-2.52)
RSRZ outliers	91569	3333 (2.60-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	379	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>20%</div> <div>• 7%</div> </div> </div>
1	B	379	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>• 6%</div> </div> </div>
1	C	379	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>19%</div> <div>• 6%</div> </div> </div>
1	D	379	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>• 6%</div> </div> </div>
1	E	379	<div> <div>9%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>• 6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	379	<div><div></div><div>9%</div><div>72%</div><div>21%</div><div>• 6%</div></div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 32311 atoms, of which 15487 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 Aspartate Semialdehyde Dehydrogenase.

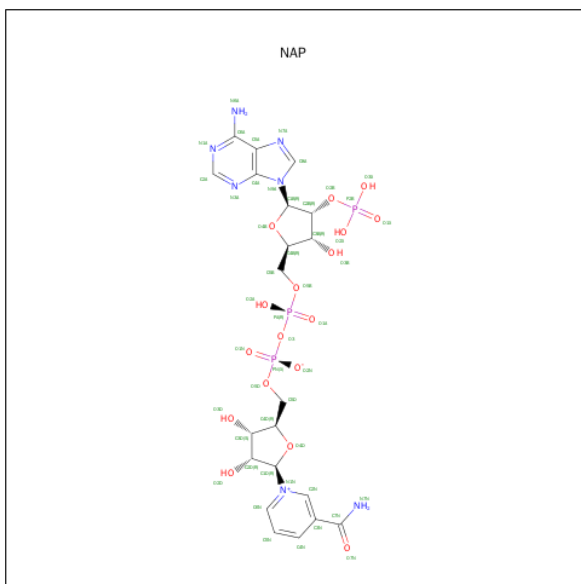
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	D	356	Total	C	H	N	O	S	0	0	0
			5061	1684	2388	467	503	19			
1	C	357	Total	C	H	N	O	S	0	5	0
			5343	1708	2632	473	511	19			
1	A	354	Total	C	H	N	O	S	0	5	0
			5272	1695	2586	467	505	19			
1	B	357	Total	C	H	N	O	S	0	0	0
			5313	1687	2634	468	505	19			
1	E	357	Total	C	H	N	O	S	0	0	0
			5317	1687	2638	468	505	19			
1	F	357	Total	C	H	N	O	S	0	0	0
			5288	1687	2609	468	505	19			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C N O P 48 21 7 17 3	0	0
3	A	1	Total C N O P 96 42 14 34 6	0	1

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	129	Total O 129 129	0	0

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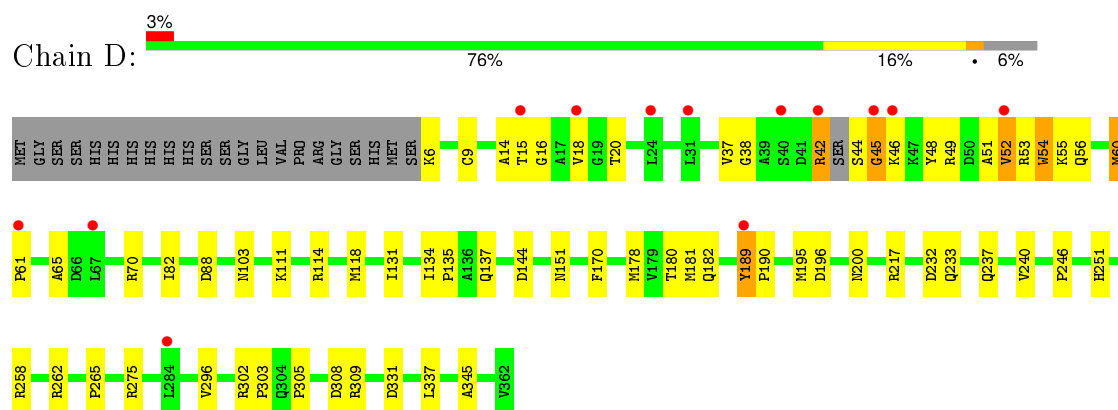
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	88	Total 88	O 88	0	0
4	A	104	Total 104	O 104	0	0
4	B	103	Total 103	O 103	0	0
4	E	64	Total 64	O 64	0	0
4	F	55	Total 55	O 55	0	0

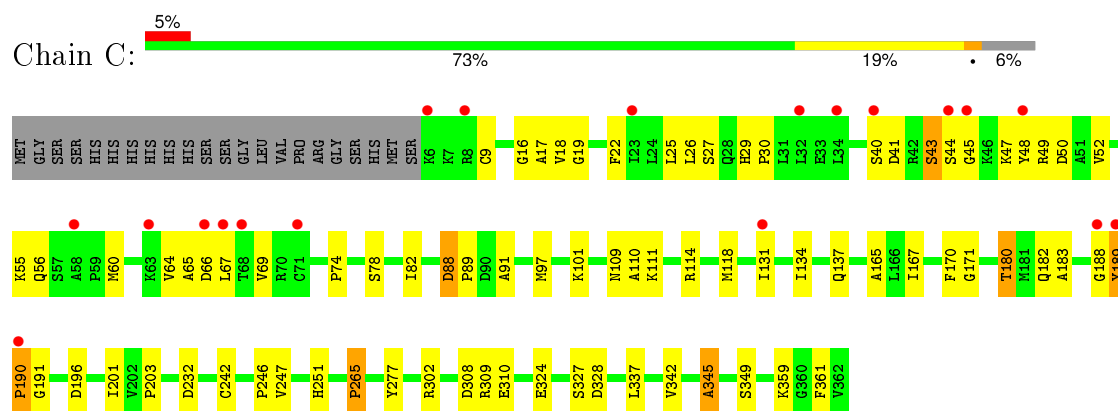
### 3 Residue-property plots [i](#)

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

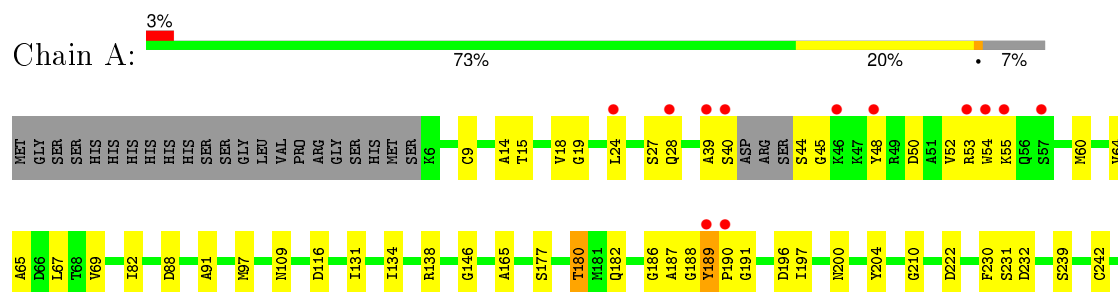
#### • Molecule 1: Aspartate Semialdehyde Dehydrogenase

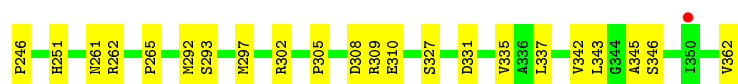


#### • Molecule 1: Aspartate Semialdehyde Dehydrogenase

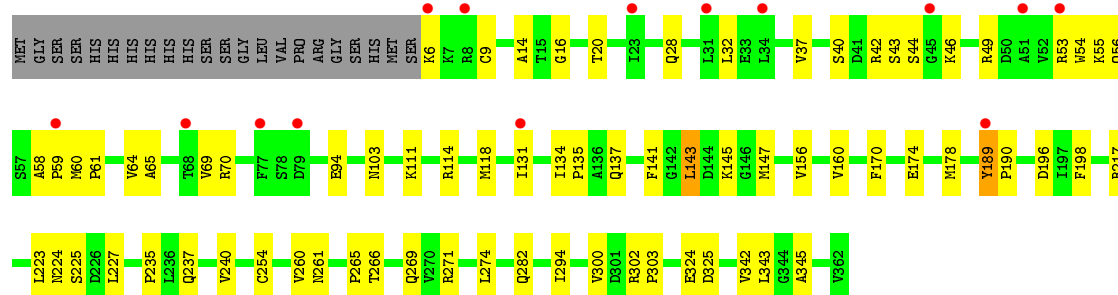
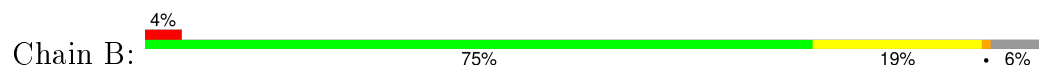


