



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:27 PM UTC

PDB ID : 3HB1 / pdb_00003hb1
Title : Crystal structure of ed-eya2 complexed with Alf3
Authors : Jung, S.K.; Jeong, D.G.; Ryu, S.E.; Kim, S.J.
Deposited on : 2009-05-03
Resolution : 2.51 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

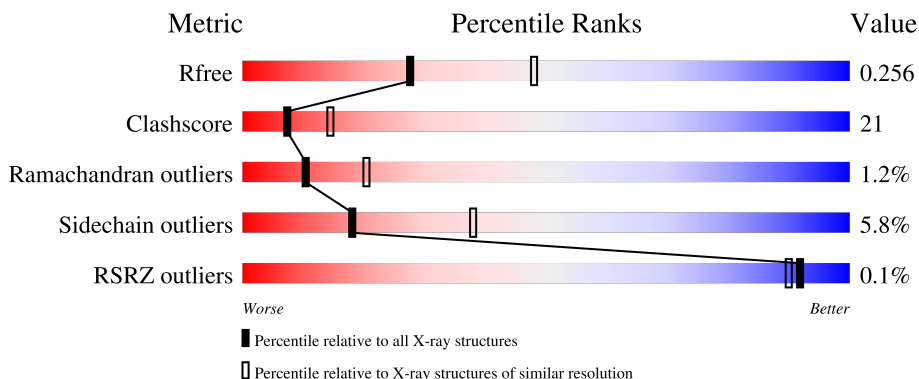
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	274	 64% 27% • 6%
1	B	274	 55% 33% • • 8%
1	C	274	 47% 40% 7% 6%
1	D	274	 55% 37% • 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8432 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.

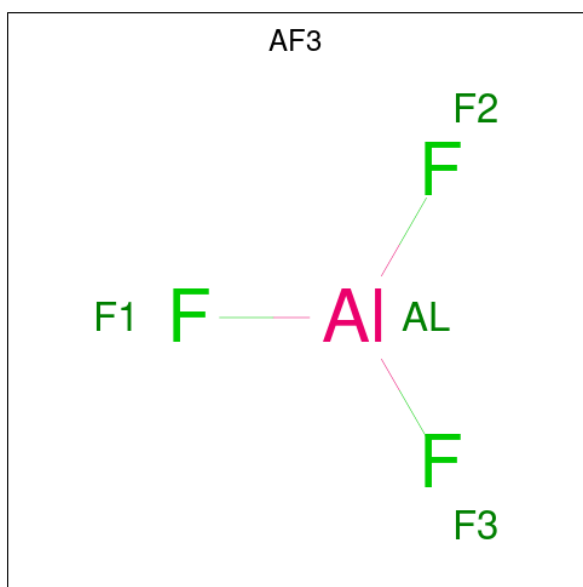
- Molecule 1 is a protein called Eyes absent homolog 2 (Drosophila).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2078	1322	355	389	12			
1	B	253	Total	C	N	O	S	0	0	0
			2049	1305	350	383	11			
1	C	258	Total	C	N	O	S	0	0	0
			2078	1322	355	389	12			
1	D	256	Total	C	N	O	S	0	0	0
			2064	1314	353	386	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	SER	-	expression tag	UNP Q86U84
A	266	HIS	-	expression tag	UNP Q86U84
A	267	MET	-	expression tag	UNP Q86U84
A	268	GLU	-	expression tag	UNP Q86U84
B	265	SER	-	expression tag	UNP Q86U84
B	266	HIS	-	expression tag	UNP Q86U84
B	267	MET	-	expression tag	UNP Q86U84
B	268	GLU	-	expression tag	UNP Q86U84
C	265	SER	-	expression tag	UNP Q86U84
C	266	HIS	-	expression tag	UNP Q86U84
C	267	MET	-	expression tag	UNP Q86U84
C	268	GLU	-	expression tag	UNP Q86U84
D	265	SER	-	expression tag	UNP Q86U84
D	266	HIS	-	expression tag	UNP Q86U84
D	267	MET	-	expression tag	UNP Q86U84
D	268	GLU	-	expression tag	UNP Q86U84

- Molecule 2 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Al	F	0	0
			4	1	3		
2	B	1	Total	Al	F	0	0
			4	1	3		
2	C	1	Total	Al	F	0	0
			4	1	3		
2	D	1	Total	Al	F	0	0
			4	1	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	58	Total	O	0	0
			58	58		

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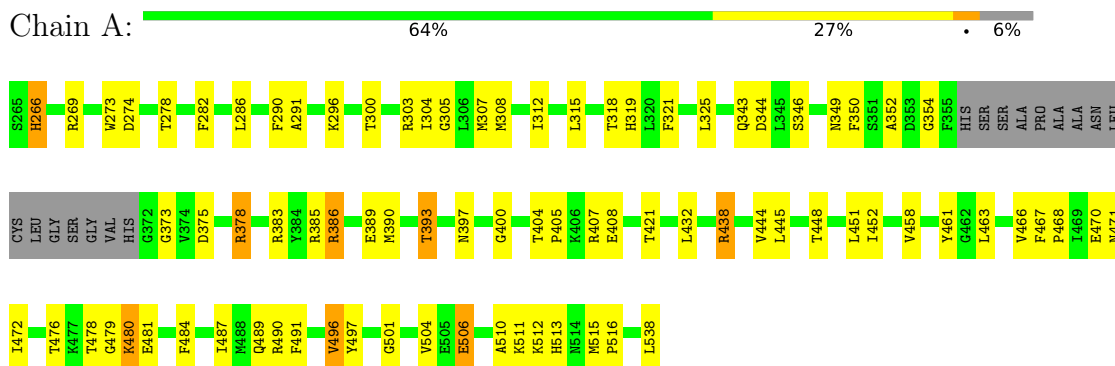
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	32	Total 32	O 32	0	0
4	C	24	Total 24	O 24	0	0
4	D	29	Total 29	O 29	0	0

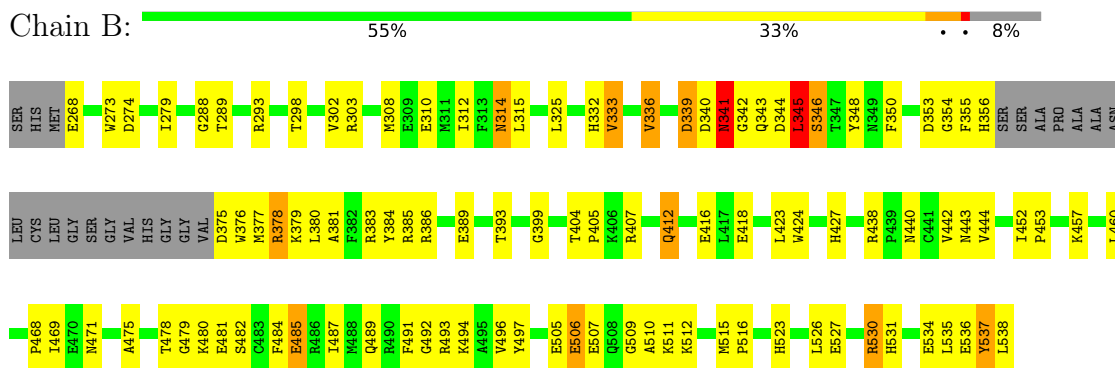
3 Residue-property plots

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.

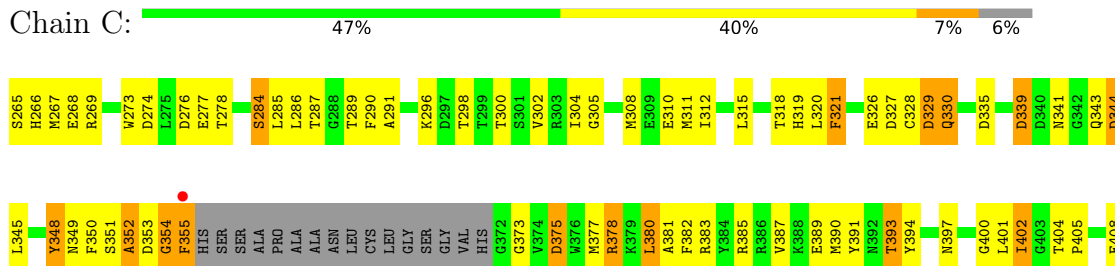
• Molecule 1: Eyes absent homolog 2 (Drosophila)



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4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	183.94Å 183.94Å 119.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.51 40.00 – 2.51	Depositor EDS
% Data completeness (in resolution range)	90.4 (40.00-2.51) 95.1 (40.00-2.51)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.200 , 0.240 0.218 , 0.256	Depositor DCC
R_{free} test set	3362 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 26.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.077 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8432	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AF3, MG

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	0.51	0/2121	1.03	14/2867 (0.5%)
1	B	0.47	0/2092	0.98	9/2829 (0.3%)
1	C	0.47	0/2121	0.97	9/2867 (0.3%)
1	D	0.48	0/2107	0.98	7/2849 (0.2%)
All	All	0.48	0/8441	0.99	39/11412 (0.3%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	537	TYR	N-CA-C	-9.13	101.25	112.38
1	A	375	ASP	N-CA-C	-8.91	102.54	113.50
1	A	438	ARG	CA-C-N	8.33	128.29	119.05
1	A	438	ARG	C-N-CA	8.33	128.29	119.05
1	C	274	ASP	N-CA-C	-8.18	98.35	110.46
1	D	537	TYR	N-CA-C	-8.17	102.57	112.54
1	B	346	SER	N-CA-C	-8.04	103.45	113.18
1	A	478	THR	N-CA-C	7.56	120.40	111.71
1	C	438	ARG	CA-C-N	7.50	127.05	119.24
1	C	438	ARG	C-N-CA	7.50	127.05	119.24
1	D	505	GLU	N-CA-C	-7.12	103.45	111.07
1	C	278	THR	N-CA-C	-7.10	102.61	112.12
1	A	274	ASP	N-CA-C	-6.90	99.73	110.42
1	D	274	ASP	N-CA-C	-6.69	100.62	110.52
1	D	438	ARG	CA-C-N	6.40	125.89	119.24
1	D	438	ARG	C-N-CA	6.40	125.89	119.24
1	B	274	ASP	N-CA-C	-6.10	100.62	110.32
1	C	353	ASP	N-CA-C	6.06	118.50	108.99
1	A	318	THR	N-CA-C	6.03	117.94	111.36
1	D	278	THR	N-CA-C	-5.93	102.51	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	438	ARG	CA-C-N	5.89	125.10	118.97
1	B	438	ARG	C-N-CA	5.89	125.10	118.97
1	A	451	LEU	N-CA-C	5.85	117.35	110.97
1	C	351	SER	N-CA-C	-5.81	105.29	112.38
1	B	336	VAL	N-CA-C	-5.70	107.72	113.20
1	A	480	LYS	N-CA-C	5.68	117.55	111.36
1	C	318	THR	N-CA-C	5.61	117.87	111.02
1	A	504	VAL	N-CA-C	5.59	116.37	110.72
1	A	479	GLY	N-CA-C	-5.53	106.09	112.29
1	C	375	ASP	N-CA-C	-5.53	105.27	112.23
1	A	273	TRP	N-CA-C	5.47	118.61	110.52
1	B	492	GLY	N-CA-C	5.37	119.23	111.24
1	A	278	THR	N-CA-C	-5.35	104.95	112.12
1	A	325	LEU	N-CA-C	5.21	118.89	112.54
1	D	342	GLY	N-CA-C	-5.18	106.28	114.10
1	B	423	LEU	N-CA-C	5.05	118.71	112.24
1	C	273	TRP	N-CA-C	5.04	117.98	110.52
1	B	314	ASN	N-CA-C	-5.01	105.89	111.36
1	A	266	HIS	N-CA-C	5.01	117.30	110.24

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	2078	0	2041	61	0
1	B	2049	0	2012	86	0
1	C	2078	0	2041	119	0
1	D	2064	0	2027	82	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	58	0	0	2	0
4	B	32	0	0	3	0
4	C	24	0	0	1	0
4	D	29	0	0	2	0
All	All	8432	0	8121	337	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 21.