#### • Molecule 1: Aspartate Semialdehyde Dehydrogenase

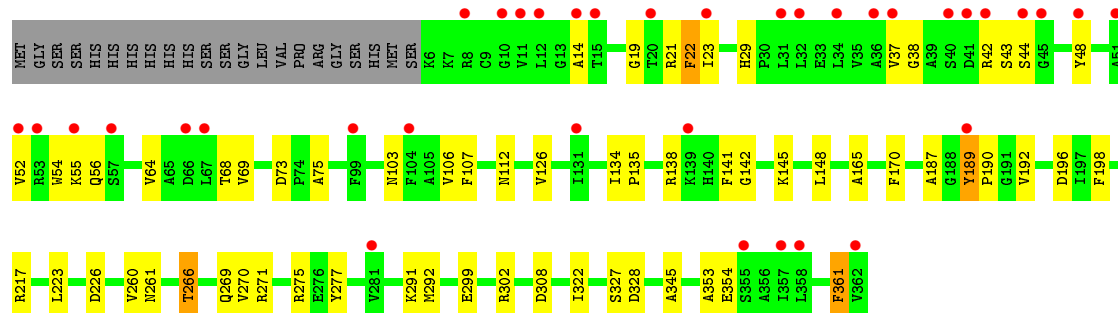
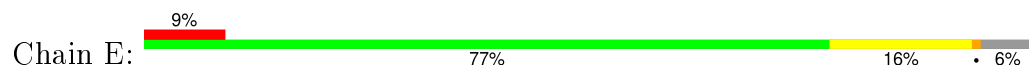




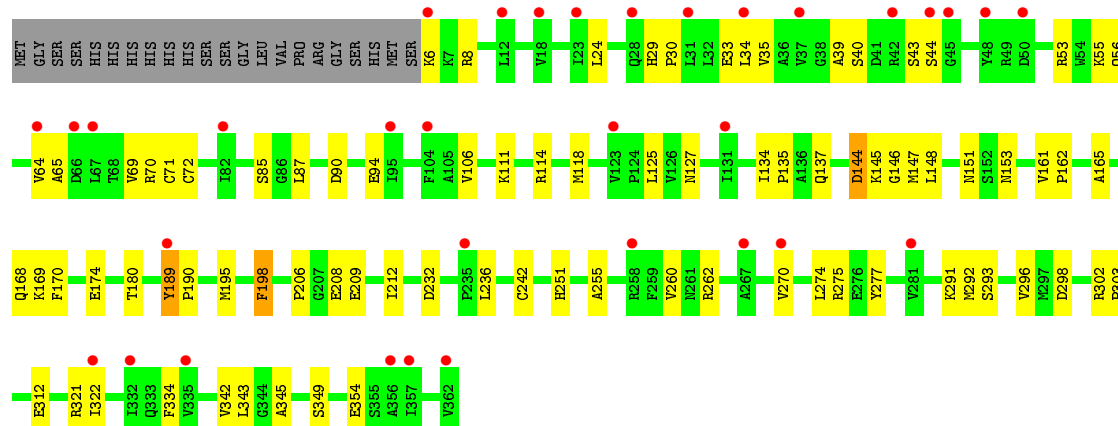
• Molecule 1: Aspartate Semialdehyde Dehydrogenase



• Molecule 1: Aspartate Semialdehyde Dehydrogenase



• Molecule 1: Aspartate Semialdehyde Dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.43Å 157.43Å 187.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.13 – 2.55 49.02 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.13-2.55) 99.7 (49.02-2.55)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.77 (at 2.54Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.227 , 0.273 0.227 , 0.272	Depositor DCC
$R_{free}$ test set	4387 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.6	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 29.4	EDS
Estimated twinning fraction	0.094 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 87511 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	32311	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.18 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.7628e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: NAP, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.28	0/2738	0.47	0/3714
1	B	0.27	0/2730	0.46	0/3703
1	C	0.27	0/2764	0.48	1/3750 (0.0%)
1	D	0.28	0/2723	0.51	2/3692 (0.1%)
1	E	0.25	0/2730	0.45	0/3703
1	F	0.25	0/2730	0.44	1/3703 (0.0%)
All	All	0.27	0/16415	0.47	4/22265 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	45	GLY	N-CA-C	8.27	133.77	113.10
1	C	27	SER	C-N-CA	7.36	140.10	121.70
1	D	70	ARG	C-N-CA	7.18	139.65	121.70
1	F	144	ASP	C-N-CA	6.97	139.12	121.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2686	2586	2707	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2679	2634	2704	67	0
1	C	2711	2632	2729	92	0
1	D	2673	2388	2698	97	0
1	E	2679	2638	2704	65	1
1	F	2679	2609	2704	76	2
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	96	0	50	29	0
3	C	48	0	25	19	0
4	A	104	0	0	26	2
4	B	103	0	0	23	0
4	C	88	0	0	27	0
4	D	129	0	0	13	2
4	E	64	0	0	23	0
4	F	55	0	0	18	0
All	All	16824	15487	16321	488	4

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 15.