All (337) 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:C:378:ARG:HH11	1:C:378:ARG:HB2	0.99	1.15
1:D:510:ALA:HA	1:D:515:MET:HE3	1.36	1.07
1:D:489:GLN:HE22	1:D:493:ARG:HH22	1.07	0.95
1:A:513:HIS:HB2	1:A:515:MET:HE2	1.46	0.94
1:A:389:GLU:O	1:A:393:THR:HG23	1.68	0.92
1:C:378:ARG:HB2	1:C:378:ARG:NH1	1.84	0.91
1:B:345:LEU:HG	1:B:385:ARG:HH21	1.33	0.90
1:D:312:ILE:HD13	1:D:460:LEU:HD12	1.51	0.89
1:B:510:ALA:HA	1:B:515:MET:HE3	1.57	0.87
1:D:427:HIS:HD2	1:D:523:HIS:CE1	1.94	0.85
1:D:489:GLN:NE2	1:D:493:ARG:HH22	1.74	0.85
1:D:427:HIS:HD2	1:D:523:HIS:HE1	1.18	0.84
1:D:339:ASP:O	1:D:378:ARG:HA	1.78	0.83
1:C:378:ARG:HH11	1:C:378:ARG:CB	1.87	0.82
1:D:432:LEU:HB3	1:D:466:VAL:HG11	1.62	0.82
1:C:513:HIS:HB2	1:C:515:MET:HE2	1.62	0.82
1:B:345:LEU:HG	1:B:385:ARG:NH2	1.95	0.81
1:D:269:ARG:HG2	1:D:496:VAL:HG22	1.64	0.80
1:C:277:GLU:OE2	1:C:284:SER:HB2	1.83	0.79
1:C:507:GLU:O	1:C:511:LYS:HD3	1.83	0.79
1:A:349:ASN:ND2	1:A:352:ALA:HB3	2.00	0.76
1:D:308:MET:HE1	1:D:312:ILE:HD11	1.66	0.76
1:C:343:GLN:HG2	1:C:344:ASP:N	2.01	0.75
1:B:427:HIS:HD2	1:B:523:HIS:HE1	1.34	0.74
1:C:348:TYR:HD2	1:C:349:ASN:N	1.85	0.74
1:A:480:LYS:NZ	1:A:506:GLU:HG2	2.02	0.74
1:B:427:HIS:HD2	1:B:523:HIS:CE1	2.04	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:481:GLU:CD	1:D:512:LYS:HD3	2.14	0.73
1:A:432:LEU:HB3	1:A:466:VAL:HG21	1.71	0.73
1:D:489:GLN:HE22	1:D:493:ARG:NH2	1.86	0.72
1:C:343:GLN:HG2	1:C:344:ASP:H	1.55	0.72
1:A:445:LEU:HD23	1:A:472:ILE:HG23	1.71	0.72
1:C:508:GLN:HG3	1:C:512:LYS:HZ2	1.52	0.72
1:A:480:LYS:HZ2	1:A:506:GLU:HG2	1.53	0.72
1:A:397:ASN:HD21	1:A:400:GLY:HA3	1.55	0.72
1:C:385:ARG:O	1:C:389:GLU:HG3	1.90	0.71
1:D:513:HIS:HB2	1:D:515:MET:HE2	1.72	0.71
1:C:339:ASP:N	1:C:339:ASP:OD2	2.23	0.71
1:C:354:GLY:HA3	1:C:383:ARG:NH2	2.04	0.71
1:B:310:GLU:O	1:B:314:ASN:HB2	1.90	0.71
1:C:484:PHE:HB3	1:C:515:MET:HE1	1.73	0.71
1:B:333:VAL:HG21	1:B:469:ILE:HG12	1.72	0.71
1:C:508:GLN:HE21	1:C:512:LYS:NZ	1.88	0.70
1:D:427:HIS:CD2	1:D:523:HIS:HE1	2.04	0.70
1:C:285:LEU:HD11	1:C:417:LEU:HD11	1.75	0.69
1:D:308:MET:HE2	1:D:461:TYR:HE1	1.58	0.69
1:B:341:ASN:HD21	1:B:378:ARG:HG2	1.58	0.69
1:B:537:TYR:O	1:C:269:ARG:NH2	2.25	0.69
1:C:481:GLU:HG3	1:C:513:HIS:CE1	2.28	0.69
1:C:378:ARG:H	1:C:378:ARG:HD3	1.59	0.68
1:A:349:ASN:HD21	1:A:352:ALA:HB3	1.55	0.68
1:B:510:ALA:HA	1:B:515:MET:CE	2.24	0.66
1:B:385:ARG:O	1:B:389:GLU:HG3	1.96	0.66
1:B:350:PHE:HA	1:B:353:ASP:OD1	1.95	0.66
1:C:268:GLU:O	1:C:496:VAL:HG22	1.95	0.66
1:B:325:LEU:HD22	1:B:384:TYR:HE1	1.61	0.66
1:C:300:THR:O	1:C:304:ILE:HG12	1.95	0.66
1:A:458:VAL:HG13	1:A:463:LEU:HB2	1.78	0.65
1:B:480:LYS:HD2	1:B:505:GLU:HB3	1.78	0.65
1:B:481:GLU:O	1:B:485:GLU:HG2	1.95	0.65
1:B:375:ASP:CG	1:B:376:TRP:H	2.02	0.65
1:B:484:PHE:CD1	1:B:515:MET:HE1	2.31	0.65
1:A:300:THR:O	1:A:304:ILE:HD13	1.96	0.65
1:C:380:LEU:HD23	1:C:381:ALA:N	2.11	0.64
1:D:448:THR:HG23	1:D:480:LYS:HE2	1.78	0.64
1:B:516:PRO:HB3	1:C:538:LEU:CD2	2.28	0.64
1:D:339:ASP:OD1	1:D:377:MET:HB3	1.98	0.64
1:B:336:VAL:HG11	1:B:380:LEU:HD12	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:ASP:OD2	1:B:377:MET:HE3	1.98	0.64
1:A:397:ASN:ND2	1:A:400:GLY:HA3	2.13	0.63
1:A:386:ARG:O	1:A:390:MET:HG2	1.97	0.63
1:A:269:ARG:HG2	1:A:496:VAL:CG2	2.29	0.63
1:D:468:PRO:HG2	1:D:471:ASN:HB2	1.80	0.63
1:C:383:ARG:O	1:C:387:VAL:HG23	1.98	0.63
1:D:484:PHE:O	1:D:488:MET:HG3	1.99	0.62
1:D:308:MET:HE2	1:D:461:TYR:CE1	2.34	0.62
1:A:269:ARG:HG2	1:A:496:VAL:HG22	1.82	0.62
1:C:452:ILE:HB	1:C:453:PRO:HD3	1.83	0.61
1:A:385:ARG:O	1:A:389:GLU:HG3	1.99	0.61
1:B:339:ASP:HB3	1:B:377:MET:HB3	1.81	0.61
1:C:508:GLN:CG	1:C:512:LYS:HZ2	2.14	0.61
1:C:290:PHE:CE2	1:C:421:THR:HA	2.36	0.60
1:C:315:LEU:C	1:C:315:LEU:HD23	2.26	0.60
1:C:508:GLN:HE21	1:C:512:LYS:HZ2	1.49	0.60