All (488) 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:D:15:THR:HB	1:D:52:VAL:HG21	1.18	1.11
1:C:196:ASP:OD1	1:A:55:LYS:HE2	1.50	1.10
1:A:187[B]:ALA:O	3:A:402[B]:NAP:H3D	1.52	1.10
1:C:196:ASP:OD1	1:A:55:LYS:CE	2.01	1.07
1:D:53:ARG:NH1	1:D:60:MET:SD	2.26	1.06
1:C:60:MET:SD	4:C:546:HOH:O	2.15	1.04
1:D:217:ARG:NH2	4:D:503:HOH:O	1.90	1.03
1:D:44:SER:HB3	1:D:45:GLY:HA3	1.38	1.03
1:C:196:ASP:OD1	1:A:55:LYS:NZ	1.91	1.01
1:A:187[A]:ALA:N	1:A:188[A]:GLY:HA2	1.75	1.00
1:A:97:MET:SD	4:A:593:HOH:O	2.19	0.99
1:C:49:ARG:N	4:C:501:HOH:O	1.93	0.98
1:A:187[B]:ALA:N	3:A:402[B]:NAP:O3D	1.97	0.97
1:D:331:ASP:OD1	4:D:501:HOH:O	1.82	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:71:CYS:SG	4:F:534:HOH:O	2.25	0.95
1:D:15:THR:HB	1:D:52:VAL:CG2	1.95	0.95
1:E:21:ARG:NH2	4:E:502:HOH:O	1.91	0.95
1:E:271:ARG:NH2	4:E:504:HOH:O	2.00	0.95
1:A:50:ASP:OD1	4:A:501:HOH:O	1.84	0.94
1:D:195:MET:O	4:D:502:HOH:O	1.86	0.93
1:B:43:SER:O	4:B:501:HOH:O	1.85	0.93
1:A:55:LYS:NZ	1:A:189[A]:TYR:CE1	2.35	0.93
1:A:55:LYS:NZ	1:A:189[A]:TYR:CZ	2.38	0.92
1:E:38:GLY:O	4:E:501:HOH:O	1.89	0.91
1:B:94:GLU:OE2	4:B:502:HOH:O	1.88	0.91
1:D:53:ARG:CA	1:D:54:TRP:HB3	2.00	0.91
1:E:75:ALA:N	4:E:505:HOH:O	2.02	0.91
1:F:206:PRO:O	4:F:501:HOH:O	1.89	0.91
1:F:151:ASN:ND2	1:F:349:SER:OG	2.04	0.90
1:D:275:ARG:HD3	4:D:511:HOH:O	1.72	0.90
1:A:91:ALA:HB2	3:A:402[B]:NAP:N6A	1.88	0.89
1:A:189[B]:TYR:CB	1:A:190[B]:PRO:CD	2.51	0.89
1:C:26:LEU:N	4:C:504:HOH:O	2.04	0.89
1:A:189[B]:TYR:HB3	1:A:190[B]:PRO:HD3	1.56	0.88
1:C:189[B]:TYR:HB3	1:C:190[B]:PRO:HD3	1.54	0.88
1:B:70:ARG:NE	4:B:504:HOH:O	1.99	0.87
1:D:42:ARG:O	4:D:504:HOH:O	1.91	0.87
1:D:53:ARG:CB	1:D:54:TRP:HB3	2.05	0.87
1:D:54:TRP:CZ3	1:D:56:GLN:HB2	2.09	0.86
1:D:53:ARG:HA	1:D:54:TRP:HB3	1.57	0.86
1:D:38:GLY:O	4:D:505:HOH:O	1.92	0.86
1:D:52:VAL:O	1:D:53:ARG:HG3	1.74	0.85
1:D:54:TRP:CE3	1:D:56:GLN:HB2	2.11	0.85
1:A:189[A]:TYR:N	3:A:402[A]:NAP:O1N	2.09	0.84
1:A:232:ASP:OD1	4:A:502:HOH:O	1.94	0.84
1:A:64:VAL:HG23	1:A:67:LEU:HD12	1.60	0.83
1:A:189[B]:TYR:HB3	1:A:190[B]:PRO:CD	2.09	0.83
1:E:223:LEU:N	4:E:506:HOH:O	2.07	0.82
1:A:177:SER:OG	4:A:503:HOH:O	1.96	0.82
1:B:224:ASN:OD1	4:B:503:HOH:O	1.97	0.82
1:A:53:ARG:HE	1:A:189[A]:TYR:HE2	1.28	0.81
1:E:68:THR:OG1	4:E:503:HOH:O	1.97	0.81
1:F:125:LEU:HD13	1:F:293:SER:HB3	1.62	0.81
1:A:222:ASP:O	4:A:504:HOH:O	1.98	0.80
1:E:48:TYR:CE1	1:E:52:VAL:HG21	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:ASN:HB3	3:C:402:NAP:H6N	1.64	0.79
1:F:232:ASP:OD1	4:F:502:HOH:O	1.99	0.79
1:C:109:ASN:HB3	3:C:402:NAP:C6N	2.12	0.79
1:A:53:ARG:NE	1:A:189[A]:TYR:CE2	2.51	0.79
1:C:74:PRO:O	4:C:502:HOH:O	2.01	0.79
1:A:189[B]:TYR:HB2	1:A:190[B]:PRO:HD2	1.65	0.79
1:A:231:SER:O	4:A:504:HOH:O	2.01	0.79
1:C:196:ASP:CG	1:A:55:LYS:HZ3	1.86	0.78
1:F:298:ASP:OD1	4:F:503:HOH:O	1.99	0.78
1:C:109:ASN:CB	3:C:402:NAP:H6N	2.14	0.78
1:C:189[B]:TYR:CB	1:C:190[B]:PRO:CD	2.62	0.77
1:E:141:PHE:N	4:E:509:HOH:O	2.17	0.77
1:C:189[B]:TYR:HB3	1:C:190[B]:PRO:CD	2.15	0.76
1:D:53:ARG:NH2	1:D:60:MET:SD	2.57	0.76
1:B:40:SER:OG	4:B:505:HOH:O	2.03	0.76
1:C:109:ASN:HB3	3:C:402:NAP:C5N	2.15	0.76
1:C:56:GLN:O	4:C:503:HOH:O	2.03	0.76
1:A:55:LYS:NZ	1:A:189[A]:TYR:OH	2.16	0.75
1:D:53:ARG:HB3	1:D:54:TRP:CD1	2.22	0.75
1:C:189[A]:TYR:CB	4:C:510:HOH:O	2.34	0.75
1:A:265:PRO:O	4:A:506:HOH:O	2.05	0.74
1:A:54:TRP:CZ3	1:A:60:MET:HB3	2.22	0.74
1:D:258:ARG:HE	1:D:262:ARG:NH2	1.86	0.74
1:A:116:ASP:OD2	4:A:505:HOH:O	2.04	0.74
1:A:222:ASP:N	4:A:504:HOH:O	2.18	0.74
1:D:53:ARG:CZ	1:D:60:MET:SD	2.75	0.74
1:A:187[A]:ALA:N	1:A:188[A]:GLY:CA	2.50	0.74
1:C:189[A]:TYR:HB2	4:C:510:HOH:O	1.87	0.73
1:F:262:ARG:NH1	4:F:506:HOH:O	2.21	0.73
1:A:293:SER:OG	4:A:507:HOH:O	2.05	0.73
1:B:54:TRP:CZ3	1:B:60:MET:HB2	2.24	0.73
1:C:55:LYS:NZ	1:A:196:ASP:OD1	2.20	0.72
1:C:109:ASN:HB3	3:C:402:NAP:H5N	1.70	0.72
1:F:236:LEU:N	4:F:507:HOH:O	2.22	0.72
1:C:180:THR:HG21	1:C:182:GLN:OE1	1.90	0.71
1:A:60:MET:SD	4:A:602:HOH:O	2.47	0.71
1:A:40:SER:OG	1:A:44:SER:HB3	1.89	0.71
1:A:180:THR:HG21	1:A:182:GLN:OE1	1.91	0.71
1:D:233:GLN:OE1	4:D:506:HOH:O	2.07	0.70
1:C:69:VAL:O	4:C:505:HOH:O	2.08	0.70
1:B:237:GLN:OE1	4:B:506:HOH:O	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:LYS:HG2	4:A:597:HOH:O	1.90	0.70
1:C:67:LEU:O	4:C:506:HOH:O	2.09	0.70
1:B:9:CYS:SG	4:B:593:HOH:O	2.49	0.70
1:C:232:ASP:OD1	4:C:507:HOH:O	2.10	0.69
1:B:16:GLY:O	4:B:507:HOH:O	2.09	0.69
1:B:223:LEU:HD12	4:B:580:HOH:O	1.92	0.69
1:D:232:ASP:OD1	4:D:507:HOH:O	2.09	0.69
1:B:28:GLN:OE1	1:B:28:GLN:N	2.25	0.69
1:D:53:ARG:HB3	1:D:54:TRP:HB3	1.74	0.69
1:E:48:TYR:CZ	1:E:52:VAL:HG21	2.28	0.69
1:F:189:TYR:CB	1:F:190:PRO:CD	2.71	0.69
1:D:189:TYR:CB	1:D:190:PRO:CD	2.71	0.68
1:B:227:LEU:O	4:B:508:HOH:O	2.11	0.68
1:D:54:TRP:CZ3	1:D:56:GLN:CB	2.77	0.68
1:A:40:SER:HB3	4:A:532:HOH:O	1.91	0.68
1:A:292:MET:SD	4:A:591:HOH:O	2.50	0.68
1:C:109:ASN:OD1	1:C:349:SER:OG	2.11	0.68
1:D:180:THR:HG22	1:D:182:GLN:HG3	1.76	0.68
1:E:170:PHE:O	4:E:507:HOH:O	2.13	0.67
1:A:60:MET:HE2	1:A:65:ALA:HB2	1.75	0.67
1:D:189:TYR:HB3	1:D:190:PRO:HD3	1.75	0.67
1:F:8:ARG:HB2	1:F:35:VAL:HG21	1.75	0.67
1:C:47:LYS:C	4:C:501:HOH:O	2.33	0.67
1:D:302:ARG:NH2	1:D:308:ASP:OD1	2.26	0.67
1:C:25:LEU:N	4:C:504:HOH:O	2.26	0.66
1:F:298:ASP:CG	4:F:503:HOH:O	2.34	0.66
1:C:180:THR:CG2	1:C:182:GLN:HG3	2.26	0.66
1:F:275:ARG:HE	1:F:296:VAL:HG11	1.59	0.65
1:A:189[B]:TYR:HB2	1:A:190[B]:PRO:CD	2.23	0.65
1:A:261:ASN:O	4:A:508:HOH:O	2.13	0.65
2:C:401:SO4:O3	3:C:402:NAP:N7N	2.30	0.65
1:A:53:ARG:NH2	3:A:402[B]:NAP:H4N	2.11	0.65
1:D:189:TYR:CB	1:D:190:PRO:HD3	2.26	0.65
1:A:310:GLU:OE1	4:A:509:HOH:O	2.14	0.65
1:F:134:ILE:HD12	1:F:147:MET:HB2	1.78	0.65
1:E:189:TYR:CB	1:E:190:PRO:CD	2.74	0.65
1:D:189:TYR:O	4:D:509:HOH:O	2.14	0.65
1:A:53:ARG:HH21	3:A:402[B]:NAP:C4N	2.10	0.64
1:C:89:PRO:HD3	3:C:402:NAP:O3D	1.97	0.64
1:D:44:SER:CB	1:D:45:GLY:HA3	2.07	0.64
1:C:111:LYS:HA	1:C:114:ARG:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:291:LYS:O	1:F:292:MET:HB3	1.97	0.64
1:B:6:LYS:N	4:B:515:HOH:O	2.32	0.63
1:F:53:ARG:NH1	4:F:511:HOH:O	2.31	0.63
1:B:189:TYR:HB3	1:B:190:PRO:HD3	1.79	0.63
1:D:42:ARG:C	1:D:44:SER:HB2	2.19	0.63
1:E:142:GLY:N	4:E:509:HOH:O	2.32	0.63
1:C:55:LYS:HZ3	1:A:196:ASP:CG	2.02	0.62
1:D:258:ARG:HE	1:D:262:ARG:HH22	1.47	0.62
1:B:324:GLU:O	4:B:509:HOH:O	2.16	0.62
1:D:52:VAL:O	1:D:53:ARG:CG	2.44	0.62
1:F:291:LYS:N	1:F:312:GLU:OE2	2.33	0.62
1:A:53:ARG:HH21	3:A:402[B]:NAP:H4N	1.64	0.62
1:A:109:ASN:O	3:A:402[A]:NAP:H6N	1.99	0.62
1:A:327:SER:O	1:B:237:GLN:NE2	2.33	0.61
3:A:402[B]:NAP:H6N	3:A:402[B]:NAP:O1A	1.99	0.61
1:A:109:ASN:ND2	3:A:402[A]:NAP:C6N	2.63	0.61
1:D:14:ALA:HB3	1:D:37:VAL:HG13	1.82	0.61
1:B:118:MET:HE2	1:B:137:GLN:HA	1.81	0.61
1:F:189:TYR:HB3	1:F:190:PRO:HD3	1.83	0.61
1:B:46:LYS:O	1:B:69:VAL:HG12	2.01	0.61
1:D:54:TRP:CG	1:D:54:TRP:O	2.54	0.60
1:D:15:THR:HG21	1:D:42:ARG:HD2	1.84	0.60
1:C:49:ARG:HA	4:C:546:HOH:O	2.02	0.60
1:E:73:ASP:HB3	4:E:505:HOH:O	2.02	0.60
1:D:302:ARG:HH21	1:D:308:ASP:CG	2.05	0.60
1:A:53:ARG:NE	1:A:189[A]:TYR:HE2	1.93	0.60
1:C:16:GLY:HA3	3:C:402:NAP:O1A	2.02	0.59
1:A:189[A]:TYR:CD1	1:A:190[A]:PRO:HA	2.37	0.59
1:E:277:TYR:O	4:E:508:HOH:O	2.17	0.59
1:D:48:TYR:CE2	1:D:53:ARG:HD2	2.37	0.59
1:C:40:SER:HB2	3:C:402:NAP:C2A	2.32	0.59
1:D:9:CYS:HB3	1:D:82:ILE:HB	1.85	0.59
1:E:189:TYR:HB3	1:E:190:PRO:HD3	1.85	0.59
1:B:217:ARG:NH2	4:B:506:HOH:O	2.35	0.59
1:D:42:ARG:O	1:D:44:SER:HB2	2.02	0.58
1:F:146:GLY:N	4:F:508:HOH:O	2.27	0.58
1:F:170:PHE:O	4:F:505:HOH:O	2.17	0.58
1:D:180:THR:CG2	1:D:182:GLN:CG	2.81	0.58
1:F:43:SER:HB2	1:F:44:SER:HA	1.85	0.58
1:B:20:THR:N	4:B:507:HOH:O	2.36	0.58
2:A:401:SO4:O1	3:A:402[A]:NAP:C6N	2.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:THR:CG2	1:D:182:GLN:HG3	2.34	0.58
1:F:275:ARG:NE	1:F:296:VAL:HG11	2.19	0.58
1:E:55:LYS:CE	1:F:195:MET:O	2.52	0.58
1:D:178:MET:HG3	1:D:240:VAL:HG23	1.86	0.58
1:D:88:ASP:HB3	4:D:526:HOH:O	2.03	0.58
1:B:43:SER:HA	1:B:44:SER:HB2	1.86	0.58
1:D:189:TYR:HB2	1:D:190:PRO:CD	2.34	0.58
1:D:52:VAL:O	1:D:52:VAL:HG23	2.04	0.57
1:A:53:ARG:NH2	1:A:190[A]:PRO:HD3	2.19	0.57
1:C:180:THR:HG23	1:C:182:GLN:HG3	1.85	0.57
1:E:42:ARG:NE	4:E:515:HOH:O	2.36	0.57
1:D:16:GLY:O	1:D:20:THR:HG23	2.04	0.57
1:A:18:VAL:HG12	3:A:402[B]:NAP:O1N	2.04	0.57
1:B:189:TYR:CB	1:B:190:PRO:HD3	2.35	0.57
1:A:9:CYS:HB3	1:A:82:ILE:HB	1.87	0.57
1:A:64:VAL:O	1:A:67:LEU:HB2	2.04	0.56
1:B:189:TYR:CG	1:B:190:PRO:HD3	2.40	0.56
1:D:48:TYR:CD2	1:D:53:ARG:HD2	2.40	0.56
1:A:187[A]:ALA:H	1:A:188[A]:GLY:HA2	1.64	0.56
1:F:189:TYR:CB	1:F:190:PRO:HD3	2.35	0.56
1:D:53:ARG:HH22	1:D:60:MET:CE	2.18	0.56
1:A:186:GLY:H	3:A:402[B]:NAP:H4D	1.70	0.56
1:A:18:VAL:CG1	3:A:402[B]:NAP:O1N	2.53	0.56
1:C:91:ALA:HB2	3:C:402:NAP:N6A	2.20	0.56
1:B:111:LYS:HA	1:B:114:ARG:HG3	1.88	0.56
1:B:14:ALA:HB3	1:B:37:VAL:HG13	1.88	0.56
1:A:180:THR:HG23	1:A:182:GLN:HG3	1.88	0.55
3:A:402[A]:NAP:H2N	3:A:402[A]:NAP:H52N	1.87	0.55
3:A:402[B]:NAP:PA	3:A:402[B]:NAP:H52N	2.47	0.55
1:E:55:LYS:NZ	1:F:195:MET:O	2.40	0.55
1:D:54:TRP:CZ2	1:D:60:MET:N	2.74	0.55
1:C:47:LYS:NZ	1:C:66:ASP:O	2.39	0.55
1:D:246:PRO:HG2	1:C:246:PRO:HG2	1.87	0.55
1:E:23:ILE:CG2	1:E:64:VAL:HG11	2.36	0.55
1:A:210:GLY:N	4:A:517:HOH:O	2.31	0.55
1:F:189:TYR:HB2	1:F:190:PRO:CD	2.36	0.55
1:B:118:MET:CE	1:B:137:GLN:HA	2.35	0.55
1:E:189:TYR:CB	1:E:190:PRO:HD3	2.36	0.54
1:F:255:ALA:HB3	1:F:334:PHE:CZ	2.42	0.54
1:A:64:VAL:HA	1:A:67:LEU:HD12	1.89	0.54
1:F:145:LYS:N	4:F:508:HOH:O	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:ILE:C	1:C:201:ILE:HD12	2.27	0.54
1:D:53:ARG:NH2	1:D:60:MET:CB	2.70	0.54
1:D:18:VAL:HG13	4:D:510:HOH:O	2.08	0.54
1:D:180:THR:HG21	1:D:182:GLN:CG	2.38	0.54
1:F:43:SER:CB	1:F:44:SER:HA	2.38	0.54
1:B:178:MET:HG3	1:B:240:VAL:HG23	1.90	0.54
1:B:134:ILE:HD12	1:B:147:MET:HB2	1.90	0.53
1:E:198:PHE:CE1	1:F:198:PHE:CE1	2.97	0.53
1:B:32:LEU:HD22	4:B:593:HOH:O	2.07	0.53
1:D:180:THR:HG22	1:D:182:GLN:CG	2.39	0.53
1:F:260:VAL:N	4:F:514:HOH:O	2.41	0.53
1:D:53:ARG:HH22	1:D:60:MET:HE2	1.73	0.53
1:F:180:THR:HG22	1:F:242:CYS:HA	1.91	0.53
1:C:55:LYS:NZ	4:C:510:HOH:O	2.25	0.53
1:A:48:TYR:CZ	1:A:52:VAL:HG11	2.44	0.53
1:A:88:ASP:HB2	3:A:402[A]:NAP:H51A	1.91	0.53
1:E:54:TRP:N	4:E:512:HOH:O	2.40	0.53
1:E:42:ARG:NH2	1:E:69:VAL:HG11	2.23	0.53
1:C:48:TYR:CZ	1:C:52:VAL:HG11	2.44	0.53
1:F:118:MET:HE2	1:F:137:GLN:HA	1.91	0.53
1:D:60:MET:HE1	1:D:65:ALA:HB2	1.91	0.52
1:C:49:ARG:CA	4:C:501:HOH:O	2.50	0.52
1:A:54:TRP:CH2	1:A:60:MET:HB3	2.43	0.52
1:B:54:TRP:N	4:B:519:HOH:O	2.42	0.52