1:B:481:GLU:OE2	1:B:512:LYS:HD3	2.02	0.60
1:C:302:VAL:HB	1:D:412:GLN:NE2	2.16	0.60
1:C:348:TYR:HD2	1:C:348:TYR:C	2.10	0.60
1:C:513:HIS:CB	1:C:515:MET:HE2	2.32	0.60
1:D:442:VAL:HG23	4:D:25:HOH:O	2.00	0.60
1:D:448:THR:HG23	1:D:480:LYS:CE	2.32	0.60
1:A:510:ALA:HA	1:A:515:MET:HE3	1.84	0.60
1:C:478:THR:HB	1:C:482:SER:OG	2.02	0.59
1:B:412:GLN:O	1:B:416:GLU:HG3	2.01	0.59
1:C:308:MET:HA	1:C:308:MET:HE3	1.85	0.59
1:B:375:ASP:N	1:B:378:ARG:HD2	2.17	0.58
1:D:268:GLU:HA	1:D:440:ASN:O	2.03	0.58
1:B:485:GLU:O	1:B:489:GLN:HG3	2.04	0.58
1:B:427:HIS:CD2	1:B:523:HIS:HE1	2.19	0.58
1:B:452:ILE:HB	1:B:453:PRO:HD3	1.85	0.58
1:C:507:GLU:HG3	1:C:511:LYS:NZ	2.18	0.58
1:C:414:ARG:HH11	1:C:414:ARG:HB3	1.69	0.58
1:D:480:LYS:HD2	1:D:505:GLU:HB3	1.85	0.58
1:C:348:TYR:C	1:C:348:TYR:CD2	2.82	0.57
1:A:404:THR:CG2	1:A:405:PRO:HA	2.34	0.57
1:A:513:HIS:CB	1:A:515:MET:HE2	2.29	0.57
1:D:355:PHE:HB3	1:D:383:ARG:NH2	2.20	0.57
1:B:389:GLU:O	1:B:393:THR:HG23	2.05	0.57
1:A:303:ARG:O	1:A:307:MET:HG3	2.04	0.57
1:C:339:ASP:OD1	1:C:377:MET:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:508:GLN:NE2	1:C:512:LYS:NZ	2.52	0.57
1:C:450:GLN:O	1:C:453:PRO:HD2	2.04	0.57
1:C:510:ALA:HA	1:C:515:MET:HE3	1.87	0.56
1:A:291:ALA:HA	1:A:296:LYS:HB2	1.86	0.56
1:D:319:HIS:O	1:D:390:MET:HE1	2.06	0.56
1:C:350:PHE:HD2	1:C:383:ARG:NH1	2.03	0.56
1:C:339:ASP:O	1:C:378:ARG:HA	2.06	0.56
1:D:507:GLU:HG3	1:D:511:LYS:HE3	1.88	0.56
1:D:321:PHE:O	1:D:325:LEU:HG	2.06	0.55
1:D:375:ASP:O	1:D:379:LYS:HG3	2.06	0.55
1:A:308:MET:HE2	1:A:461:TYR:CE1	2.42	0.55
1:C:496:VAL:HG23	1:C:496:VAL:O	2.05	0.55
1:D:468:PRO:HG2	1:D:471:ASN:CG	2.31	0.55
1:D:339:ASP:OD2	1:D:339:ASP:N	2.35	0.55
1:A:538:LEU:CD2	1:D:516:PRO:HB3	2.37	0.54
1:C:391:TYR:CD2	1:C:469:ILE:HB	2.43	0.54
1:C:470:GLU:CD	1:C:470:GLU:H	2.15	0.54
1:B:509:GLY:HA2	1:B:512:LYS:HD2	1.87	0.54
1:A:290:PHE:CE2	1:A:421:THR:HA	2.43	0.54
1:A:319:HIS:HE1	4:A:78:HOH:O	1.90	0.54
1:C:339:ASP:OD1	1:C:377:MET:HE3	2.08	0.54
1:C:501:GLY:HA3	1:C:506:GLU:OE1	2.09	0.53
1:D:448:THR:O	1:D:476:THR:HG22	2.08	0.53
1:B:268:GLU:HG2	1:B:494:LYS:HE2	1.91	0.53
1:B:340:ASP:CG	1:B:341:ASN:H	2.14	0.53
1:A:308:MET:HE3	1:A:312:ILE:HG13	1.89	0.53
1:D:307:MET:O	1:D:310:GLU:HB3	2.09	0.53
1:D:350:PHE:HD2	1:D:383:ARG:NH1	2.07	0.53
1:A:282:PHE:HB3	4:A:76:HOH:O	2.08	0.53
1:A:484:PHE:HB3	1:A:515:MET:HE1	1.91	0.53
1:C:418:GLU:OE1	1:C:423:LEU:HA	2.08	0.53
1:B:303:ARG:NH2	1:B:416:GLU:OE1	2.37	0.53
1:C:382:PHE:HE2	1:C:385:ARG:NH2	2.07	0.53
1:A:300:THR:HG22	1:A:304:ILE:HD13	1.90	0.52
1:B:268:GLU:HA	1:B:440:ASN:O	2.09	0.52
1:D:303:ARG:NH2	1:D:416:GLU:OE1	2.41	0.52
1:B:325:LEU:HD22	1:B:384:TYR:CE1	2.43	0.52
1:A:404:THR:HG23	1:A:408:GLU:OE2	2.10	0.52
1:A:470:GLU:CD	1:A:470:GLU:H	2.17	0.52
1:A:349:ASN:HD21	1:A:352:ALA:CB	2.23	0.52
1:B:377:MET:HB2	1:B:378:ARG:HH21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:THR:CG2	1:C:405:PRO:HA	2.40	0.52
1:A:444:VAL:HG11	1:A:487:ILE:HD13	1.90	0.52
1:B:273:TRP:HB3	1:B:279:ILE:HD11	1.91	0.52
1:D:501:GLY:HA3	1:D:506:GLU:OE1	2.09	0.52
1:B:535:LEU:O	1:B:536:GLU:HB2	2.07	0.52
1:D:507:GLU:O	1:D:511:LYS:HG3	2.09	0.52
1:A:321:PHE:CE1	1:A:386:ARG:HG2	2.45	0.51
1:A:349:ASN:ND2	1:A:352:ALA:H	2.08	0.51
1:B:332:HIS:ND1	1:B:333:VAL:N	2.59	0.51
1:C:355:PHE:C	1:C:355:PHE:CD1	2.88	0.51
1:D:481:GLU:OE1	1:D:512:LYS:HD3	2.09	0.51
1:B:507:GLU:HG2	1:B:511:LYS:HE2	1.93	0.51
1:D:308:MET:CE	1:D:312:ILE:HD11	2.39	0.51
1:B:536:GLU:C	1:B:538:LEU:N	2.64	0.51
1:D:307:MET:HE2	1:D:413:LEU:HD13	1.91	0.51
1:D:468:PRO:HG2	1:D:471:ASN:CB	2.40	0.51
1:C:510:ALA:HB1	1:C:515:MET:O	2.10	0.51
1:C:480:LYS:HG3	1:C:505:GLU:OE2	2.10	0.50
1:D:385:ARG:O	1:D:389:GLU:HG3	2.10	0.50
1:B:487:ILE:O	1:B:491:PHE:HD1	1.95	0.50
1:C:320:LEU:HD22	1:C:387:VAL:HG13	1.93	0.50