1:A:305:PRO:O	1:A:309:ARG:HG2	2.09	0.52
1:D:237:GLN:NE2	1:C:327:SER:O	2.42	0.52
1:B:53:ARG:NH2	4:B:520:HOH:O	2.42	0.52
1:C:9:CYS:HB3	1:C:82:ILE:HB	1.92	0.52
1:B:134:ILE:N	1:B:135:PRO:HD2	2.25	0.52
1:A:109:ASN:HD21	3:A:402[A]:NAP:C6N	2.23	0.52
1:B:60:MET:CE	1:B:65:ALA:HA	2.40	0.52
1:A:15:THR:OG1	3:A:402[A]:NAP:O1X	2.28	0.52
1:C:78:SER:N	4:C:502:HOH:O	2.43	0.52
1:F:6:LYS:NZ	1:F:33:GLU:OE2	2.31	0.52
1:D:53:ARG:HB3	1:D:54:TRP:CB	2.39	0.51
1:C:47:LYS:HB3	4:C:501:HOH:O	2.09	0.51
1:A:24:LEU:HD11	1:A:54:TRP:CH2	2.45	0.51
1:A:39:ALA:HB3	1:A:69:VAL:HG11	1.92	0.51
1:B:49:ARG:HG3	1:B:65:ALA:HB1	1.92	0.51
1:F:189:TYR:HB3	1:F:190:PRO:CD	2.40	0.51
1:D:302:ARG:HB3	1:D:303:PRO:HA	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:LYS:HA	1:D:114:ARG:HG3	1.92	0.51
1:D:53:ARG:HB3	1:D:54:TRP:CG	2.45	0.51
1:A:186:GLY:O	3:A:402[A]:NAP:N7N	2.44	0.51
1:B:189:TYR:CD2	1:B:190:PRO:HD3	2.46	0.51
1:C:170:PHE:CG	1:C:265:PRO:HG3	2.46	0.51
1:E:196:ASP:OD1	1:F:55:LYS:HE3	2.11	0.51
1:C:302:ARG:NH1	1:C:308:ASP:OD1	2.44	0.51
1:D:54:TRP:CZ2	1:D:60:MET:HB2	2.45	0.51
3:A:402[B]:NAP:O1A	3:A:402[B]:NAP:H52N	2.10	0.51
1:C:191[B]:GLY:O	4:C:508:HOH:O	2.15	0.51
1:D:44:SER:HB3	1:D:45:GLY:CA	2.26	0.51
1:F:87:LEU:N	1:F:87:LEU:HD12	2.24	0.51
1:C:189[B]:TYR:HB2	1:C:190[B]:PRO:CD	2.41	0.50
1:A:15:THR:OG1	3:A:402[B]:NAP:O1X	2.27	0.50
1:A:24:LEU:HD11	1:A:54:TRP:CZ2	2.46	0.50
1:A:362:VAL:O	4:A:510:HOH:O	2.19	0.50
1:D:275:ARG:HG3	1:D:296:VAL:HG21	1.92	0.50
1:C:165:ALA:HB2	1:C:277:TYR:CD1	2.46	0.50
1:D:6:LYS:N	4:D:523:HOH:O	2.45	0.50
1:A:180:THR:CG2	1:A:182:GLN:HG3	2.41	0.50
1:F:34:LEU:HD23	1:F:64:VAL:CG1	2.41	0.50
1:C:69:VAL:HG12	4:C:505:HOH:O	2.11	0.50
1:E:189:TYR:HB3	1:E:190:PRO:CD	2.42	0.50
1:F:24:LEU:CD1	1:F:56:GLN:HG2	2.41	0.50
1:E:361:PHE:HD1	1:E:361:PHE:N	2.09	0.50
1:C:18:VAL:HG13	1:C:19:GLY:N	2.27	0.50
1:E:189:TYR:HB2	1:E:190:PRO:CD	2.42	0.50
1:A:230:PHE:N	4:A:513:HOH:O	2.23	0.49
1:A:204:TYR:CE2	1:B:300:VAL:HG22	2.47	0.49
1:E:361:PHE:N	1:E:361:PHE:CD1	2.79	0.49
1:D:55:LYS:HD2	1:B:196:ASP:OD1	2.12	0.49
1:E:302:ARG:NH1	1:E:308:ASP:OD2	2.44	0.49
1:A:309:ARG:HG3	1:A:310:GLU:HG2	1.95	0.49
1:C:47:LYS:CB	4:C:501:HOH:O	2.61	0.49
1:C:189[B]:TYR:HB2	1:C:190[B]:PRO:HD2	1.95	0.49
1:F:174:GLU:HB2	1:F:260:VAL:HG13	1.94	0.48
1:C:69:VAL:C	4:C:505:HOH:O	2.51	0.48
1:C:44:SER:HA	4:C:505:HOH:O	2.13	0.48
1:D:182:GLN:HB3	1:D:251:HIS:CE1	2.48	0.48
1:C:131:ILE:O	1:C:134:ILE:HG12	2.13	0.48
1:F:118:MET:CE	1:F:137:GLN:HA	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:29:HIS:NE2	1:E:354:GLU:OE2	2.45	0.48
1:C:25:LEU:CA	4:C:504:HOH:O	2.61	0.48
1:F:255:ALA:HB3	1:F:334:PHE:CE1	2.49	0.48
1:C:308:ASP:HB2	1:C:337:LEU:CD2	2.43	0.48
1:C:109:ASN:HB2	3:C:402:NAP:H6N	1.95	0.48
1:A:39:ALA:CB	1:A:69:VAL:HG11	2.44	0.48
1:D:305:PRO:O	1:D:309:ARG:HD3	2.14	0.47
1:B:61:PRO:O	1:B:64:VAL:HG12	2.14	0.47
1:D:51:ALA:O	1:D:52:VAL:C	2.53	0.47
1:C:189[B]:TYR:CB	1:C:190[B]:PRO:HD3	2.29	0.47
1:D:14:ALA:N	4:D:505:HOH:O	2.28	0.47
1:E:299:GLU:HB2	1:E:302:ARG:HG3	1.97	0.47
1:F:90:ASP:HB2	4:F:545:HOH:O	2.13	0.47
1:B:9:CYS:HB3	4:B:593:HOH:O	2.15	0.47
1:B:260:VAL:HG23	1:B:261:ASN:OD1	2.15	0.47
1:C:55:LYS:NZ	4:C:509:HOH:O	2.20	0.47
1:C:91:ALA:CB	3:C:402:NAP:N6A	2.77	0.47
1:E:68:THR:CB	4:E:503:HOH:O	2.61	0.47
1:D:49:ARG:HA	1:D:53:ARG:NH1	2.29	0.47
1:D:54:TRP:HZ2	1:D:60:MET:N	2.12	0.46
1:A:187[B]:ALA:O	3:A:402[B]:NAP:C3D	2.43	0.46
3:A:402[B]:NAP:H5N	4:A:571:HOH:O	2.14	0.46
1:B:174:GLU:HB2	1:B:260:VAL:HG12	1.97	0.46
1:F:165:ALA:HA	1:F:277:TYR:CD1	2.50	0.46
1:A:27:SER:O	1:A:28:GLN:HB2	2.14	0.46
1:E:103:ASN:OD1	1:E:145:LYS:N	2.42	0.46
1:B:302:ARG:HB3	1:B:303:PRO:HA	1.98	0.46
1:C:110:ALA:HA	3:C:402:NAP:O2D	2.14	0.46
1:C:345:ALA:HB2	3:C:402:NAP:C4N	2.46	0.46
1:B:189:TYR:CB	1:B:190:PRO:CD	2.93	0.46
1:D:53:ARG:HA	1:D:54:TRP:CB	2.29	0.46
1:A:40:SER:HG	1:A:44:SER:HB3	1.80	0.46
1:E:107:PHE:CE2	1:E:353:ALA:HA	2.50	0.46
1:E:260:VAL:HG13	1:E:261:ASN:N	2.31	0.46
1:E:52:VAL:HG12	4:E:512:HOH:O	2.14	0.46
1:D:114:ARG:HD3	1:D:151:ASN:O	2.15	0.46
1:C:167:ILE:HA	1:C:171:GLY:O	2.15	0.46
1:C:43:SER:HB3	1:C:44:SER:HA	1.97	0.46
1:A:297:MET:HE1	1:A:302:ARG:NH1	2.31	0.46
1:F:168:GLN:NE2	4:F:504:HOH:O	2.17	0.45
1:D:51:ALA:O	1:D:53:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:GLY:N	3:A:402[B]:NAP:H4D	2.31	0.45
1:C:44:SER:HB2	1:C:45:GLY:HA2	1.97	0.45
1:E:43:SER:HB2	1:E:44:SER:CA	2.46	0.45
1:E:43:SER:HB2	1:E:44:SER:HA	1.98	0.45
1:A:165:ALA:O	4:A:511:HOH:O	2.21	0.45
1:A:231:SER:N	4:A:504:HOH:O	2.34	0.45
1:A:182:GLN:HG2	1:A:251:HIS:CD2	2.52	0.45
1:F:106:VAL:CG2	1:F:148:LEU:HD13	2.46	0.45
1:A:64:VAL:HA	1:A:67:LEU:CD1	2.46	0.45
1:A:18:VAL:HG13	1:A:19:GLY:N	2.31	0.45
1:F:134:ILE:N	1:F:135:PRO:HD2	2.31	0.45
1:F:24:LEU:HD11	1:F:56:GLN:HG2	1.97	0.45
1:F:342:VAL:HG12	1:F:343:LEU:N	2.32	0.45
1:D:52:VAL:C	1:D:53:ARG:HG3	2.36	0.45
1:A:91:ALA:HB2	3:A:402[B]:NAP:C6A	2.47	0.45
1:E:19:GLY:O	1:E:22:PHE:HB2	2.17	0.45
1:D:170:PHE:CG	1:D:265:PRO:HG3	2.52	0.45
1:C:309:ARG:HG3	1:C:310:GLU:HG2	1.98	0.45
1:D:60:MET:HG2	1:D:61:PRO:N	2.32	0.45
1:E:187:ALA:CB	1:E:192:VAL:HG23	2.47	0.45
1:D:103:ASN:OD1	1:D:144:ASP:N	2.46	0.45
1:E:43:SER:CB	1:E:44:SER:HA	2.47	0.44
1:E:266:THR:O	1:E:270:VAL:HG23	2.18	0.44
1:C:182:GLN:HG2	1:C:251:HIS:CD2	2.52	0.44
1:A:239:SER:OG	1:B:325:ASP:OD2	2.22	0.44
1:B:225:SER:N	1:E:226:ASP:OD2	2.40	0.44
1:F:39:ALA:O	1:F:40:SER:OG	2.28	0.44
1:A:331:ASP:OD1	4:A:512:HOH:O	2.21	0.44
1:A:14:ALA:HA	1:A:19:GLY:HA3	1.99	0.44
1:F:43:SER:HA	1:F:44:SER:C	2.38	0.44
1:C:40:SER:HB3	1:C:41:ASP:HA	1.99	0.44
1:F:34:LEU:HD23	1:F:64:VAL:HG12	1.99	0.44
1:D:60:MET:SD	1:D:65:ALA:HB2	2.58	0.44
1:B:43:SER:HB2	1:B:44:SER:C	2.38	0.44
1:C:18:VAL:CG1	1:C:19:GLY:N	2.80	0.44
1:D:180:THR:HG22	1:D:181:MET:N	2.33	0.44
1:C:48:TYR:CE1	1:C:52:VAL:HG11	2.53	0.44
1:F:64:VAL:HG23	1:F:65:ALA:N	2.33	0.44
1:B:141:PHE:CB	1:B:143:LEU:HD21	2.47	0.44
1:F:165:ALA:HA	1:F:277:TYR:CE1	2.53	0.44
1:E:37:VAL:HG13	4:E:501:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:327:SER:O	1:E:328:ASP:HB2	2.17	0.44
1:E:291:LYS:N	1:E:291:LYS:HD2	2.32	0.44
1:C:50:ASP:N	4:C:501:HOH:O	2.32	0.43
1:C:88:ASP:HA	3:C:402:NAP:O3D	2.18	0.43
1:E:134:ILE:HB	1:E:135:PRO:HD3	2.00	0.43
1:A:189[B]:TYR:CB	1:A:190[B]:PRO:HD2	2.27	0.43
1:B:189:TYR:HB3	1:B:190:PRO:CD	2.47	0.43
1:E:106:VAL:CG2	1:E:148:LEU:HD13	2.48	0.43
1:D:196:ASP:OD1	1:B:55:LYS:HE3	2.18	0.43
1:C:17:ALA:HB3	3:C:402:NAP:O1N	2.18	0.43
1:E:23:ILE:HG21	1:E:64:VAL:HG11	2.00	0.43
1:A:204:TYR:CE2	1:B:300:VAL:CG2	3.00	0.43
1:C:183:ALA:HB1	1:C:247:VAL:O	2.19	0.43
1:C:40:SER:CB	3:C:402:NAP:C2A	2.97	0.43
1:F:144:ASP:HB3	4:F:508:HOH:O	2.18	0.43
1:E:126:VAL:O	4:E:510:HOH:O	2.21	0.43
1:F:39:ALA:HB3	1:F:69:VAL:HG11	2.00	0.43
1:B:271:ARG:NH2	4:B:513:HOH:O	2.29	0.43
1:A:189[A]:TYR:HA	1:A:191[A]:GLY:N	2.34	0.43
1:F:111:LYS:HA	1:F:114:ARG:NE	2.34	0.43
1:A:308:ASP:HB2	1:A:337:LEU:CD2	2.48	0.43
1:B:189:TYR:C	1:B:189:TYR:CD1	2.92	0.43
1:E:55:LYS:HZ2	1:F:195:MET:HB3	1.84	0.43
1:B:274:LEU:HB3	1:B:294:ILE:HG21	2.01	0.43
1:E:322:ILE:O	4:E:504:HOH:O	2.22	0.42
1:F:85:SER:OG	1:F:87:LEU:CD1	2.67	0.42
1:C:97:MET:CE	1:C:101:LYS:HE2	2.49	0.42
1:F:208:GLU:O	1:F:212:ILE:HG12	2.19	0.42
1:A:131:ILE:O	1:A:134:ILE:HG12	2.19	0.42
1:D:53:ARG:CA	1:D:54:TRP:CB	2.77	0.42
1:F:262:ARG:HD3	4:F:506:HOH:O	2.20	0.42
1:B:58:ALA:HB1	1:B:59:PRO:HA	2.01	0.42
1:F:85:SER:OG	1:F:87:LEU:HD13	2.19	0.42
1:D:15:THR:CB	1:D:42:ARG:HH11	2.33	0.42
1:C:18:VAL:HG12	3:C:402:NAP:O2N	2.19	0.42
1:F:145:LYS:CG	4:F:508:HOH:O	2.68	0.42
1:B:178:MET:HA	1:B:254:CYS:O	2.20	0.42
1:E:275:ARG:CG	1:E:292:MET:HE3	2.50	0.42
1:E:75:ALA:HB3	4:E:505:HOH:O	2.19	0.42
1:C:327:SER:O	1:C:328:ASP:HB2	2.20	0.42
1:A:335:VAL:CG2	4:A:585:HOH:O	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:TRP:O	1:D:54:TRP:CD2	2.73	0.42
1:C:188[A]:GLY:O	3:C:402:NAP:O1N	2.36	0.42
1:D:180:THR:CG2	1:D:182:GLN:HG2	2.49	0.42
1:B:189:TYR:CG	1:B:190:PRO:CD	3.02	0.42
1:D:48:TYR:O	1:D:53:ARG:HD3	2.19	0.42
1:C:359:LYS:HB3	1:C:361:PHE:CE2	2.55	0.42
1:F:29:HIS:NE2	1:F:354:GLU:OE2	2.53	0.42
1:A:242:CYS:HB2	4:A:559:HOH:O	2.20	0.42
1:F:165:ALA:CB	1:F:277:TYR:CD1	3.03	0.42
1:C:196:ASP:CG	1:A:55:LYS:NZ	2.59	0.42
1:E:55:LYS:CE	1:F:195:MET:C	2.88	0.42
1:D:200:ASN:O	1:D:246:PRO:HD3	2.18	0.42
1:A:204:TYR:CD2	1:B:300:VAL:HG22	2.55	0.42
1:F:69:VAL:HG12	1:F:70:ARG:N	2.35	0.42
1:A:138:ARG:NH1	4:A:514:HOH:O	2.25	0.42
1:A:189[A]:TYR:HA	1:A:191[A]:GLY:H	1.85	0.42
1:B:94:GLU:HG2	4:B:502:HOH:O	2.19	0.42
1:C:43:SER:HB3	4:C:505:HOH:O	2.18	0.42
1:E:145:LYS:O	4:E:511:HOH:O	2.22	0.42
1:E:14:ALA:HA	1:E:19:GLY:HA3	2.01	0.42
1:B:170:PHE:CG	1:B:265:PRO:HG3	2.54	0.42
1:F:127:ASN:N	1:F:127:ASN:OD1	2.53	0.42
1:E:138:ARG:C	4:E:509:HOH:O	2.57	0.41
1:F:43:SER:CB	1:F:44:SER:CA	2.98	0.41
1:C:242:CYS:HB2	4:C:545:HOH:O	2.19	0.41
1:C:118:MET:HE2	1:C:137:GLN:HA	2.02	0.41
1:B:131:ILE:O	1:B:134:ILE:HG12	2.20	0.41
1:F:6:LYS:HE2	1:F:33:GLU:HB2	2.02	0.41
1:E:302:ARG:NH1	1:E:308:ASP:CG	2.73	0.41
1:E:266:THR:HG22	1:E:269:GLN:OE1	2.21	0.41
1:B:342:VAL:HG12	1:B:343:LEU:N	2.35	0.41
1:A:342:VAL:HG12	1:A:343:LEU:N	2.35	0.41
1:C:29:HIS:HA	1:C:30:PRO:HD3	1.94	0.41
1:F:302:ARG:HB3	1:F:303:PRO:HA	2.02	0.41
1:F:270:VAL:O	1:F:274:LEU:HG	2.20	0.41
1:A:186:GLY:CA	3:A:402[B]:NAP:H4D	2.50	0.41
1:E:43:SER:N	4:E:515:HOH:O	2.52	0.41
1:D:118:MET:HE2	1:D:137:GLN:HA	2.03	0.41
1:D:134:ILE:N	1:D:135:PRO:HD2	2.35	0.41
1:A:40:SER:HA	3:A:402[B]:NAP:H2A	2.03	0.41
1:D:251:HIS:O	1:D:337:LEU:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:GLN:OE1	4:B:511:HOH:O	2.22	0.41
1:F:161:VAL:HB	1:F:162:PRO:HD3	2.01	0.41
1:C:188[A]:GLY:HA3	1:C:189[A]:TYR:HA	1.95	0.41
1:D:303:PRO:O	1:C:203:PRO:HG3	2.21	0.41
1:F:168:GLN:HG3	1:F:169:LYS:N	2.35	0.41
1:B:266:THR:HG22	1:B:269:GLN:HG3	2.02	0.41
1:A:64:VAL:CG2	1:A:67:LEU:HD12	2.41	0.41
1:B:224:ASN:CG	4:B:503:HOH:O	2.53	0.41
1:B:20:THR:HG23	4:B:507:HOH:O	2.21	0.41
1:E:302:ARG:NH2	4:E:526:HOH:O	2.54	0.41
1:C:64:VAL:HG13	1:C:65:ALA:N	2.35	0.41
1:F:145:LYS:HG2	4:F:508:HOH:O	2.20	0.40
1:E:165:ALA:HB2	1:E:277:TYR:CD1	2.56	0.40
1:D:131:ILE:O	1:D:134:ILE:HG12	2.22	0.40
1:B:156:VAL:HG22	1:B:160:VAL:HG13	2.03	0.40
1:A:186:GLY:HA3	3:A:402[A]:NAP:N7N	2.36	0.40
1:A:197:ILE:HG13	1:A:197:ILE:O	2.22	0.40
1:D:189:TYR:HB3	1:D:190:PRO:CD	2.39	0.40
1:E:55:LYS:HE3	1:F:195:MET:C	2.41	0.40
1:F:198:PHE:HA	1:F:198:PHE:HD1	1.81	0.40
1:B:103:ASN:HB3	1:B:145:LYS:HB3	2.04	0.40
1:A:200:ASN:O	1:A:246:PRO:HG3	2.21	0.40
1:E:54:TRP:CZ2	1:E:56:GLN:HG3	2.57	0.40