1:D:373:GLY:O	1:D:377:MET:HG2	2.10	0.50
1:B:375:ASP:CG	1:B:376:TRP:N	2.70	0.50
1:D:310:GLU:O	1:D:314:ASN:HB2	2.12	0.50
1:D:427:HIS:CD2	1:D:523:HIS:CE1	2.85	0.50
1:C:319:HIS:O	1:C:390:MET:HE1	2.12	0.50
1:C:481:GLU:HG3	1:C:513:HIS:HE1	1.73	0.50
1:A:350:PHE:HB3	1:A:383:ARG:NH1	2.26	0.50
1:B:507:GLU:O	1:B:511:LYS:HG3	2.12	0.50
1:C:315:LEU:HD23	1:C:315:LEU:O	2.12	0.50
1:C:348:TYR:CD2	1:C:349:ASN:N	2.74	0.50
1:C:483:CYS:O	1:C:487:ILE:HG13	2.11	0.49
1:B:340:ASP:OD1	1:B:341:ASN:N	2.35	0.49
1:A:266:HIS:CD2	1:D:514:ASN:HB3	2.46	0.49
1:C:511:LYS:HD2	1:C:511:LYS:N	2.27	0.49
1:C:311:MET:HE1	1:C:410:TRP:HB2	1.94	0.49
1:C:375:ASP:HA	1:C:378:ARG:CZ	2.42	0.49
1:C:404:THR:HG23	1:C:408:GLU:OE2	2.13	0.49
1:A:496:VAL:CG2	1:A:496:VAL:O	2.60	0.49
1:B:336:VAL:HG12	1:B:381:ALA:HB2	1.94	0.49
1:B:496:VAL:HG11	1:C:267:MET:HE3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:MET:HE2	1:A:461:TYR:HE1	1.78	0.49
1:A:350:PHE:HB3	1:A:383:ARG:HH12	1.76	0.49
1:B:344:ASP:C	1:B:346:SER:H	2.21	0.49
1:B:312:ILE:HD13	1:B:457:LYS:HG2	1.95	0.49
1:B:339:ASP:O	1:B:378:ARG:HA	2.13	0.48
1:B:468:PRO:HG2	1:B:471:ASN:CG	2.37	0.48
1:C:507:GLU:HG3	1:C:511:LYS:HZ3	1.77	0.48
1:A:321:PHE:HE1	1:A:386:ARG:HG2	1.79	0.48
1:B:530:ARG:NH2	4:B:85:HOH:O	2.45	0.48
1:C:390:MET:HA	1:C:393:THR:OG1	2.13	0.48
1:B:507:GLU:CG	1:B:511:LYS:HE2	2.44	0.48
1:B:268:GLU:HG2	1:B:494:LYS:CE	2.43	0.48
1:C:468:PRO:HG2	1:C:471:ASN:OD1	2.13	0.48
1:D:426:THR:O	1:D:430:LYS:HG2	2.14	0.48
1:B:298:THR:O	1:B:302:VAL:HG23	2.13	0.48
1:C:468:PRO:HG2	1:C:471:ASN:CG	2.38	0.48
1:D:489:GLN:NE2	1:D:493:ARG:NH2	2.53	0.48
1:C:530:ARG:NH1	1:C:534:GLU:OE1	2.36	0.48
1:C:291:ALA:HA	1:C:296:LYS:HB2	1.96	0.48
1:B:444:VAL:HG11	1:B:487:ILE:HD13	1.97	0.47
1:C:345:LEU:HD21	1:C:382:PHE:CD2	2.49	0.47
1:B:345:LEU:CG	1:B:385:ARG:HH21	2.15	0.47
1:C:414:ARG:HB3	1:C:414:ARG:NH1	2.28	0.47
1:C:312:ILE:HD13	1:C:457:LYS:HG2	1.97	0.47
1:B:288:GLY:HA2	4:B:61:HOH:O	2.15	0.47
1:C:350:PHE:HD2	1:C:383:ARG:HH11	1.61	0.47
1:C:382:PHE:HE2	1:C:385:ARG:HH21	1.63	0.47
1:A:468:PRO:HG2	1:A:471:ASN:CG	2.40	0.47
1:C:508:GLN:NE2	1:C:512:LYS:HZ2	2.10	0.47
1:D:389:GLU:O	1:D:393:THR:HG23	2.14	0.47
1:B:308:MET:CE	1:B:460:LEU:HD13	2.45	0.47
1:A:344:ASP:OD2	1:A:346:SER:HB2	2.15	0.47
1:A:404:THR:HG22	1:A:405:PRO:HA	1.97	0.47
1:B:531:HIS:O	1:B:534:GLU:HB2	2.15	0.46
1:C:330:GLN:HG2	1:C:335:ASP:HB2	1.98	0.46
1:D:269:ARG:HH12	1:D:538:LEU:HA	1.81	0.46
1:B:343:GLN:O	1:B:385:ARG:NH2	2.49	0.46
1:B:399:GLY:CA	1:B:407:ARG:HG3	2.46	0.46
1:C:329:ASP:OD1	1:C:452:ILE:HG12	2.16	0.46
1:B:355:PHE:HB2	1:B:383:ARG:HH21	1.81	0.45
1:C:404:THR:HG23	1:C:405:PRO:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:430:LYS:HB2	1:D:530:ARG:HD2	1.97	0.45
1:C:444:VAL:HG11	1:C:487:ILE:HD13	1.98	0.45
1:A:491:PHE:HB2	1:A:497:TYR:OH	2.16	0.45
1:B:527:GLU:HA	1:B:527:GLU:OE1	2.16	0.45
1:C:339:ASP:C	1:C:378:ARG:HG3	2.41	0.45
1:C:484:PHE:CB	1:C:515:MET:HE1	2.44	0.45
1:D:397:ASN:ND2	1:D:400:GLY:HA3	2.31	0.45
1:D:434:LEU:O	1:D:438:ARG:HG3	2.17	0.45
1:B:442:VAL:HG22	1:B:443:ASN:N	2.32	0.45
1:B:493:ARG:NH2	1:C:265:SER:OG	2.49	0.45
1:D:308:MET:O	1:D:312:ILE:HG12	2.16	0.45
1:D:439:PRO:HG2	4:D:26:HOH:O	2.17	0.45
1:C:341:ASN:OD1	1:C:343:GLN:HB2	2.17	0.45
1:A:481:GLU:HB2	1:A:513:HIS:HE1	1.82	0.45
1:B:336:VAL:HG12	1:B:336:VAL:O	2.17	0.44
1:B:386:ARG:CG	1:B:386:ARG:HH11	2.31	0.44
1:C:354:GLY:HA3	1:C:383:ARG:HH21	1.80	0.44
1:C:394:TYR:CG	1:C:401:LEU:HB2	2.51	0.44
1:A:438:ARG:NH2	1:A:538:LEU:HG	2.32	0.44
1:B:386:ARG:HH11	1:B:386:ARG:HG2	1.81	0.44
1:D:481:GLU:OE2	1:D:512:LYS:HD3	2.17	0.44
1:D:336:VAL:HG23	1:D:381:ALA:HA	2.00	0.44
1:B:480:LYS:HD3	1:B:506:GLU:HG3	2.00	0.44
1:A:506:GLU:H	1:A:506:GLU:HG3	1.29	0.44
1:D:404:THR:N	1:D:405:PRO:HD2	2.33	0.44
1:D:452:ILE:HB	1:D:453:PRO:HD3	1.99	0.44