All (4) 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)
4:D:518:HOH:O	4:A:548:HOH:O[2_565]	1.82	0.38
4:D:518:HOH:O	4:A:529:HOH:O[2_565]	2.05	0.15
1:F:209:GLU:OE1	1:F:321:ARG:HH22[4_465]	1.58	0.02
1:E:112:ASN:ND2	1:F:94:GLU:OE1[6_345]	2.18	0.02

## 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	355/379 (94%)	331 (93%)	19 (5%)	5 (1%)	14	25
1	B	355/379 (94%)	339 (96%)	12 (3%)	4 (1%)	17	33
1	C	360/379 (95%)	340 (94%)	14 (4%)	6 (2%)	11	20
1	D	352/379 (93%)	328 (93%)	20 (6%)	4 (1%)	17	33
1	E	355/379 (94%)	330 (93%)	23 (6%)	2 (1%)	30	52
1	F	355/379 (94%)	327 (92%)	24 (7%)	4 (1%)	17	33
All	All	2132/2274 (94%)	1995 (94%)	112 (5%)	25 (1%)	19	30

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	52	VAL
1	D	54	TRP
1	D	189	TYR
1	C	189[A]	TYR
1	C	189[B]	TYR
1	A	189[A]	TYR
1	A	189[B]	TYR
1	B	189	TYR
1	E	189	TYR
1	F	189	TYR
1	E	345	ALA
1	F	72	CYS
1	A	345	ALA
1	B	345	ALA
1	D	345	ALA
1	C	190[A]	PRO
1	C	190[B]	PRO
1	C	345	ALA
1	B	42	ARG
1	F	30	PRO
1	A	45	GLY
1	B	235	PRO
1	F	345	ALA
1	C	342	VAL
1	A	146	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	294/314 (94%)	291 (99%)	3 (1%)	82	93
1	B	295/314 (94%)	292 (99%)	3 (1%)	82	93
1	C	297/314 (95%)	291 (98%)	6 (2%)	63	84
1	D	294/314 (94%)	291 (99%)	3 (1%)	82	93
1	E	295/314 (94%)	291 (99%)	4 (1%)	74	89
1	F	295/314 (94%)	291 (99%)	4 (1%)	74	89
All	All	1770/1884 (94%)	1747 (99%)	23 (1%)	76	90