1:B:475:ALA:HB1	1:B:479:GLY:C	2.43	0.44
1:B:536:GLU:C	1:B:538:LEU:H	2.25	0.44
1:C:382:PHE:CE2	1:C:385:ARG:NH2	2.86	0.44
1:D:269:ARG:NH1	1:D:538:LEU:O	2.50	0.44
1:C:435:ILE:HG23	1:C:441:CYS:HB3	2.00	0.43
1:D:438:ARG:NH2	1:D:533:LEU:O	2.50	0.43
1:A:404:THR:HG23	1:A:405:PRO:HA	2.00	0.43
1:A:480:LYS:HZ3	1:A:506:GLU:HG2	1.82	0.43
1:B:399:GLY:HA3	1:B:407:ARG:HG3	2.00	0.43
1:C:486:ARG:O	1:C:490:ARG:HB2	2.18	0.43
1:D:327:ASP:OD1	1:D:328:CYS:N	2.50	0.43
1:D:506:GLU:H	1:D:506:GLU:HG3	1.38	0.43
1:C:319:HIS:O	1:C:320:LEU:HD23	2.18	0.43
1:C:394:TYR:CD2	1:C:401:LEU:HB2	2.54	0.43
1:C:448:THR:HG23	1:C:480:LYS:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:451:LEU:O	1:C:455:LEU:HG	2.17	0.43
1:C:434:LEU:HD23	1:C:533:LEU:HB2	2.01	0.43
1:D:345:LEU:O	1:D:348:TYR:HB3	2.18	0.43
1:D:435:ILE:HB	1:D:443:ASN:HD21	1.83	0.43
1:C:349:ASN:O	1:C:352:ALA:HB3	2.19	0.43
1:D:376:TRP:O	1:D:379:LYS:HB2	2.19	0.43
1:A:343:GLN:O	1:A:385:ARG:NH2	2.52	0.43
1:A:511:LYS:O	1:A:512:LYS:C	2.60	0.43
1:C:397:ASN:HD21	1:C:400:GLY:HA3	1.84	0.43
1:D:271:PHE:CE1	1:D:435:ILE:HD12	2.54	0.43
1:A:349:ASN:HD21	1:A:352:ALA:H	1.67	0.42
1:C:519:ARG:HG2	1:C:520:ILE:N	2.33	0.42
1:A:467:PHE:HB3	1:A:472:ILE:HD11	2.01	0.42
1:C:298:THR:HB	1:D:415:ALA:HB1	2.02	0.42
1:B:348:TYR:HE2	1:B:350:PHE:HA	1.83	0.42
1:C:458:VAL:HG13	1:C:463:LEU:HB2	2.00	0.42
1:A:407:ARG:NH1	1:A:408:GLU:OE1	2.50	0.42
1:B:404:THR:N	1:B:405:PRO:HD2	2.33	0.42
1:D:353:ASP:C	1:D:353:ASP:OD1	2.61	0.42
1:B:491:PHE:HB2	1:B:497:TYR:OH	2.19	0.42
1:C:480:LYS:HZ3	1:C:506:GLU:HG2	1.84	0.42
1:C:497:TYR:O	1:C:516:PRO:HG2	2.19	0.42
1:C:308:MET:CE	1:C:311:MET:HB2	2.49	0.42
1:D:394:TYR:CD2	1:D:401:LEU:HB2	2.55	0.42
1:A:448:THR:HG23	1:A:480:LYS:HE3	2.02	0.41
1:C:345:LEU:HD21	1:C:382:PHE:CE2	2.55	0.41
1:A:286:LEU:HD21	1:A:305:GLY:C	2.44	0.41
1:A:497:TYR:O	1:A:516:PRO:HG2	2.20	0.41
1:B:289:THR:O	1:B:293:ARG:HG3	2.21	0.41
1:C:326:GLU:C	1:C:328:CYS:H	2.27	0.41
1:C:450:GLN:HG3	4:C:50:HOH:O	2.20	0.41
1:B:308:MET:HE1	1:B:460:LEU:HD13	2.02	0.41
1:C:511:LYS:N	1:C:511:LYS:CD	2.83	0.41
1:D:399:GLY:CA	1:D:407:ARG:HG3	2.50	0.41
1:B:336:VAL:HG11	1:B:380:LEU:CD1	2.48	0.41
1:B:496:VAL:HG11	1:C:267:MET:CE	2.51	0.41
1:C:345:LEU:HG	1:C:385:ARG:NH1	2.36	0.41
1:D:407:ARG:O	1:D:410:TRP:HB3	2.20	0.41
1:B:308:MET:HE2	1:B:312:ILE:HG13	2.02	0.41
1:C:287:THR:OG1	1:C:289:THR:HG23	2.21	0.41
1:A:496:VAL:O	1:A:496:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:LEU:HD21	1:C:305:GLY:C	2.44	0.41
1:C:328:CYS:O	1:C:329:ASP:C	2.63	0.41
1:D:535:LEU:O	1:D:536:GLU:HB2	2.20	0.41
1:C:276:ASP:HB3	1:C:277:GLU:OE1	2.20	0.41
1:C:530:ARG:HG2	1:C:530:ARG:HH11	1.85	0.41
1:D:394:TYR:CG	1:D:401:LEU:HB2	2.56	0.41
1:D:477:LYS:HG2	1:D:478:THR:HG23	2.03	0.41
1:B:354:GLY:H	1:B:379:LYS:NZ	2.18	0.41
1:C:402:ILE:HD12	1:C:402:ILE:HA	1.82	0.41
1:D:339:ASP:OD1	1:D:377:MET:HE3	2.21	0.41
1:D:345:LEU:HG	1:D:385:ARG:HH22	1.86	0.41
1:A:378:ARG:H	1:A:378:ARG:HG2	1.56	0.41
1:B:418:GLU:HG2	4:B:9:HOH:O	2.20	0.41
1:B:424:TRP:CD1	1:B:424:TRP:C	2.98	0.40
1:D:345:LEU:O	1:D:346:SER:C	2.61	0.40
1:D:424:TRP:CD1	1:D:424:TRP:C	3.00	0.40
1:B:482:SER:HA	1:B:485:GLU:HG3	2.03	0.40
1:D:323:ASN:H	1:D:323:ASN:ND2	2.19	0.40
1:A:501:GLY:HA3	1:A:506:GLU:OE1	2.22	0.40
1:B:516:PRO:HB3	1:C:538:LEU:HD23	2.03	0.40
1:B:516:PRO:HB3	1:C:538:LEU:HD22	2.02	0.40
1:C:315:LEU:HD12	1:C:402:ILE:HD13	2.04	0.40
1:C:343:GLN:H	1:C:385:ARG:NH2	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	254/274 (93%)	243 (96%)	9 (4%)	2 (1%)	16	31
1	B	249/274 (91%)	228 (92%)	17 (7%)	4 (2%)	7	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	254/274 (93%)	235 (92%)	14 (6%)	5 (2%)	6	10
1	D	252/274 (92%)	235 (93%)	16 (6%)	1 (0%)	30	49
All	All	1009/1096 (92%)	941 (93%)	56 (6%)	12 (1%)	10	20

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	339	ASP
1	B	341	ASN
1	B	342	GLY
1	C	321	PHE
1	C	352	ALA
1	D	353	ASP
1	A	373	GLY
1	C	327	ASP
1	A	354	GLY
1	B	345	LEU
1	C	354	GLY
1	C	373	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	226/237 (95%)	216 (96%)	10 (4%)	25	50
1	B	223/237 (94%)	211 (95%)	12 (5%)	20	41
1	C	226/237 (95%)	205 (91%)	21 (9%)	8	18
1	D	224/237 (94%)	215 (96%)	9 (4%)	28	54
All	All	899/948 (95%)	847 (94%)	52 (6%)	18	38

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	315	LEU
1	A	378	ARG
1	A	386	ARG
1	A	393	THR
1	A	452	ILE
1	A	476	THR
1	A	489	GLN
1	A	490	ARG
1	A	496	VAL
1	A	506	GLU
1	B	315	LEU
1	B	333	VAL
1	B	341	ASN
1	B	345	LEU
1	B	356	HIS
1	B	378	ARG
1	B	412	GLN
1	B	478	THR
1	B	485	GLU
1	B	506	GLU
1	B	526	LEU
1	B	530	ARG
1	C	266	HIS
1	C	284	SER
1	C	310	GLU
1	C	321	PHE
1	C	329	ASP
1	C	330	GLN
1	C	339	ASP
1	C	344	ASP
1	C	348	TYR
1	C	355	PHE
1	C	378	ARG
1	C	380	LEU
1	C	393	THR
1	C	402	ILE
1	C	466	VAL
1	C	470	GLU
1	C	478	THR
1	C	489	GLN
1	C	490	ARG
1	C	498	VAL
1	C	506	GLU