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	42	ARG
1	D	46	LYS
1	D	60	MET
1	C	22	PHE
1	C	43	SER
1	C	88	ASP
1	C	180	THR
1	C	265	PRO
1	C	324	GLU
1	A	180	THR
1	A	262	ARG
1	A	346	SER
1	B	56	GLN
1	B	143	LEU
1	B	198	PHE
1	E	22	PHE
1	E	217	ARG
1	E	266	THR
1	E	361	PHE
1	F	153	ASN
1	F	198	PHE
1	F	251	HIS

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Mol	Chain	Res	Type
1	F	322	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	29	HIS
1	A	109	ASN
1	E	333	GLN
1	F	151	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

9 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	A	401	-	4,4,4	0.25	0	6,6,6	0.21	0
3	NAP	A	402[A]	-	45,52,52	0.82	1 (2%)	55,80,80	1.37	1 (1%)
3	NAP	A	402[B]	-	45,52,52	0.82	1 (2%)	55,80,80	1.43	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	B	401	-	4,4,4	0.23	0	6,6,6	0.19	0
2	SO4	C	401	-	4,4,4	0.22	0	6,6,6	0.11	0
3	NAP	C	402	-	45,52,52	0.81	1 (2%)	55,80,80	1.37	2 (3%)
2	SO4	D	401	-	4,4,4	0.12	0	6,6,6	0.16	0
2	SO4	E	401	-	4,4,4	0.14	0	6,6,6	0.14	0
2	SO4	F	401	-	4,4,4	0.16	0	6,6,6	0.15	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	401	-	-	0/0/0/0	0/0/0/0
3	NAP	A	402[A]	-	-	0/27/67/67	0/5/5/5
3	NAP	A	402[B]	-	-	0/27/67/67	0/5/5/5
2	SO4	B	401	-	-	0/0/0/0	0/0/0/0
2	SO4	C	401	-	-	0/0/0/0	0/0/0/0
3	NAP	C	402	-	-	0/27/67/67	0/5/5/5
2	SO4	D	401	-	-	0/0/0/0	0/0/0/0
2	SO4	E	401	-	-	0/0/0/0	0/0/0/0
2	SO4	F	401	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	NAP	C5A-C4A	3.12	1.47	1.40
3	A	402[A]	NAP	C5A-C4A	3.14	1.47	1.40
3	A	402[B]	NAP	C5A-C4A	3.14	1.47	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402[A]	NAP	N3A-C2A-N1A	-6.59	123.70	128.87
3	C	402	NAP	N3A-C2A-N1A	-6.59	123.70	128.87
3	A	402[B]	NAP	N3A-C2A-N1A	-6.51	123.76	128.87
3	C	402	NAP	C4D-O4D-C1D	2.01	111.78	109.64
3	A	402[B]	NAP	C4B-O4B-C1B	2.02	111.79	109.64
3	A	402[B]	NAP	C4D-O4D-C1D	2.15	111.92	109.64
3	A	402[B]	NAP	O4D-C1D-N1N	3.26	111.62	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	SO4	1	0
3	A	402[A]	NAP	10	0
3	A	402[B]	NAP	19	0
2	C	401	SO4	1	0
3	C	402	NAP	19	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

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	354/379 (93%)	0.42	13 (3%) 45 42	20, 39, 78, 111	0
1	B	357/379 (94%)	0.41	14 (3%) 43 40	20, 44, 94, 113	0
1	C	357/379 (94%)	0.52	19 (5%) 30 28	18, 42, 92, 111	0
1	D	356/379 (93%)	0.35	13 (3%) 45 42	18, 39, 88, 112	0
1	E	357/379 (94%)	0.64	36 (10%) 9 7	24, 52, 101, 116	0
1	F	357/379 (94%)	0.70	33 (9%) 11 9	30, 61, 101, 116	0
All	All	2138/2274 (94%)	0.51	128 (5%) 25 22	18, 47, 93, 116	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	189	TYR	11.7
1	F	45	GLY	9.9
1	C	189[A]	TYR	9.7
1	E	48	TYR	7.5
1	C	45	GLY	7.3
1	E	45	GLY	7.1
1	A	189[A]	TYR	6.3
1	C	67	LEU	5.9
1	E	42	ARG	5.5
1	D	52	VAL	5.1
1	F	322	ILE	5.1
1	E	189	TYR	5.0
1	C	188[A]	GLY	5.0
1	B	51	ALA	4.6
1	C	190[A]	PRO	4.6
1	F	281	VAL	4.2
1	F	37	VAL	4.2
1	D	189	TYR	4.1
1	C	66	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	53	ARG	4.0
1	F	42	ARG	4.0
1	E	40	SER	3.9
1	B	8	ARG	3.7
1	E	11	VAL	3.7
1	B	59	PRO	3.6
1	E	31	LEU	3.5
1	A	55	LYS	3.5
1	D	45	GLY	3.5
1	E	44	SER	3.4
1	B	34	LEU	3.3
1	B	45	GLY	3.3
1	E	357	ILE	3.2
1	F	270	VAL	3.2
1	C	44	SER	3.1
1	B	31	LEU	3.1
1	F	48	TYR	3.1
1	E	362	VAL	3.1
1	B	23	ILE	3.0
1	F	66	ASP	3.0
1	F	44	SER	3.0
1	A	39	ALA	2.9
1	E	10	GLY	2.9
1	E	41	ASP	2.9
1	F	104	PHE	2.9
1	E	34	LEU	2.9
1	F	362	VAL	2.8
1	E	14	ALA	2.8
1	E	52	VAL	2.8
1	E	53	ARG	2.8
1	E	131	ILE	2.7
1	C	6	LYS	2.7
1	F	131	ILE	2.7
1	A	190[A]	PRO	2.7
1	F	23	ILE	2.7
1	E	55	LYS	2.7
1	E	15	THR	2.7
1	F	34	LEU	2.6
1	D	284	LEU	2.6
1	E	20	THR	2.6
1	E	99	PHE	2.6
1	F	267	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	79	ASP	2.6
1	F	332	ILE	2.5
1	C	34	LEU	2.5
1	B	68	THR	2.5
1	E	281	VAL	2.5
1	A	57	SER	2.5
1	E	51	ALA	2.5
1	F	123	VAL	2.5
1	E	67	LEU	2.5
1	E	139	LYS	2.5
1	D	46	LYS	2.5
1	D	67	LEU	2.4
1	C	63	LYS	2.4
1	B	6	LYS	2.4
1	C	32	LEU	2.4
1	A	46	LYS	2.4
1	F	235	PRO	2.4
1	D	31	LEU	2.4
1	F	357	ILE	2.4
1	E	8	ARG	2.4
1	E	36	ALA	2.4
1	F	356	ALA	2.4
1	C	8	ARG	2.3
1	C	23	ILE	2.3
1	F	28	GLN	2.3
1	A	40	SER	2.3
1	A	54	TRP	2.3
1	F	18	VAL	2.3
1	C	131	ILE	2.3
1	E	57	SER	2.3
1	D	18	VAL	2.3
1	C	48	TYR	2.3
1	B	189	TYR	2.3
1	D	42	ARG	2.3
1	C	71	CYS	2.3
1	C	68	THR	2.2
1	E	12	LEU	2.2
1	F	31	LEU	2.2
1	E	104	PHE	2.2
1	A	28	GLN	2.2
1	C	58	ALA	2.2
1	D	24	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	40	SER	2.2
1	B	131	ILE	2.2
1	E	358	LEU	2.2
1	E	37	VAL	2.2
1	F	335	VAL	2.2
1	D	15	THR	2.2
1	F	82	ILE	2.2
1	B	77	PHE	2.2
1	B	53	ARG	2.1
1	F	6	LYS	2.1
1	F	95	ILE	2.1
1	E	32	LEU	2.1
1	A	24	LEU	2.1
1	A	350	ILE	2.1
1	E	66	ASP	2.1
1	E	355	SER	2.1
1	F	12	LEU	2.1
1	A	48	TYR	2.1
1	E	23	ILE	2.1
1	F	64	VAL	2.0
1	F	67	LEU	2.0
1	D	40	SER	2.0
1	F	258	ARG	2.0
1	F	50	ASP	2.0
1	D	61	PRO	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors



of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAP	A	402[A]	48/48	0.76	0.39	1.78	55,72,77,79	48
3	NAP	A	402[B]	48/48	0.76	0.39	1.45	51,71,75,77	48
3	NAP	C	402	48/48	0.74	0.38	1.38	70,76,85,88	48
2	SO4	C	401	5/5	0.98	0.20	0.28	40,43,50,58	0
2	SO4	D	401	5/5	0.98	0.13	-0.71	30,35,37,40	0
2	SO4	A	401	5/5	0.98	0.13	-1.27	43,50,58,59	0
2	SO4	B	401	5/5	0.97	0.14	-1.30	32,36,38,46	0
2	SO4	E	401	5/5	0.95	0.13	-1.70	37,50,53,55	0
2	SO4	F	401	5/5	0.97	0.12	-2.26	45,53,57,60	0

## 6.5 Other polymers

There are no such residues in this entry.