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Mol	Chain	Res	Type
1	D	302	VAL
1	D	315	LEU
1	D	330	GLN
1	D	333	VAL
1	D	339	ASP
1	D	386	ARG
1	D	414	ARG
1	D	496	VAL
1	D	526	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	319	HIS
1	A	323	ASN
1	A	330	GLN
1	A	349	ASN
1	A	397	ASN
1	A	412	GLN
1	A	508	GLN
1	B	314	ASN
1	B	319	HIS
1	B	341	ASN
1	B	392	ASN
1	B	412	GLN
1	B	427	HIS
1	B	433	ASN
1	B	450	GLN
1	B	514	ASN
1	B	523	HIS
1	C	266	HIS
1	C	330	GLN
1	C	397	ASN
1	C	412	GLN
1	C	450	GLN
1	C	508	GLN
1	D	323	ASN
1	D	356	HIS
1	D	392	ASN
1	D	397	ASN
1	D	412	GLN
1	D	427	HIS

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Mol	Chain	Res	Type
1	D	450	GLN
1	D	489	GLN
1	D	508	GLN
1	D	514	ASN
1	D	523	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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	AF3	A	801	-	0,3,3	-	-	-		
2	AF3	B	802	-	0,3,3	-	-	-		
2	AF3	D	804	-	0,3,3	-	-	-		
2	AF3	C	803	-	0,3,3	-	-	-		

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	258/274 (94%)	-1.37	0 100 100	21, 35, 59, 73	0
1	B	253/274 (92%)	-1.17	0 100 100	27, 46, 80, 80	0
1	C	258/274 (94%)	-1.14	1 (0%) 88 86	28, 47, 80, 80	0
1	D	256/274 (93%)	-1.22	0 100 100	25, 42, 78, 80	0
All	All	1025/1096 (93%)	-1.22	1 (0%) 92 90	21, 42, 79, 80	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	355	PHE	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	B	702	1/1	0.98	0.03	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AF3	B	802	4/4	0.99	0.04	44,46,46,50	0
2	AF3	C	803	4/4	0.99	0.05	44,47,49,49	0
2	AF3	D	804	4/4	0.99	0.05	43,47,48,50	0
2	AF3	A	801	4/4	0.99	0.04	41,42,44,45	0
3	MG	A	701	1/1	1.00	0.02	26,26,26,26	0
3	MG	C	703	1/1	1.00	0.01	24,24,24,24	0
3	MG	D	704	1/1	1.00	0.01	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.